Supplementary Material (Motherwell et al.)

7. Discussion of results and methodology by each participant

Each subsection has been prepared by the named author. The principal programs used are given in parentheses after the author surname

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7.1 *Ammon (MOLPAK/WMIN/DMAREL)*

General Procedures

Our basic procedures for structure predictions had been given in the previous paper (Lommerse et al., 2000), but will be briefly outlined here. Structure prediction is a three step process: (1) construct a so-called search probe, a geometry optimized model, for the molecule of interest; (2) determine thousands of hypothetical packing structures with predetermined symmetries for the search probe; (3) refine the best of the hypothetical structures by minimization of the crystal lattice energies.

Step (1): A preliminary model was built with the PC Spartan Pro program (Wavefunction Inc., 1999) followed by ab initio geometry optimization with either the Gaussian94 (Frisch et al., 1995) or Gaussian98W (Frisch et al., 1998) programs. The optimizations used the non-local DFT method and 6-31G* basis sets (B3LYP/6-31G* option in Gaussian). The optimized structures were modified by adjusting C(sp3)-H, C(sp2)-H and N-H lengths to the standard values of 1.098, 1.084 and 1.013 Å, respectively, to give the search probe models.

Step (2): Detailed analyses of many triclinic, monoclinic and orthorhombic crystal structures revealed a relatively small number of common molecular coordination geometries or patterns with 14 as the most prevalent coordination number. The MOLPAK program (Holden, Du & Ammon, 1993) was designed to build the highest density, hypothetical packing arrangements from the search probe and known coordination geometries. There are 29 commonly used geometries which span the following space groups (# of geometries): P1 (1), P-1 (2), P21 (2), P21/c (5), C2 (1), Cc (1), C2/c (3), P212121 (2), P21212 (3), Pna21 (3), Pca21 (2), Pbcn (2) and Pbca (2). For each geometry, all unique orientations of a search probe are utilized by rotations of 180° in 10° steps about three Eulerian axes leading to 6859 (193) hypothetical packing arrangements. The packing calculations were accelerated by the use of only the repulsive term of a standard 6-12 potential and predetermined repulsion energy thresholds. The drawbacks of this repulsion-only procedure are evident in H-bonded structures and caused a particular problem for (IV).

Step (3): For each of the 29 coordination geometries, the 150-200 highest density packing arrangements were refined by lattice energy minimization with the WMIN (Busing,1981) (single charge per atom electrostatic model) or DMAREL3 (Willock, Price, Leslie & Catlow,1995) (distributed multipole charge model) programs. The three structures contained functionality not originally recognized by the programs. For WMIN, force field coefficients were determined for the imide functionality in (IV), Br in (V) and sulfonimine (-SO2-N=C) functionalities in (V) and (VI). New coefficients for S, Br and H-N (H on N) were determined for DMAREL3.

Results

Attempts to predict the structure for (IV) based on the ab initio search probe model were unsuccessful. The structure of (IV) has a strong intermolecular O…H-N bond of 2.11 Å (based on the observed N-H length of 0.87 Å); the H…O distance is 1.97 Å with a more realistic N-H of 1.013 Å. To a large extent, this failure can be attributed to the inability of the repulsion-only docking potential used in MOLPAK to yield an appropriate set of initial hypothetical structures for refinement.

However, a search probe based on the experimental structure with C-H and N-H bond adjusted to 1.098 and 1.013 Å, respectively, and a MOLPAK + WMIN search did yield the correct crystal structure. This solution (E = -25.92 kcal/mol) was far from that with the lowest energy of –27.23 kcal/mol. A MOLPAK + DMAREL3 run failed to duplicate this success, perhaps because the preliminary refinement stage of WMIN involves a step minimization and provides a reasonably large convergence radius**.** A DMAREL3 calculation

starting with the WMIN refined structure gave a correct result with O…H of 1.95 Å. The reasons for the failure of the ab initio search probe and partially successful use of the experimental search probe are unclear given that both models are virtually identical. Perhaps blame can be placed with the MOLPAK potential which is just on the edge of being unable to handle a structure with the strong H-bonding of (IV).

The structure of (V) was readily determined with a search probe model obtained by geometry optimization with Gaussian94. From a MOLPAK + WMIN calculation, the solutions with the three lowest lattice energies in acentric space groups were C2 (-32.58 kcal/mol), Cc (-31.72) and P212121 (-31.64). The C2 solution was rejected as being unlikely based on a low crystal density of 1.558 g/cc compared to a volume additivity prediction (Ammon, 2001) of 1.651 g/cc. The correct solution was P212121. It should be noted that the lowest energy solution for the racemate was in P21/c at –34.34 kcal/mol.

The two lowest energy, acentric space group solutions from a MOLPAK + DMAREL3 calculations for (V) were Cc (-33.54 kcal/mol) followed by the correct P212121 (-33.40). Again the lowest energy solution for the racemate was P21/c at –34.37 kcal/mol. The DMAREL3 calculations used newly determined force field coefficients for S and Br; it is probable that an improved prediction could have resulted from the determination of specific cross-terms interactions for Br with H, C, N, O, S and Br. The results reported by Price for (V), which are more elegant than those reported here, indicate the importance of an anisotropic potential for Br.

It should be noted the original submission of results for (V) did not recognize that the structure is a pure enantiomer limited to Sonhke space groups. The top three solutions submitted were in space groups P21/c, P21/c and Cc. The correct P212121 solution was fourth.

Predictions for (VI) used two possible conformations, both of which were quite far from the experimental. However, with the observed structure as the search probe, a test of the MOLPAK + WMIN and MOLPAK + DMAREL3 procedures found the correct structure as the second lowest energy for WMIN and lowest energy for DMAREL3.

7.2 ***Dunitz & Schweizer (Zip-Promet)***

Compound IV

As a preliminary guide to choosing between dimeric and catemeric hydrogen-bonded crystal structures for this compound, we made a CSD search for molecules similar to (IV). The search fragment was defined as a glutarimide moiety substituted with 4-connected C atoms at the 3- and 5-positions of the ring. This search produced five hits (BAHFIZ, LERDIF, PIVFIJ, RERYES, YUFYED), all containing centrosymmetric or pseudo-centrosymmetric hydrogen-bonded dimers in the respective crystal structures.

The crystal structure generation for (IV) was therefore limited to space groups P-1, P21/c, C2/c and Pbca. Molecular dimensions were taken from results of an ab initio calculation (MACSPARTAN, 6-31* basis set, assuming molecular Cs symmetry). In most of the calculations, and especially in the final ones, library potentials were supplemented by R-1 terms over atomic point charges obtained by a fit to the electrostatic potential. Contrary to our expectation based on the result of the CSD search, most of the low-energy structures generated by PROMET contained catemeric hydrogen-bonded arrangements rather than dimeric ones. Nevertheless, influenced by the result of the CSD search, we focussed our attention on the relatively few dimeric structures generated by the program and finally selected the three lowest energy structures of this type as our predictions.

After the experimental structure had been announced, re-examination of our listing of calculated structures revealed that the lowest energy structure obtained in our calculations was indeed close to the experimental structure although cell dimensions were somewhat expanded, presumably due to inaccurate potentials. Clearly, in this case we would have done better not to use the CSD as a guide.

7.**3** ***Dzyabchenko (PMC)***

The PMC program (Dzyabchenko *et al*., 1999, Dzyabchenko, 2001) has been designed to minimize the potential energy of a crystal composed of several generally distinct molecular units with fixed internal geometry, interacting with one another *via* only the non-bonded atom-atom potentials of van der Waals (6-12

/ 6-exp type) and electrostatic type. These units can be defined as integral molecules or fragments of a flexible molecule within which they are additionally held together by the 'link' potentials of quadratic type to preserve standard geometry around such a link.

The molecular geometry of IV and V was taken basically the same with that reported for chemical analogues of these compounds found in the CSD (Allen *et al*.,1991): glutarimide (Petersen, 1971) and its 4,4-dimethyl derivative (Bocelli & Grenier-Loustalot, 1981) for IV, and camphorsulphonimine (Chakraborty *et al*., 1997) for V. Molecule VI was constructed from three rigid fragments: the central SO_2 group, the phenyl ring and the planar heteroaromatic system, their geometry was taken from the crystal structures of cis (Basak *et al.*, 1984) and trans (Bar, 1985) isomers of the 4-phenylamino analogue. The list of non-bonded atom-atom potential parameters used in this work is reported in Supplementary Material. The net atomic charges were calculated for free molecules IV-VI with *Gaussian* 98 (Frisch et.al., 1998) at the 6-31G level. Preliminary, the accuracy of this force-field was assessed by its application to the known crystal structures of the named analogues, whose minimized structures were compared by energy with other minima from the respective ab initio searches (although restricted to the P21/c, Pbca, and P-1 space groups only because of time limitations).

The strategy of global search followed essentially that described in an early paper on benzene structures (Dzyabchenko, 1984). For IV and VI, the space groups $P2_1/c$, *Pbca*, *P*-1, $C2/c$, $P2_12_12_1$, $P2_1$, $Pna2_1$, *Cc*, and *C*2 have been selected. In addition, to avoid structures with large beta angles, the list of monoclinic groups was extended with some in non-standard settings: $P2_1/n$, $C2/n$, $I2/c$, *Cn*, *Ic*, and *I*2. For enantiomorphous V only $P2_12_12_1$ and $P2_1$ were selected. The starting cells were taken rectangular, their dimensions allowed the cell shape to be one of the four selected types ('cubic', 'brick', 'plate', and 'stick') and scaled to give the density 1.2 - 1.5 times as great as the minimized-structure density. The starting centre-of-molecule positions were taken at the eight vertices of the asymmetric unit of the Cheshire-group cell (Hirshfeld, 1968): 0,0,0; 1/4,1/4,1/4; 0,1/4,1/4; 1/4,0,1/4; 1/4,1/4,0; 1/4,0,0; 0,1/4,0; and 0,0,1/4. The starting orientations were assigned within the symmetry-adapted ranges of the three Euler angles (Hirshfeld, 1968; Dzyabchenko, 1983, 1984), with a 30-degree step in each angle. The starting grid structures were optimised with the *VA09* procedure (Fletcher, 1972) with analytical 1st derivatives. The optimised structures were sorted by energy. The same-energy minima were compared with each other with CRYCOM to screen out the non-unique solutions.

Results of ab initio search

Compound IV. The three lowest-energy structures submitted as ab initio predictions contained hydrogen-bonded (HB) dimers closed cyclically about the symmetry centres. This is in contrast to the experimental structure ranked 31, stabilised with H-bonds in infinite chains mediated by the glide planes. Remarkably, most other structures, of those predicted lower in energy than I-31, contained cyclic dimers as well, while minor portion was represented by motifs with HB-chains mediated by a screw axis or a glide plane. Overall, the dimeric packings were more stable then the packings built of infinite chains. Of the chain packings, those due to a screw axis were more stable than the glide-plane ones. This packing hierarchy looks reasonable from the point of view of stabilization energy caused by the electrostatic interactions. For comparison, the chains in glutarimide are mediated by screw axis while the chains in its dimethyl derivative are glide-plane. To explain the observation of chains rather than more stable dimers, one can suggest that the former are favoured kinetically when crystallised from polar media.

Compound V. The energy differences of the several most stable minima are rather small here again, and the ranking could be affected by the thermal factor ignored in this calculation. At the same time, the ranking was found sensitive to small variation in the van der Waals potentials for bromine.

Compound VI. It was initially intended to perform the global search with a set of fixed conformations first and then refine the minima found with flexible molecule. However, it was soon understood that such a stepwise strategy was not in fact optimal with our software, and we turned to the flexible-molecule minimizations straightforwardly from the grid structures. Of the two isomers considered, the trans isomer has been correctly selected as more stable in solid state. However, the observed structure occurred as a less symmetrical and rather loosely packed than the predicted *Pbca* structures. It was identified on the powder-assisted step as one of the energy minima, rather high in energy and heavily distorted with respect to the experimental structure.

Powder-assisted results for IV-VI

The powder spectra treated with the powder-indexing program TREOR (Werner *et. al.* 1985) has resulted in cell parameters and space group symmetry which made it possible to recognise the true solutions for IV and V among the structures found ab initio. The correct structure of VI was also found at this stage, though

additional refinement of the ab initio $P2_1/c$ structures was in fact necessary by the energy minimisation based on the true cell dimensions.

To conclude, the ab initio search has defined the three observed structures as local energy minima, of energy rankings beyond 3. To improve these results, more accuracy in the force field for V (bromine), and of VI (adding a torsional potential) is necessary. With regard to IV, the result could hardly be improved without taking into consideration the kinetic factor. With the experimental powder cell parameters, the force-field pitfalls become of less significance, for the energy-based prediction delivers the structures correctly in the three test cases.

This table is intended for supplementary material to Section 4.3 Dzyabchenko (PMC)

Table PMC-1. Non-bonded potential parameters for IV-VI

Atom pair [a,b]		Type	r_0, A	ε, kcal/mol	α, A^{-1}
H	H	6-12	2.930	-0.0359	
H	C	6-12	3.315	-0.0474	
H	N	6-12	3.460	-0.0357	
H	O	6-12	2.75	-0.0400	
H	S	6-12	3.540	-0.0787	
H	Br	6-exp	3.900	-0.1000	3.55
H	H*	6-12	2.805	-0.0467	
C	C	6-12	3.700	-0.0722	
C	N	6-12	3.845	-0.0567	
C	O	6-12	3.410	-0.1170	
C	S	6-12	3.925	-0.1263	
C	Br	6-exp	4.200	-0.2000	3.50
C	H*	6-12	3.190	-0.0597	
N	N	6-12	3.990	-0.0450	
N	O	6-12	3.555	-0.0906	
N	S	6-12	4.070	-0.1007	
N	Br	6-exp	4.200	-0.2000	3.50
N	H*	6-12	3.335	-0.0445	
O	O	6-12	3.120	-0.2001	
O	S	6-12	3.635	-0.1996	
O	Br	6-exp	4.100	-0.2000	3.50
O	H*	6-12	1.900	-1.1100	
S	S	6-12	4.150	-0.2257	
S	Br	6-exp	4.300	-0.3000	3.50
S	H*	6-12	3.415	-0.0977	
Br	Br	6-exp	4.500	-0.5000	3.60
Br	H*	6-exp	3.349	-0.1407	3.55
H*	H*	6-12	2.680	-0.0614	

[a]H and H* stand for hydrogens attached to carbon and nitrogen, respectively. [b] Shortened bond length of 1.5Å was accepted for C-Br to adapt anisotropy of bromine interactions.

7.4 *Erk (SySe/PP)*

All calculations were performed using CERIUS^2 version 4.2 (Accelrys Inc., 2001). The Dreiding2.21force field (Mayo, Olafson & Goddard, 1990) was used in all cases. Bonding parameters for sulfur were changed to achieve a better match of the bonding situation in sulfur containing molecules. Electrostatics were calculated by Ewald summation based on atom charges. Two charge models, MNDO-ESP (Besler, Merz & Kollman, 1990) and charge equilibration charges (QEQ) (Rappe & Goddard, 1991), were evaluated by checking their suitability to reproduce the crystal structures of related molecules. The molecules used for evaluation and the charge model applied in the simulation are listed in *Table*.

For each of the three molecules a systematic search (SySe) (Erk, 1999) and the Polymorph Predictor (Verwer & Leusen, 1998) were used to generate initial packings. For the SySe the molecular model was placed in a rectangular unit cell large enough to allow the molecules to be rotated without interference with their symmetry related copies. The molecular model was centered at (¼, ¼, ¼) and aligned in such a way that its maximum moment of inertia was parallel to the a-axis. Structures were generated by changing the orientation of the molecule in steps of 30° with respect to each axis, which is usually sufficient to perform an exhaustive global minimization. However, in the present case the structure generation procedure was repeated with the molecule initially turned by 15°. The packing energy of these low density structures was minimized using the CERIUS^2 module Crystal-Packer step by step, first with respect to the cell axis (permuting the order of the axis), secondly the cell angles (as required by the crystal system) and finally the orientation of the molecule. A representative *tcl* script for CERIUS^2 4.2 as used in the CSP is given in the annex. In the case of molecule VI the resulting packings were further minimized allowing full molecular flexibility.

Polymorph Predictor runs were performed once for each space group considered. A representative tcl script file for these runs is also in the annex. In a subsequent stage, all generated structures were energy minimized allowing the full flexibility of the molecule.

The results of the SySe , molecules IV,V, were clustered by having identical energy components and the same density within limits of 0.1 kcal/mol and 0.001 g/cm^3 respectively. In the cases where molecular flexibility has been considered (Polymorph Predictor, SySe molecule VI), structures were clustered based on a radial distribution function. To avoid the loss of results, the most selective parameters were chosen for the clustering.

Molecule IV

The CSD entry GLUTIM was used as a reference for molecule IV. The molecular geometry calculated using PM3 was found to match almost perfectly the experimentally determined one. For the same reason MNDO-ESP charges were found to be superior to QEQ atom charges. A Polymorph Predictor test run in space group $P2_1/c$ followed by clustering after the simulated annealing procedure did not yield the correct structure. Upon minimisation of all generated packings, the experimentally determined catemer structure was on the list of calculated structures. However it was ranked by energy at place #38 (highly selective clustering which did not remove all redundant packings suggested rank #95).

Using the same force field as for the GLUTIM validation, structures for IV were calculated using the SySe and with the Polymorph Predictor in all 10 space groups. Additionally, structures were predicted with the SySe using the centrosymmetric hydrogen bonded dimer as a fixed unit.

In the SySe with one molecule as the modeling unit 20160 packings have been generated and were energy minimized within 46 hours and 35 minutes CPU time on a 270 MHz R12000 SGI O^2 workstation. In the Polymorph Predictor run 24771 structures were generated and minimized within 125 hours and 9 minutes. The higher demand in CPU time for the Polymorph Predictor is presumably due to the more costly minimization of the molecular structure as well as the crystal packing. The time factor between both methods depends highly on the complexity of the space group and ranges from close to unity for P $\bar{1}$ to almost four in Pbcn.

The three best structures ranked by energy of these different approaches were compared and it was found that they were basically identical for the Polymorph Predictor and the 2 SySe runs. The three lowest energy structures were proposed for the test. The minimum energy structure corresponding to the experimental structure was found by both methods. It was ranked by the force field of SySe 6 kcal/mol and by the Polymorph Predictor (considering full flexibility) 5.5 kcal/mol above the respective global minimum.

Molecule V

Force field validation for V was carried out using the CSD structures ROLBOJ and SURJOE. Because of the poor geometrical accuracy of the sulfone group, Dreiding2.21 was modified as follows: bond minimum S_3-O_2 = 143 pm, angle minimum X-S_3-X = 90°, torsion X-C_3-S_3-X, 2 kcal/mol, 3 periods, minimum at 0°.

The molecular model for V was derived from the coordinates of the structure of SURJOE, to which the bromine atom was added. The positions of the bromine and the hydrogen atoms have been optimized. QEQ charges in combination with the modified Dreiding force field were found to yield sufficiently accurate structures for both validation models.

Runs in the SySe and the Polymorph Predictor were carried out in the two space groups considered. Again the three lowest energy structures were identical for both methods and were proposed. Only in the SySe procedure the structure correlating with the experimental structure was found. However the geometrical similarity of experimental and calculated structure was very poor. The "correct" calculated structure was 4.6 kcal/mol above the global minimum. Any obvious reasons for the failure of the Polymorph Predictor could not be found. However, the calculated structure corresponding to the experimental packing was found to be 5.3 kcal/mol higher in energy than the global minimum in the current run.

Molecule VI

Force field validation was carried out using the isomeric series of sulfapyridine polymorphs (BEWKUJ). Because of poor geometrical accuracy, the force field was modified further (including the modifications for V) as follows: bond minimum S_3-N_2 = 160 pm, torsion X-S_3-C_R-X, 30 kcal/mol, 2 periods, minimum at 0°. This modified force field in combination with QEQ atom charges calculated with the molecular geometry of the respective isomer yielded good matching packings for all BEWKUJ polymorphs (E- and Z-diastereoisomers).

The molecular model for the E-Isomer was calculated using the modified Dreiding force field. The model for the Z-isomer was constructed from BEWKUJ04 by moving the amino group and optimizing the amino nitrogen and all hydrogen atom positions. Thus a representative configuration for the phenyl group in VI should have been ensured. For both models QEQ atom charges were calculated.

SySe runs were performed for both isomers in all space groups followed by minimizations of all unique structures allowing full molecular flexibility. Polymorph Predictor runs were carried out in the 5 most promising space groups only. Energy ranking of the calculated structures was found to be nonsensical. The lowest energy structures were all crowded with an irrationally high number of hydrogen bonds and other objective selection criteria could not be found. Finally three subjectively selected structures were proposed. Both methods yielded the packing corresponding to the experimental structure at 2.7 (SySe) and 2.1 kcal/mol (Polymorph Predictor) above the global minimum

Mol V Polymorph Predictor.log
mol2_start.msi

Tcl script und input file for Polymorph Predictor run on molecule V.

SySe	molecular model	charge model	space groups considered	global minimum	exptl. min calculated	molecular flexibility
Mol IV	PM3	MNDO-ESP	all	-108.2	-102.3	no
Mol V	modified SURJOE	QEQ	$P2_1$, $P2_12_12_1$	-138.0	-133.4	no
E-Mol VI	modified Dreiding	QEQ	all	-141.9	-121.2	no

				-14.0	-11.3	yes
Z-Mol VI	BEWKUJ04	QEQ	all	not eval.	not eval.	yes

PolPred

Mol IV	PM3	MNDO-ESP	all	-109.0	-103.5	yes
Mol V	modified SURJOE	QEQ	$P2_1$, $P2_12_12_1$	-137.3	-132.0	yes
E-Mol VI	modified Dreiding	QEQ	$P\ 2_1/c$, $P\ \bar{1}$ C2/c, P bca $P\ 2_12_12_1$	-16.2	-14.1	yes
Z-Mol VI	BEWKUJ04	QEQ	$P\ 2_1/c$, $P\ \bar{1}$ C2/c, P bca $P\ 2_12_12_1$	not eval.	not eval.	yes

7.5 *Gavezzotti (Zip-Promet)*

Compound V

The program package used was Zip-Promet in its standard formulation, as described in the previous paper (Acta B, previous results). The molecular model for V was taken from the crystal structure of the un-brominated compound in the CSD, ROLBOJ. Hydrogen positions were standardized: staggered methyl hydrogens, all C-H's 1.08 Å. The bromine atom was added at C-Br 1.91 Å and reasonable bond angles. Potentials used were the chargeless UNI set (Gavezzotti & Filippini, 1994). Molecular volume is 201 $Å^3$ and molecular surface 227 $Å^2$, so the expected average cell volume per molecule is 201/0.7 = 287 $Å^3$. The expected lattice energy is (0.322 x 227 + 37.2) = 110 kJ/mol (Gavezzotti,1994). In space group $P2_1$ three searches were performed: 1) standard: 1384 structures reduced to 47 after cycles of optimization and sorting; 2) shortest screw translation 5 Å: 989 structures reduced to 31 after optimization and sorting. 3) shortest screw translation 7 Å: 1618 structures, reduced to 22 after optimization and sorting. After further merging and sorting, 84 final optimized crystal structures were left, of which 21 crystal structures between E = -100 and E = -109.3 kJ/mol. In space group $P2_12_12_1$ two searches were performed: 1) standard search: 13455 structures reduced to 50 after merging and optimization; 2) shortest screw translation 5: 3873 structures. After final merging and sorting, 71 independent optimized crystal structures were left of which 36 structures between E = -100 and E = -110.4 kJ/mol.

Comments

A crystal structure close but not quite similar to the experimental one was found with energy rank 14; the difference is presumably due to slight differences in the molecular model. The rank became 4 when the energy minimisation was repeated including point charge parameters from a standard MO 6-31G calculation with Mulliken population analysis. However, the absolute values of energies and the densities obtained in the calculations with point charges were too high. A search run using the experimental cell parameters and space group quickly found the correct crystal structure. In post-analysis, energy minimization of the experimental crystal structure gave E = -108.2 kJ/mol, or 2.2 kJ/mol less stable than the best calculated structure. However, such small energy differences can hardly be considered significant, being almost within the error window of the search and optimization routines.

7.6 *Hofmann (FlexCryst)*

FlexCryst performs three steps. First, a large number of crystal structures is generated. Secondly, the structures are scored and sorted according their score. Finally, high ranking structures are refined.

The generation follows the nuclei concept of Gavezzotti. First, chains are constructed. These are extended to planes fulfilling the constraints of an assumed space group. Finally, these planes are stacked to result in three-dimensional crystal structures. The scan for favorable structures is executed in the discrete space, i.e. the space is superimposed with a mesh. For each vector that connects two mesh points and represents a unit cell vector, the energy of the resulting chain, plane or structure is scored. The mesh size (1A) is chosen to trade off the accuracy of the search against the required computing time.

The scoring function is trained on existing crystal structure data. The training procedure optimizes the scoring function for the discrimination between observed structures and distorted structures (decoys), that are not observed in nature. This function performs better than statistical potentials and, at present, has the same quality as common force fields. The score is much faster to evaluate for the trained potentials as the energy expression of force fields. It is in this approach just the vector product between weight factors and occurring intermolecular distances. The score of the function is proportional to the energy values computed by force fields and the energy of a given structure can be obtained by multiplying the score by a factor.

Structure refinement is performed via reduction of the grid constant. The algorithm of structure generation requires, that cell vectors are lying on whole-numbered grid points. During the refinement the adjacent grid point on the finer grid sh (0.1 A) are screened for structures with a lower score until the refinement converges in a local minimum.

Ab initio results

The main goal of FlexCryst is producing an approximate structure among the 1000 high ranking structures for further refinement with highly accurate methods. The calculations have been redone with the correct structure and have been restraint to the correct space group. In this case the program succeeded in the two cases of structure IV (rank 358) and structure V (rank 746). The third structure is too heavily distorted and no similar structure has been generated. An attractive property of FlexCryst is the very short calculation times for this application (roughly 3h for structure IV and 1h for structure V).

Powder assisted results

The 'experimental' powder pattern and the calculated powder patterns were compared automatically. For similarity we used a combined similarity measurement of the differences in the powder diffraction profile and the crystal structure energy. The structures were refined to optimize the similarity measurement. For the first two structures we retained a similar cell and a similar powder diffraction. But the orientation of the molecules in the cell shows different stacking patterns.

Finally we tested Flexcryst for crystal structure determination after successful indexing of the powder pattern. In all three cases the structure ranked first is similar to the experimental structure. The huge difference in the score for the experimental structure (-162.27) and the calculated structure (-173.11) for example VI reflects the inaccuracy of this structure.

7.7 *Leusen (PP-CVFF)*

The search for crystal packing alternatives was performed using the Polymorph Predictor (PP) technology as implemented in the Cerius^2 molecular modeling environment (Verwer & Leusen, 1998, Accelrys Inc., 2000). In contrast to the contributions of Verwer and Mooij, who utilized the Dreiding force field (Mayo, Olafson & Goddard, 1990) in combination with non-transferable, quantum mechanically derived atomic charges (Verwer) or atomic multipoles (Mooij) to rank the various potential polymorphs, the Consistent Valence Force Field (CVFF) (Dauber-Osguthorpe et al., 1988) was used for this submission. In CVFF, atomic charges are assigned from bond increments which were fitted together with all other parameters in the original force field fitting procedure. All parameters in CVFF are therefore fully transferable. The advantages are twofold. Firstly, the charge assignment is instantaneous, thus saving computer time – although this saving is insignificant in view of the computer time needed for the polymorph simulations. Secondly, the CVFF atomic charges are independent of molecular conformation, which enables a direct comparison of lattice energies calculated for conformational polymorphs. A major drawback of the electrostatic treatment in CVFF is its lack of accuracy in comparison to specifically derived, non-transferable, electrostatic models. CVFF uses a Lennard-Jones 12-6 potential to describe van der Waals interactions, and it does not have a special hydrogen bond term. To describe intra-molecular interactions, the force field features the usual diagonal terms to represent bond stretching, angle bending, rotation around torsions, and out-of-plane interactions. In addition, CVFF has a number of cross terms to represent couplings between deformations of internal coordinates, e.g., stretch-stretch, bend-bend, and stretch-bend-stretch couplings. The force field was chosen for this contribution in order to compare the results obtained with different electrostatic models: ‘cheap’ atomic charges from bond increments versus ‘expensive’ atomic charges and multipoles from high-level quantum mechanical calculations. Prior to the disclosure of the experimental crystal structures the expectation was that CVFF would perform worse than the two Dreiding submissions because of its simple electrostatic model, with the possible exception of the flexible molecule VI, where the consistency of the CVFF charges with the rest of the force field, together with its more sophisticated intra-molecular potentials, might tip the balance in its favor.

All polymorph simulations were carried out with one molecule in the asymmetric unit and Ewald summation of both the van der Waals r^{-6} and electrostatic terms. Molecules were kept rigid during the initial Monte

Carlo Simulated Annealing (MCSA) search, but were treated as fully flexible during the final lattice energy minimization step. CVFF was used without any modifications for all three compounds.

For molecule IV, the MCSA search was performed in the ten space groups specified. The sampling proved difficult, and it was necessary to run the search six times to ensure that all relevant minima were located. Based on previous experience, this indicates that the compound is difficult to crystallize. A total of 47,138 crystal structures were lattice energy minimized with respect to all degrees of freedom. The energy separation between the various crystal packing alternatives was very small: 28 **structures were found within 1 kcal/mol of the global minimum structure. This suggests that the compound may well show** polymorphic behavior. The three lowest energy structures were submitted with relative energies of 0, 0.06, and 0.11 kcal/mol per asymmetric unit. When the powder diffraction data was released and compared to powder patterns simulated for the list of predicted structures, a good fit was found with the third submitted structure. Comparison with the experimental structure revealed that the thirds submitted structure was indeed correct. This result is in line with expectations for this simple and rigid molecule.

For the enantiomerically pure molecule V, only three space groups had to be considered: $P2_12_12_1$, $P2_1$, and C2. Sampling was straightforward: all relevant minima were located in each of the three runs performed. A total of 16,920 structures were optimized. Only four structures were found within 1 kcal/mol of the global minimum. The three lowest energy structures were submitted with relative energies of 0, 0.17, and 0.82 kcal/mol asymmetric unit. Upon release of the powder diffraction data, it became clear that the experimentally determined structure was not among the three submitted, but it was found by powder pattern comparison as structure 70 (ranked by calculated lattice energy) with an energy difference of 2.48 kcal/mol relative to the global minimum. This significant error is larger than anticipated and may be attributed to the 'exotic' =N-SO_2- group for which the force field is not well parameterized, compounded by the presence of a bromine substituent.

Conformational analysis with CVFF on molecule VI revealed four low-energy conformers. For the cis (S-N=C-N at 0°) isomer, two conformers were identified with relative energies of 0 and 0.5 kcal/mol in the gas phase (Ph-S-N=C at 180° and 71°, respectively, and Ph-Ph-S-N at 90° and 63°, respectively). For the trans (S-N=C-N at 180°) isomer there were two additional conformers with relative energies of 1.1 and 3.1 kcal/mol (Ph-S-N=C at 180° and 71°, respectively, and Ph-Ph-S-N at 90° and 56°, respectively). The search for possible crystal structures was carried out for each of the four conformers in each of the ten space groups specified. Sampling did not pose any problems as all relevant minima were found in each of the three runs performed. A total of 138,559 crystal structures were lattice energy minimized with respect to all degrees of freedom. Only four structures were found within 1 kcal/mol of the global minimum structure. The three lowest energy structures, all three containing the cis isomer, were submitted with relative energies of 0, 0.26, and 0.93 kcal/mol asymmetric unit. Comparison of the powder pattern with those of the list of predicted structures did not yield any obvious fits. After disclosure of the experimental structure, it became clear that this structure had not been sampled because CVFF proved inadequate for molecule VI: the CVFF minimized experimental structure has a lattice energy of 9.16 kcal/mol above the global minimum located in the search. It is not surprising that the structure was not found, since the MCSA procedure is designed to explore the low-energy region of phase space, while it tries to avoid high-energy regions. The magnitude of the error in calculated lattice energy, however, is alarming. The error cannot be explained solely by the presence of the 'exotic' =N-SO_2- function (which is also present in molecule V, where the error in lattice energy is 2.48 kcal/mol). Comparison of the gas phase conformational analysis to high-level quantum mechanical calculations suggests that CVFF makes an error of several kcal/mol in the conformational energies. A contributing factor is the balance between forming an intra-molecular hydrogen bond in structures containing the cis isomer *versus* establishing an inter-molecular hydrogen bond in structures containing the trans isomer. CVFF seems to erroneously favor structures with the intra-molecular hydrogen bond.

7.8 *PackStar Lommerse*

It has been established that the crystal lattice energy is generally the most important parameter which determines the formation of the final crystal structure from the dissolved state, melted state or gas phase. Indeed, most programs applied in this and previous crystal structure prediction (Lommerse et al., 2000) work relatively successful on the assumption that an experimental crystal structure will have the lowest possible lattice energy for a given molecular structure. However, the neglected entropy effects and kinetic factors may be decisive to select the correct prediction from a series of calculated, and in terms of lattice energy,

nearly equivalent crystal structures. Using statistical information of real crystal structures, PackStar attempts to account implicitly for these effects .

Two aspects of PackStar have changed since CSP1999. Firstly, the initial random sampling of crystal structures is now based on simple fitting of hard-sphere molecules in a unit cell. Subsequently, the highest density structures are optimised on basis of the more expensive PackStar cost calculation. The second change is that the interaction between interacting groups and atoms has been extended from 0.5 Å up to 1.0 Å. All statistical IsoStar data still act on interactions distances less then or equal to 0.5 Å (CSP1999), but an artificial 'attractive' function has been added: $F(r) = (1.0 - r)^e$ where r is the shortest intermolecular distance between interacting groups minus the sum of the van der Waals radii of interacting atoms and e=2.718. In effect, it means that there is an extra contribution of 1.0 to the propensity for van der Waals contacts between interacting fragments which gradually diminishes to 0.0 for a intermolecular interaction at r = 1.0 Å, the fixed boundary of the interaction space. There is no fundamental physical reasoning behind this function, but it has been empirically tested and found to work satisfactorily.

Crystal structure predictions were run for compounds IV and V only, as PackStar cannot handle flexible molecules. IsoStar central and contact group information was stored in grids, for which the mesh was optimised such that at least four contacts in each grid cube are present if the interaction would have been completely random. The following contact groups were used (mesh of the grid in brackets). Compound I, any aliphatic C-H (0.30 Å), methylene (0.60 Å), any C=O (0.50 Å) and any N-H (0.40 Å). For compound IV: methyl, methylene, any C-H any C-Br, any C=O (to mimic S=O), aromatic/N-sp2 and substituted aromatic carbon, all in a grid of mesh 0.50 Å. No contact group representations for the remaining three adjacent ring-bridging carbons were available for this compound.

The (fixed) conformations of the compounds were calculated using GAUSSIAN98 at the 6311-G basis set level. Initial hard-sphere searches for each compound were performed starting from cubic boxes. Cell parameters, orientation and positions in agreement with space group symmetry were density optimised. For each spacegroup 1000 different high density structures were stored. A structure was considered different if at least one of the differences of following parameters exceeded a certain limit: either cell length > 1.6 Å (compound IV) / 1.9 Å (compound V), or cell angle > 18^o, or fractional position in cell > 0.1 or rotational position in cell > 72^o. The 200 densest structures were optimised using the PackStar cost function. Due to time constraints, this procedure was applied only once for compound IV in space groups C2, Cc, P-1, P21, P212121, P21/c, Pbca, Pbcn and Pna21 (1800 final minima ranked by PackStar cost), and for compound V three times in space groups P21 and P212121 (1200 ranked minima). The lowest cost structures were analysed visually. In general all C-H…H-C contacts were considered to be bad, as well as C…C contacts.

CSD analysis suggested that in general planar CO-NH-CO- containing compounds prefer dimer formation in crystal structures, whereas non-planar compounds, like compound IV, often form chains throughout the structure. However, the first 40 crystal structures of compound IV all had dimer motives, so two dimers and only one chain structure were chosen.

For compound V many C-H…O=S were considered to be important, especially if the hydrogen is more 'acidic' (C-H adjacent to the SO_2 group).

None of the selected structures were near the experimental coordinates Even if the search method had been successful in identifying the correct solutions, the correct structures would not have been chosen on basis of the PackStar cost (cost of submitted structures for compound IV: -42.4, -44.9, -48.3, calculated cost of the experimental structure is –30.8; cost of submitted structures for compound V: -40.0, -37.5, -34.3, calculated cost of the experimental structure is –29.2). Nevertheless, the author still believes in the merits of statistical approach of the crystal structure prediction problem. Much more efforts should be put in development of a better cost function, which can handle the statistical gaps. Even so, it is not likely that the statistical approach will get as accurate as well developed energy calculations. At best, statistical data could be helpful in selecting the right instances from a list of low energy structures. This has already shown to be potentially powerful in ligand protein interaction studies (Boer, Kroon, Cole, Smith & Verdonk, 2001; Verdonk, Cole, Watson, Gillet & Willett, 2001).

7.9 *Mooij (PP-Multipoles/Dreiding)*

Methods

Possible crystal packings were optimized in a model that focuses on an accurate description of electrostatic interactions, combined with full molecular flexibility. To this end atomic multipoles were combined with a generic force field, viz. Dreiding (Mayo, Olafson & Goddard, 1990). The Dreiding2.21 force field as implemented in the Cerius^2 suite of programs (Accelrys Inc., 2000) was used with the following modifications: a) the 6-exp formulation of the van der Waals potential was used, with the parameters as given in the original Dreiding paper. b) the hydrogen-bond potential was disabled; instead specific polar hydrogen 6 exp parameters were used (the FIT parameters from Coombes, Price, Willock & Lesley, 1996). This Multipoles/Dreiding model was tested on the 1999 edition of the blind test, with rather satisfactory result (Mooij & Leusen, 2001). The bond, angle, torsion, and inversion terms were left unchanged. Only for compound VI, some torsional energy terms were modified to reproduce relative DFT energies for various conformations as calculated by DMol^3 at the PW91/DNP level. The modified torsional energy terms are supplied in the supplementary material. Calculations with the Multipoles/Dreiding force field were performed using a previously described crystal energy minimizer (Mooij, van Eijck & Kroon, 1999), that uses the polarizable multipole electrostatic code as implemented in TINKER (Ponder, 2000) Ewald summation was used for all multipole-multipole interactions, as well as for the van der Waals r^{-6} term.

Multipole model

The atomic multipole models were derived by fitting to the electrostatic potential on a grid outside the van der Waals surface of the molecules. The fitting program allows for a fit to multiple conformations at the same time, a functionality that has been used for compound VI. This ESP grid was calculated by the DMol^3 program (Delly,1990; Delly, 1991; Accelrys Inc., 2000), using the PW91 (Perdew & Wang, 1992) gradient-corrected functional with the DNP basis set. Molecular geometries were optimized at the same level of theory. For compound VI both cis and trans forms were optimized in the two different C-S=N-C conformations. In addition, two geometry optimizations were performed for the cis form with the phenyl group constrained at a Phe-S-N torsional angle of 0°, which is ~90° rotated with respect to the fully optimized geometry. The optimizations for compound VI were performed at the PW91/DND level, constraining the NH_2 to be planar. The preference for non-planar NH_2 conformations in DMol^3 was suppressed to resemble the rather planar conformation that is enforced by the Dreiding force field. The multipole model for compound VI was fit to the ESP grids for all these six conformations simultaneously.

Sampling

For compounds IV and V, the 500 lowest-energy structures from both Verwer's and Leusen's lists were taken as starting points. Results were largely indifferent to the starting set: all low-energy structures were reached from both lists. The three lowest-energy structures were submitted. For compound VI a maximum of 750 structures per conformation and space group from one Polymorph Predictor run of Leusen were minimized (~20 000 structures), augmented with the 3000 most favorable structures in Leusen's final list (based on a number of Polymorph Predictor runs). In addition, the crude output of one Monte Carlo run in the space groups P 21/c and P-1 (~10 000 each) was used without full minimization in the CVFF force field. Finally, the 1000 most favorable structures from Verwer's list were also taken. The two lowest-energy structures were submitted together with the lowest-energy trans structure (7th overall).

Results and discussion

For compound IV the second most favorable structure corresponds to the experimental structure. The energy for this structure is only 0.19 kJ/mol higher than the global minimum. It is interesting to compare the result with the other multipole-based submissions (Price, and Ammon). They both used intermolecular potentials that are very similar to the one used here (note the C, H, N, and O van der Waals potentials of Dreiding are based on Williams' parameters). So, the use of rigid molecular geometries by DMAREL is the most important difference. Therefore, the problems in the prediction using these other methods indicate that it is important to allow for molecular flexibility, even for an essentially rigid molecule like this one. Another interesting observation is that Dreiding with point charges failed in the prediction for this compound (see Verwer). Analysis indicated that the high relative energy of the experimental structure could partially be attributed to the Dreiding hydrogen-bond term, and partly to the use of an electrostatic point-charge model.

For compound V, the ninth lowest-energy structure corresponds to the experimental structure. The relative energy for this structure was 6.6 kJ/mol. So, the force field appears to be substantially in error. Although force field errors had to be expected for a compound with a bromine and an SO_2 group, the large energy spread of the first three structure gave some (false) hope for the predictions for this compound: it is not often that the second and the third lowest-energy structure have relative energies of 2.8 and 4.1 kJ/mol respectively. Considering that the other multipole based models have been more successful for this

compound, it seems likely that the Br and S van der Waals parameters are the main source of error in our model. It was tempting to see a compensation of errors between errors in the isotropy of repulsion and electrostatics for bromine: successful predictions have been obtained either with isotropic repulsion and point charges (Williams), or with anisotropic repulsion and multipoles (Price). In addition, Dreiding with point charges (Verwer) performed better than Multipoles/Dreiding. Nevertheless, Price's analysis indicated that the anisotropic repulsion is not an essential factor for correct prediction, which is also supported by the DMAREL results of Ammon.

For compound VI, no structure was recognized as the experimental structure: the energy-minimized experimental structure has not been sampled in the search procedure. Afterwards, its energy turned out to be 16.6 kJ/mol relative to the global energy minimum found. Obviously, the Multipoles/Dreiding model was just not accurate enough for this compound. One of the reasons for not sampling the experimental structure is this high energy. More serious is probably that most of the structures were generated within the CVFF force field, which ranks the experimental structure at a relative energy of a much as 38 kJ/mol (see Leusen): the Monte Carlo simulated annealing procedure is not designed to sample all local minima at such high relative energies.

Powder-assisted results

The supplied powder patterns were automatically compared to simulated powder patterns for all the hypothetical structures in the list. This was done using the CMACS utility in Cerius^2. Visual inspection of the best-scoring patterns then easily led to the identification of structures for compounds IV and V. For compound VI no matching powder pattern was found. Indeed, as discussed above, the experimental structured turned out to be not present in the list of generated structures. For compound IV, the second most favorable structure, already submitted at the ab initio stage of the test, was identified as the experimental structure. For compound V, the 9th structure matched the experimental pattern, and was submitted. So, for two of the three compounds the structure could be solved based on an un-indexed powder pattern. For this purpose the exact energy ordering, of utmost importance for success at the ab initio stage, is much less important than an excellent reproduction of the geometry of the crystal packing. Obviously, the force field should be accurate enough to allow the sampling algorithm to produce the experimental packing somewhere in the list of possible crystal structures.

7.10 *Motherwell (Rancel)*

Methodology
The Rancel program was used to perform a search for low energy crystal structures in a set of named space groups, using a rigid molecular model so compound VI was not attempted. The search method is a genetic algorithm, which is run on fixed population of 100 structures, for a maximum of 100 generations, and repeating the runs for 50 random starting sets (Motherwell, 1999). In this work a deliberate emphasis was placed not on the accuracy of the force field used, but on selection from the low energy set of structures on the basis of patterns found in the CSD. The empirical potentials of Gavezzotti (Gavezzotti,1994) were used, with no electrostatic charges, as these were found to give acceptably accurate locations of minima on many molecules of similar size and chemical type in the CSD, e.g. GLUTIM, EACLEZ, but of course not reliable in energy ranking as a predictive criterion.

Results
Compound IV was modeled as a rigid body using the CSD structure HIYKEF, removing side-chains and calculating all hydrogens at idealized geometric positions with C-H 1.083, N-H 1.009. The search gave many structures where dimer or catemer H-bond motifs were present within a low energy range of 10 kJ/mole. Examination of a set of CSD molecules containing rings with –CO-NH-CO- showed that both types of motif are represented, with no clear preference. A contact distance frequency scoring function was set up using a set of molecules of similar size and functionality (AZMCHO10, DTHPIM, EACLEZ, HPTLIM, NAPOIM, PHALIM, PHPYRO, PHYPHM, SUCCIN, TUPQEA, YUFNES), and a chi-squared fit, S, of the frequency distributions was calculated as a possible indicator for the most likely polymorph. A penalty function, P, were also devised to give the lowest score for the largest number of CH…O contacts less than the van der Waals radii sum, and a combined score function Q = S + P was calculated as a criterion. The submitted structures in order of ranking were (i) the lowest Q and also the lowest global energy found, a

catemer in $P2_12_12_1$, with a closely planar chain arrangement, (ii) low Q and planar catemer in $P2_1$, and (iii) the lowest Q for a dimer in the set, in Pbca. Unfortunately the correct structure was not generated in the search, which was found in post-analysis runs, but not with the lowest Q score, so this criterion as calculated could not have succeeded.

Compound V was modeled using the de-brominated derivative, ROLBOJ, and re-calculating hydrogen postions as before. A crude approximation was used where the energy curves of Br treated as S. The selection criteria applied to the low energy sets derived for space groups $P2_1$ and $P2_12_12_1$ were as follows, (1) $P2_12_12_1$, the global lowest energy, lowest cell volume, but with little confidence as various devised scoring functions Q did not perform well, and there were close Br…O contacts not seen in CSD,
(2) $P2_12_12_1$, global energy rank 2, good scoring function, low volume, and contacts Br…O compatible with similar CSD molecules,
(3) $P2_1$, lowest energy in $P2_1$, low volume, but not lowest Q, and no Br…O contacts which were thought to be likely from CSD. Post-analysis also showed that the correct structure was not in the low energy set, and also that the Q functions would not have succeeded.

7.11 Price (MOLPAK/DMAREL)

Methodology
The main distinguishing feature of our approach was the use of accurate anisotropic atom-atom models for the intermolecular potential, including anisotropic repulsion for the Br atom in V, plus careful consideration of the mechanical and morphological properties of the low energy structures. The search for minima in the lattice energy required a rigid molecular model and so no attempt was made for VI. This molecular model was obtained by ab initio optimization using a MP2 6-31G** wavefunction for IV and a SCF 6-31G** wavefunction for V. Sets of atomic charges, dipoles, quadrupoles, octupoles and hexadecapoles were obtained by a Distributed Multipole Analysis (DMA) (Stone and Alderton 1985) of each ab initio charge density, and used to evaluate the electrostatic contribution to the lattice energy. For V, the atomic multipoles were multiplied by a factor of 0.9 to approximately correct for the neglect of electron correlation on the charge density. The only other terms used to represent the intermolecular potential were a 6-exp atom-atom repulsion-dispersion model. The empirically fitted parameters due to Williams were used for C,H,N (Williams and Cox 1984) and O (Cox, Hsu, and Williams 1981), and consistently fitted parameters for the polar hydrogen H_N (Coombes et al. 1996) were used for IV. The same parameters for C, H, N and O were used for the interactions of the hydrocarbon groups and the oxygen and nitrogen atoms for V, leaving the S and Br atom interactions to be modeled non-empirically. Since the S atom was buried, its repulsion was unlikely to be significant, and so the same parameters as used in the previous blind tests (Lommerse et al., 2000) were used. However, the Br atom seemed likely to have a major effect on the packing, and was expected to have an elliptical van der Waals surface (Nyburg and Faerman, 1985), so its interactions with all other atom-types were determined non-empirically. The dispersion coefficients were obtained using atomic polarisabilities (Miller, 1990) in the Slater-Kirkwood formulae. The repulsion parameters were determined by assuming it was proportional to the overlap between two methyl bromide molecules for Br..Br, Br..C and Br..H interactions and between methylbromide and methanesulfonamide for Br interacting with N, O and S. The proportionality parameters were obtained by fitting to the exchange-repulsion energies calculated by Intermolecular Perturbation Theory (Hayes, Hurst, and Stone 1984)for 30 randomly chosen repulsive contacts for each pair of molecules. This overlap model approach (Mitchell and Price, 2000) has the great advantage that the total molecular overlaps can be sub-divided into atom-atom contributions, using a Gaussian Multipole representation of the molecular charge densities. This allows each atom-atom contribution to be fitted separately, allowing the determination of whether the isotropic exponential form is adequate. In this case, we determined both an isotropic and anisotropic potential for Br interactions. The anisotropic Br potential corresponded to the Br atom having an elliptical shape, with the same functional form as the anisotropic Cl potential which has recently been developed using the same methodology (Mitchell et al., 2001). The atom-atom repulsion-dispersion potential for V is summarized in the Supplementary Material.

The lattice energy minima search was conducted using the starting points generated by MOLPAK (Holden, Du, & Ammon, 1993), using the latest version kindly supplied by Ammon, and then using a new version of DMAREL to find the corresponding lattice energy minima. About 1500 minimisations were carried out for IV, and only 375 in the chiral space-groups for V. The Hessian matrix was examined at the end of each minimization, and used either to lower the symmetry constraints if a saddle point had been found, or to calculate the elastic constant matrix of the minimum energy structure. The growth morphology of the low energy structures was estimated using the attachment energy model within the Cerius2 software (Accelrys Ltd, 2000).

Results

The search for IV was unsuccessful, as the MOLPAK procedure did not produce an appropriate starting point. The minimum found by using our molecular model and model potential in the experimental structure reproduces it quite well, but is 4 kJ/mol more stable than the best catemer structure found in the MOLPAK search. This appears to be because the purely repulsive MOLPAK model generates relatively few catemer starting points. We found that only 21 of the 108 $P2_1/c$ minima were catemer structures. The model potential was also deficient, as the experimental structure was 8 kJ/mol higher than the global minimum, and so outside the group of 14 low energy structures which were considered for submission. These were all dimer structures. The calculated lattice energy of the experimental structure is sensitive to the location of the hydrogen atoms, since the experimental molecular structure with the hydrogen bond lengths standardized to neutron values, produces a minimum within 4 kJ/mol of the global minimum. Thus, the use of a rigid gas phase molecular structure, with empirical hydrogen interactions at the nuclei, is not quite accurate enough for the experimental crystal structure to have appeared within the energy range of plausible structures.

We successfully predicted V as our first ranked submission. The global minimum found in the search was the experimental structure (Table 4), with a rms. cell length error of 2.6%. The lattice energy of –110.1 kJ/mol was 1.7 kJ/mol lower than any other found, hence it was submitted with about as much confidence as can reasonably be given to lattice energy search results at the moment.

The energetically favoured structures (14 structures for IV and 16 for V within 10 kJ/mol of the global minimum) did not show any marked variations in growth rate and none were particularly susceptible to mechanical distortion. Hence consideration of the kinetics of crystallite growth and mechanical stability was not helpful in distinguishing between the hypothetical low energy structures in these cases, unlike that of paracetamol (Beyer, Day, & Price, 2001).

The successful prediction of V as a clear global minimum in the lattice energy reflects the reduced number of packing motifs for this lumpy chiral molecule and the accuracy of the model intermolecular potential. The novel modeling of the anisotropic shape of the repulsive wall around Br was not crucial to the success of the model, as the experimental structure remained the global minimum, albeit by a slightly smaller margin of 1.3 kJ/mol when the isotropic Br model was used. The electrostatic energy is only a minor component of the lattice energy, with our first and second guesses having electrostatic energies of -38.1 and –39.1 kJ/mol respectively, significantly lower than the third guess at –30.2 kJ/mol. So although the realistic representation of the electrostatic energy is important, the relative strength of the dispersion contribution also needed to be reasonable. Since Ammon also found the experimental structure as the global minimum for the chiral space groups, using distributed multipoles and an empirically derived repulsion-dispersion potential, we must conclude that the relative lattice energies can be well predicted by carefully developed potentials.

The anisotropic Br potentials used in the successful prediction of V by Price

Atoms ι and κ	$C_{\iota\kappa}$ /kJ mol-1 Å	$B_{\iota\kappa}$/ Å^{-1}	$A_{\iota\kappa}$ / kJ mol-1
Br…Br	10488.71	3.9726	16984474
Br…C	4138.34	4.0950	5597582
Br.. .H	1383.02	3.8338	279723
Br…N	4433.63	4.0047	4693682
Br…O	2963.29	4.1074	4967420
Br…S	10052.46	4.1016	6580190
S…S	5790.66	3.3007	401033

The potential used had the form:

$$U = \sum_{i\in A, k\in B} A_{\iota\kappa} \exp\left(-B_{\iota\kappa}\left(R_{ik} - \rho_{\iota\kappa}\left(\Omega_{ik}\right)\right)\right) - C_{\iota\kappa} / R_{ik}^{6} + U_{elec}\left(DMA, \Omega_{ik}, R_{ik}^{n}, n \le 5\right)\Big)$$

with the anisotropy in the repulsion on Br being represented by

$$\rho_{\iota\kappa}(\Omega_{ik}) = \rho_1^{\iota}(z_i \cdot R_{ik}) + \rho_1^{\kappa}(-z_k \cdot R_{ik}) + \rho_2^{\iota}(3[z_i \cdot R_{ik}]^2 - 1)/2 + \rho_2^{\kappa}(3[z_k \cdot R_{ik}]^2 - 1)/2$$

where $\rho_1^{Br} = 0.014085$Å , $\rho_2^{Br} = -0.088952$Åand all other anisotropy coefficients being zero. The local **z** axis is along the C-Br bond, and the unit inter-atomic vector $\mathbf{R}_{ik}$ is from atom *i* of type ι to atom *k* of type κ.
The remaining repulsion-dispersion parameters were taken from (Williams & Cox, 1984, and Cox, Hsu, & Williams 1981), or the S parameters given above, assuming the combining rules used in (Williams & Cox 1984).

*7.*12 Scheraga (CRYSTALG)

Program details
The CRYSTALG program predicts crystal structures by global optimization of a potential energy function without assuming any symmetry information. The number of molecules in the unit cell (Z) is a parameter, i.e. several runs for different values of Z are carried out, and the value of Z that leads to the lowest energy per molecule is selected. In the current version of the program, we use a newly developed global optimization method, Conformation-Family Monte Carlo (CFMC) (Pillardy, Czaplewski, Wedemeyer & Scheraga,2000; Pillardy, Arnautova, Czaplewski, Gibson & Scheraga, 2001). We are still working on improving this method. The program has been tested on crystal structure prediction calculations for a number of rigid and flexible H, C, N, O-containing molecules. The CFMC method can be considered as an extension of the Monte Carlo-Minimization (MCM) method. The most important differences between the classical MCM and the CFMC are that the CFMC method does not use a single conformation for a Monte Carlo step; instead, it uses the whole family of conformations (and, consequently, only the moves *between families* are accepted or rejected). Any two structures belong to the same family of structures if they are different representations of the same crystal structure. The database of the families and structures encountered during the calculations is maintained throughout the simulation. The structure-family database for a CFMC run is initialized by successively generating a set of random structures, and the database is updated by structures generated during the MCM procedure. All structures in the database are locally minimized. A total of 5000 local minimizations was carried out for each run.

The potential energy is assumed to be a sum of pairwise interatomic interactions, and includes electrostatic, nonbonded, and torsional terms. The electrostatic interatomic interactions were modeled by the Coulomb formula in which q_i and q_j are point charges positioned on the atom sites. The electrostatic energy was calculated using the Ewald summation without including the dipole moment correction term. The atomic charges were obtained by fitting to the molecular electrostatic potential calculated *ab initio* (HF 6-31G*). The torsional energy was calculated using a third-order Fourier expansion with coefficients obtained by fitting the torsional energy to the difference between the *ab initio* and molecular mechanic (sum of nonbonded and electrostatic) profiles.

Ab initio quantum chemistry calculations were carried out for the target molecules to obtain molecular geometries. Our results showed that the two methods used [Hartree-Fock (HF) and Möller-Plesset perturbation theory up to the second order (MP2) methods with 6-31G* basis set] gave very similar values of the geometrical parameters. For both methods, the mean deviations of the bond lengths, valence and torsional angles from their experimental values did not exceed 4%. We also evaluated the relative stabilities of two possible conformations of the six-carbon ring of compound IV (boat and chair). The chair conformation was much more stable and it was chosen for further calculations.

As the first part of our crystal structure prediction procedure, we carried out a refinement of the potential parameters for some atom types present in the target molecules using our recently-developed Monte Carlo-based method for refining potential parameters (Arnautova, Pillardy, Czaplewski & Scheraga, 2002). The main idea of the method is to derive parameters that satisfy the following criteria: (1) the potential should reproduce the experimental structure within a certain accuracy; (2) the crystal structures corresponding to the lowest-energy minima found for the potential should represent possible crystal structures, and one of them, possibly the global minimum, should correspond to the observed structure; (3) the energy value for the observed structure should be close to the experimental enthalpy of sublimation. To obtain a potential satisfying these requirements, we have to optimize a vector function including three main components: the first one depends on the order and relative position of the minima; the second is the penalty function providing the best fit to heats of sublimation, and the last is a measure of similarity between the experimental and minimized experimental structures. Our method allows us to minimize all three components simultaneously for an arbitrary number of molecules.

Crystal structure prediction calculations for the three target molecules were carried out in several steps.

1. A search of the Cambridge Structural Database was carried out in order to find experimental crystal data for molecules containing functional groups and atom types similar to those in our targets (test molecules). We chose 1,2,3,6-tetrahydro-phthalimide (CSD reference code PHYPHM) as a test molecule for compound (IV), α-1,2,3,4,5,6-hexabromocyclohexane (LIDCIK) and 2,3,5,6-tetrabromonorbornane (BAVJUD) for compound (V), and 8,8-dimethyl-3,3a,4,5,6,7-hexahydro-3a,6-methanobenz(c)-isothiazole s,s-dioxide (ROLBOJ) for compounds (V) and (VI).
2. For the test molecules we carried out crystal structure prediction calculations using the AMBER (Cornell et al., 1995) and Williams (Williams & Cox, 1984) force fields in order to evaluate the quality of these potentials and effectiveness of our search method. We ran computations for Z equal to 2 and 4. In the case of PHYPHM, the molecule similar to the first target, both potentials were "good", i.e. the minimized experimental structure corresponded to the lowest minimum of the lattice energy, and structural deviations from the experimental structure were quite small. We chose the AMBER force field for crystal structure prediction of the first target. For ROLBOJ, the minimized experimental structure was minimum number three for Z=2. In the case of bromine-containing molecules, we had to obtain potential parameters for bromine because they were not included in either the Williams or the AMBER force fields. We ran several global optimization computations using the AMBER, Williams, and Dreiding (Rappe, Casewit, Colwell, Goddard & Skiff, 1992) potentials. None of them were satisfactory. The minimized experimental structures were more than 1 kcal/mol higher than the lowest minimum found, and quite large structural deviations from the experimental structure were observed for all potentials. In the case of the AMBER and Dreiding potentials utilizing the '6-12' functional form, the structural deviations were somewhat larger, and the symmetries of the experimental structures were not preserved during local minimization. It appears that the '6-exp' form of the potential is more suitable for crystal calculations of these molecules.
3. For ROLBOJ, BAVJUD and LIDCIK, we tried to improve the potential parameters using our potential optimization method. In the first round of potential optimization, the parameters for the N, S and O atoms in the ROLBOJ molecule were improved. As a result, the minimized experimental structure was found as the global minimum during global optimization carried out with the new set of parameters. In the second round, we tried to refine the parameters for bromine. Although the values of all components of our vector function were decreasing, we were not able to change the order of the minima. This result may be due to the presence of specific Br...Br interactions in the crystals of these molecules which contain a large number of bromine atoms. Use of rules for heteroatomic parameters might not enable us to obtain correct values for the parameters A_{BrBr} and B_{BrBr}. For crystal structure prediction (compounds V and VI), we used the improved parameters for N, O, S and William's (Hsu & Williams, 1980) chlorine parameters for Br.

Compound (IV). In order to predict the crystal structure of this compound, we used our global optimization CRYSTALG program with the AMBER force field. The lowest-energy minima for the molecule (PHYPHM) similar to compound (IV) were not always reproducible by our method; so, we checked the quality of our search for compound (IV) by carrying out additional systematic searches in the most common space groups provided by the organizers of this exercise. The PMC program of Dzyabchenko (Dzyabchenko, Agafonov & Davydov, 1999) was used. The lowest-energy structures found by the systematic search were subjected to subsequent energy minimization without any symmetry constraints. As a result, we submitted the list of the three lowest-energy structures obtained by both systematic (first two structures) and global (structure number three) search. All submitted structures contain dimers of molecules connected by hydrogen bonds and look plausible. The experimental structure (catemer hydrogen bond motif) was not present on this list although the structure found as minimum number three in our global search (minimum number 5 in the joint list) corresponds to the experimental structure minimized with the AMBER potentials.

Compound (V). Crystal structure prediction calculations for compound (V) were carried out using our improved Williams potential. To assess the success of the crystal structure prediction for this compound, the experimental structure was subjected to local energy minimization with the improved potential. The resulting structure was not present among the structures submitted as the predictions. It was also not found among our higher-energy structures although its energy suggests that the rank of this structure can be somewhere around 5.

Compound (VI). Our CRYSTALG program enables us to conduct a global search for flexible molecules; however, at the time of the "blind" test, the program was still under development, and this influenced the results of our predictions. Global optimization runs carried out for Z=2 and Z=4 for compound (VI) (with the

improved Williams potential supplemented by parameters of Price (Mitchell & Price, 1990) for hydrogen attached to nitrogen), produced only low-symmetry structures (number of symmetry independent molecules in the unit cell ≥2) built of molecules in the cis-conformation (C=N bond). Therefore, we carried out a systematic search in the most common space groups considering only the more stable cis-conformation. Energy minimization of the experimental structure (with molecules in the trans-conformation) with our potential showed that it is much more stable than any structure that we found.

Table Scheraga. Potential parameters for N, O, and S before and after improvement (*A* in kcal·mol^{-1}·Å^{6}, *B* in kcal·mol^{-1}, *C* in Å^{-1}). Parameters for H and C were taken from D.E. Williams, S.R. Cox. *Acta Crystallogr.* 1984, B40, 404; parameters for hydrogen H* attached to nitrogen were taken from J.B.O. Mitchell, S.L. Price. *J. Comput. Chem*. 1990, 11, 1217.

Atom type	Parameter	initial	improved
H	***A***	32.60	32.60
	B	2861.140	2861.14
	C	3.74	3.74
H*	***A***	5.14	5.14
	B	1202.10	1202.10
	C	2.73	2.73
C	***A***	583.13	583.13
	B	88370.69	88370.69
	C	3.60	3.60
N	***A***	329.45	270.64
	B	60833.89	101388.51
	C	3.78	3.78
O	***A***	268.55	153.17
	B	54986.62	48514.29
	C	3.96	3.96
S	***A***	2788.48	2006.96
	B	41424.47	56525.26
	C	2.90	2.90

$$E_{ij} = -\frac{A_{ij}}{r_{ij}^6} + B_{ij}\exp(-C_{ij}r_{ij}) + \frac{q_i q_j}{r_{ij}}$$

7.13 Schmidt (CRYSCA)

CRYSCA program

The program CRYSCA ("Crystal Structure Calculations") performs global energy optimisations for flexible molecules, starting from random crystal structures (Schmidt, 1995; Schmidt & Englert, 1996; Schmidt, 1999). The starting set consists of several hundred random crystal structures with random values for lattice parameters, orientation and position of the molecules as well as for the intramolecular degrees of freedom. The user selects, which intramolecular degrees of freedom (distances, angles or rotations) are to be considered. All starting values are inside sensible ranges. The crystal symmetry is included from the beginning. All crystallographic symmetries can be handled, including scarce space groups, molecules on special positions, supersymmetries, disorders etc.. For crystal structure predictions, where the space group is not known, all common space groups are tested separately. The energy is minimised by a special steepest-descent algorithm. The minima are sorted according to energy, and checked for higher symmetries, meaningful molecular conformations and reliable intermolecular interactions. The packings having the lowest energy are regarded as 'predicted' crystal structures.

The molecular geometries are constructed with respect to crystal structure data of similar compounds or fragments, which were found by extensive CSD searches. In addition, quantum mechanical calculations were carried out. For compound IV and compound V, the geometry calculated by AM1 showed similar bond distances and angles as found in the CSD. These AM1 geometries were chosen as a basis for the energy minimisations. For compound V the calculated S=O, C-CH_3 and C-Br distances were corrected manually to correspond to the values from the CSD. Molecule VI was constructed according to the crystal data of form(ii) of sulfapyridine (Bar & Bernstein, 1985, CSD reference code BEWKUJ11). In all cases the positions of the hydrogen atoms were idealised with C-H and N-H distances of 1.04 and 1.01 Å, resp.

Molecules IV and V were treated as rigid. For molecule VI three intramolecular degrees of freedom were considered: (1) rotation around the S-N bond, (2) rotation around the Ph-S bond, (3) twisting around the N=C double bond. Intramolecular van der Waals interactions between C and H atoms were included, to prevent the two 6-membered rings to come too close together. The twisting around the N=C double bond was described by a harmonic potential with a force constant of $f = 0.1\ kJ{\cdot}mol^{-1} \cdot (°)^{-2}$ and a minimum at 0° or 180° for the cis and trans conformations, resp. For the rotations around the single bonds (1) and (2), CSD searches were carried out to determine the preferred conformations in the solid state. For both rotations, the torsion angles C-S-N=C (for (1)) and C-C-S-N (for (2)) typically adopt values between 60° and 90°. The intramolecular potentials were chosen in order to represent these distributions: Harmonic potentials were set up with $f = 0.01\ kJ{\cdot}mol^{-1} \cdot (°)^{-2}$ and minima at 60° for (1) and 90° for (2), resp. With these intramolecular potentials, the energy minimum of a single molecule VI (trans conformation) converged at torsion angles of 76.5° each for (1) and (2); these values lie well inside the experimental torsion angle distributions.

The lattice energy is calculated by CRYSCA by the formula

$$E = \frac{1}{2} \sum_i \sum_j \left(-A_{ij} r_{ij}^{-6} + B_{ij}\, e^{-C_{ij} r_{ij}} + \frac{1}{4\pi\varepsilon\varepsilon_0} \frac{q_i\, q_j}{r_{ij}} \right)$$

where A, B, and C are empirical van der Waals parameters (Schmidt & Englert, 1996, Schmidt, 1999), q resembles the atomic charge, and r_{ij} stands for the interatomic distance between the atoms i and j. The dielectric constant ε is set to 1.0. Van der Waals parameters for bromine were taken from Giglio (1970), after test calculations on three model compounds showed, that these parameters should work fairly well. For sulphur, the following parameters were used: A(S...S)= 6000 $kJ{\cdot}mol^{-1}{\cdot}Å^6$, B(S...S)= $1{\cdot}10^6\ kJ{\cdot}mol^{-1}$, C(S...S) = 3.56 $Å^{-1}$.

The charges are calculated for compound IV by the charge-iteration procedure using the program ICON (Howell *et al.*, 1977), and scaled by 1.1. It had been shown (Schmidt, 1995), that these charges generally work well in combination with the applied van der Waals parameters. For compound V and VI, charges were calculated by the Gasteiger method and scaled by 0.5. For the N-H groups in IV and VI, the charge separation between hydrogen and nitrogen was increased manually in order to get a better description of hydrogen bond interactions.

The energy minimisations were carried out in the common space groups $P2_1/c$, P-1, $P2_12_12_1$, C2/c, $P2_1$, Pbca, $Pna2_1$, Pbcn, Cc and C2. For molecule V only the solutions in , $P2_12_12_1$, $P2_1$, and C2 were relevant because the compound was enantiomerically pure. Molecule VI was calculated in $P2_1/c$, P-1, C2/c and Cc only due to computer time limitations.

For compound IV, preliminary calculations in $P2_1/c$ showed, that all low-energy packings consisted of 'dimers': two CONH groups form an 8-membered hydrogen-bonded ring around an inversion centre. This structural motif seemed to be much more advantageous than a chain topology of hydrogen bonds. Consequently, only space groups having an inversion centre were considered further ($P2_1/c$, P-1, C2/c, Pbca, Pbcn). Although the experimental structure shows a chain topology, it was found in the calculations. The structure was not predicted *a priori* because of slightly worse energy (see table 6), but it could easily be recognised by comparison of the experimental and the calculated X-ray powder diagrams.

Compound V correct structure was found in the calculations, too, but with a non-favourable energy. Hence the structure could not be predicted *a priori*. The comparison with the given experimental X-ray powder diagram did not help, because the diagram of the calculated correct packing was not similar to the diagram of the experimental structure. The reason for the distortion of the packing might be that the van der Waals interactions of the bromine atoms are not well described by the atom-atom potential method.

Compound VI was not found in the crystal structure predictions, because the experimental structure shows an unusual conformation: The torsion angle C-C-S-N, describing the rotation around the Ph-S bond, exhibits a value of 27°, which is by far outside the range given by other similar compounds (60° to 90°). Correspondingly, the used harmonic intramolecular potential is not suitable; the calculated intramolecular energy would be about +40 $kJ \cdot mol^{-1}$. This prevents the crystal structure from being found as a minimum with reasonable energy. When the intramolecular potential for the rotation around the Ph-S bond is neglected, the crystal structure can be found (see Table 8). In many cases, it is useful to look into the CSD in order to focus the search on those conformations, which are statistically preferred in the solid state. However, for compound VI, this approach led to an exclusion of the correct solution.

7.14 *Van Eijck (UPACK)*

Structure generation

The random search technique implemented in the UPACK program (van Eijck & Kroon, 2000) was used. The two torsional degrees of freedom in compound VI were set to random values in each starting structure, but *cis* and *trans* forms about S-N=C-N were treated separately. For each compound 5000 structures were generated in each of the qualifying space groups, and subjected to a preliminary energy minimization with fully flexible molecules. This was sufficient to find all low-energy structures several times, except for compound VI in space group $P2_1/c$ where 10000 additional structures had to be created. Equivalent structures were removed by clustering, after which the energy minimization was continued for structures within an energy window of 30 kJ/mol. A second clustering delivered the final lists of possible structures.

Force fields

Models of the free molecules were constructed by geometry optimisation of suitable molecular fragments at the 6-31G* level, combined with average geometrical parameters from the CSD database (Allen & Kennard, 1993). Force field parameters for bond distances and bond angles were adjusted to reproduce these geometries, and reasonable values were guessed for the corresponding force constants. Charges were obtained from ESP fittings, using MOLDEN (Schaftenaar & Noordik, 2000) on wave functions for the complete molecules (STO-6G for compound V and 6-31G** for compounds IV and VI). Since these charges were expected to overestimate the true values, an overall dielectric constant of 1.5 was employed. All torsional angles involving sp^2 C and N atoms were restrained to planarity with aid of a harmonic potential. The dihedral force constants for the puckering of the five-membered ring C-C-C=N-S in compound V were set to zero. Intermolecular Lennard-Jones parameters were taken from the all-atom OPLS force field (Jorgensen et al, 1996), augmented with values from GROMOS96 (van Gunsteren et al, 1996) for bromine and sulphur. Mixing parameters from different force fields is generally not a good idea, but no better method could be implemented within a reasonable amount of time.

Initially no dihedral angle force constants were defined for the angles ψ = C-C-S-N and φ = C-S-N-C in compound VI. In the database 82 fragments $PhSO_2N{=}C$ were found which were not embedded in a larger

ring structure. Both ψ and φ showed maxima around 90°; for ψ the distribution ranged between 30° and 150°, for φ between 70° and 170°. To determine the necessary torsional parameters, 1000 preliminary structures were generated in $P2_1/c$. After energy minimisation it was found that the distribution of φ-values corresponded nicely with the histogram from the database, but the ψ-values were almost evenly distributed. A better correspondence was obtained by adding a term $V_\psi \cos 2\psi$, with $V_\psi = 1$ kcal/mol.

In order to test the force field, preliminary structure predictions were done for related molecules found in the database. For compound IV AZMCHO and GLUTIM represent the glutarimide fragment. ROLBOJ corresponds to compound V with Br replaced by H; BRMACA and REZNIT were studied to find a possible improvement for the van der Waals parameters of the bromine atom. For compound VI no suitable fragments were found. The results (Table Eijck-1 of the Supplementary Material), although no worse than might be expected from the ad-hoc force field, were not encouraging: there were too many low-energy structures to obtain anything like a reliable structure prediction. In all cases the correspondence between the observed and calculated cell parameters and molecular positions was reasonable.

For the most promising structures of GLUTIM ab initio energies were calculated, as detailed recently (van Eijck et al**,** 2001a). Here intramolecular energies were obtained directly at the 6-31G* level, whereas intermolecular energies came from the parameterization developed by Coombes et al (1996). In this model the experimental structure ranked second in the list of energies.

The corrections from energies to free energies (at 300 K) were also estimated. This was done by calculating the harmonic frequencies of the lattice vibrations (van Eijck, 2001) from the force-field. For unsaturated hydrogen-bonded systems this approach has led to improved ab initio structure predictions (van Eijck et al**,** 2001b). Here, however, the ab initio results for GLUTIM deteriorated upon considering the free energy (although all empirical rankings improved). So for compound IV no corrections to free energies were applied.

Results

The number of structures within 10 kJ/mol was 160 for compound IV and 106 for compound V. For compound VI the conformation around the S-N=C-N bond may be either *cis* or *trans*. The two possibilities might correspond to chemically distinct substances, but both cases were investigated as no experimental information was available. Neglecting any possible torsional force constants for the double bond, the global minimum was found for the *cis* form. The best *trans* structure was 8.5 kJ/mol higher in energy. There were 15 *cis* structures and 166 *trans* structures within 10 kJ/mol of their respective global minima. For compound IV, ab initio energies were calculated in the same way as for GLUTIM. For all compounds the three submitted structures were selected with the criterion that they should occur consistently with low (free) energy on all available lists. For compound VI one *trans* structure was included.

After the submission, the simulated powder diffraction diagrams of the experimental structures were compared visually with similar diagrams for the hypothetical structures. For compound IV an almost perfect match was seen for a structure in space group $P2_1/c$. This structure was the fifth in energy, and it was identified with near certainty. But for compounds V and VI no satisfactory match was found, and structures with remotely acceptable powder diffraction diagrams were selected without much confidence.

Post-analysis

The observed structures were energy-minimized to enable comparison with the lists of generated structures. All three were found to be present. Furthermore, the energies of all structures proposed by the other participants were minimized. All structures within 10 kJ/mol from the respective global minima were present. For compounds IV and V only one structure was missing, indicating that the search was essentially complete. However, for compound VI about half of all submitted structures were not traceable in the list.

The geometry differences between observed and "predicted" structures are given in Tables 6-8. It is seen that structure IV is well reproduced. Contrarily, structure V is deformed to such an extent that the powder diffraction pattern was not recognized. The main reason for this failure is that the puckering of the five-membered ring C-C-C=N-S is all wrong. No potential had been set for the five dihedral angles involved; if they had been restrained to the values observed in ROLBOJ the results would have been much better. Structure VI is reasonably well reproduced, apart from the peculiar bond distances.

The rankings and energy differences with respect to the global minima are given in Table Eijck-2 of the Supplementary Material. For compound IV the first submitted structure had the lowest empirical energy as well as the lowest ab initio energy, and it was disappointing that it was not the observed polymorph. Eight

other participants have also submitted variants of this structure (Table 9). Consideration of the free energy would have given no improvement. Contrarily, for compound V use of the free energy criterion led to submission of the correct structure as the first choice. However, this structure is correct only in the sense that it is identical with the energy-minimized experimental structure, but is was not good enough to allow recognition of the corresponding powder diffraction pattern. For structure VI the relative energy is unexpectedly large. Nevertheless, the calculated powder diffraction pattern might well have been recognized if the inspection of these diagrams had not been given up after about 250 structures.

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(Free) energy differences ΔA, ΔE (kJ/mol) and rankings R_E, R_A refer to the energy-minimized experimental structure with respect to the global (free) energy minimum at 300 K.

Table Eijck-1. Results of preliminary crystal structure predictions.

	Space group	ΔE	R_E	ΔA	R_A
AZMCHO	*Pccn*	3.1	15	2.1	5
GLUTIM	$P2_1/c$	2.6	32	1.8	13
GLUTIM (ab initio)	$P2_1/c$	0.5	2	2.4	5
ROLBOJ	$P2_1$	9.1	32	7.7	21
BRMACA	$P2_1/c$	0	1		
BRMACA01	*Pccn*	3.0	47		
REZNIT	$C2/c$	8.1	6		

Table Eijck-2. Status of the experimental structures in the blind test.

		ΔE	R_E	ΔA	R_A	Submitted
IV		2.0	5	2.4	12	Only after powder data
IV (ab initio)		2.0	6	2.8	12	
V		1.2	4	0	1	As first choice
VI (*trans* only)	13.0	340	11.0	278		
VI (*trans* + *cis*)	21.3	413	20.1	358	No	

7.15 Verwer (MSI-PP/Dreiding)

The method used is similar to that used by Leusen, and by Mooij, since all three use the Accelrys Polymorph Predictor to obtain their structures, which has been described elsewhere (Leusen, 1996; Leusen *et al*., 1999). The difference is in the ranking of predicted structures, where different force fields and charge models have been used. In this case, the Dreiding 2.21 force field (Mayo *et al*., 1990) was used, in combination with atomic charges fitted to the MEPs of the optimized molecules.

Dreiding is a generic force field, which uses force constants and geometric parameters based on simple hybridization considerations rather than the particular combination of atoms involved in the bond, angle, or torsion. Despite its simplicity, encouraging results where obtained in the 1999 blind test (Lommerse *et al*., 2000). Atomic charges where obtained by optimizing the molecules at the HF 6-31G* level using Gaussian94 (Frisch *et al*., 1995), and fitting atomic charges to the resulting MEP, using the molecular dipole moment as an additional constraint. The ChelpG method (Breneman and Wiberg, 1990) was used to do so. The atomic radius of bromine had to be supplied by hand for the calculation on molecule V, and was set to 1.85 Å. Molecule VI has two rotatable torsions, and the possibility of cis-trans tautomerization around the CN double bond. Based on a very limited (9 hits) search in the CSD (Allen *et al*., 1991) and time considerations, it was decided to do the quantum mechanical calculations on the conformer which has ∠(CSNC)= 180º, ∠ (CCSN)= ±90º, and S-N=C-N trans. Predictions were carried out on each model applying space-group symmetry, taking a single molecule per asymmetric unit, and were repeated until no new structures of low energy were found, to ensure that sampling, which is based on a Monte Carlo algorithm, could be considered complete.

For molecule IV, predictions where carried out in the 10 suggested space groups, and had to be repeated 8 times to achieve completeness. In total ca. 88000 structures were generated and optimized, leading to ca. 3400 structures that were considered unique after optimization. Structures ranked 1, 2, and 3 were selected, with relative energies of 0, 0.25 and 0.38 kcal/mol. The correct structure was in the predicted set, ranked 209, with a relative energy of 1.30 kcal/mol, deviations in cell parameters of 1-2%, and small deviations in atomic positions. Given the type of molecule, the ranking was worse than expected.

Molecule V was used in predictions in only those three space groups in the top ten which lack inversions and mirrors. To prevent the SO_2 group from heavily deforming, the NSO_2 unit was defined to be rigid in the energy minimizations. Three prediction runs in the allowed space groups were done, all yielding the same set of low-energy structures. In total ca. 11500 structures were optimized, producing a set of ca. 2000 unique structures. Structures ranked 1, 2, and 4 were selected (number 3 turns out to be indistinguishable from number 2), with relative energies of 0, 0.088 and 0.094 kcal/mol. The correct structure was predicted ranked 6, at a relative energy of 0.30 kcal/mol, in close geometric correspondence. Given earlier experience with the Dreiding force field, this is an expected result.

As with molecule V, the SO2 group in molecule VI had to be put into a rigid NSO_2 unit to avoid large geometric deviations. The CSD search suggested that the phenyl group may rotate ca. 30º both ways from the optimized position, which can be easily achieved from this starting point. Besides its value used in the quantum mechanical calculation, the C-S-N=C torsion has two additional energy minima, which are symmetry related. To avoid the energy barrier involved from hampering a complete sampling of structures, this other conformer was also used as initial structure in the predictions. Two prediction runs in ten space groups turned out to be sufficient to obtain adequate sampling starting from one conformer, producing a number of structures where the molecule had obtained the different conformation described above as well. A run starting from the other conformation produced no new structures. Apparently, the energy barrier is small enough to be overcome during optimization, after all. About 39000 structures were generated and optimized, and ca. 6000 unique structures were obtained. Energy calculations on this molecule turned out to be problematic: structures ranked 1, 2, 5, and 6 by energy all had a very unlikely orientation of the phenyl ring, and were therefore discarded. Structures ranked 3, 4 and 7 were selected, with relative energies of 0, 0.08 and 0.26 kcal/mol. The correct structure turned out not to be in the predicted set, which is surprising given earlier results with the polymorph predictor, and most likely due to the inadequate performance of the force field for this molecule. The correct structure was calculated to have a relative energy of 7.79 kcal/mol, ranking it at position 733 had it been added to the set. In our experience, sampling of structures with such high energies is usually far worse compared to the low-energy range. After optimization, cell parameters were off by up to 4.2 % and 4.3º, but the molecular conformation was retained quite well. Given the type of the molecule a slightly better, but still inadequate result was expected.

7.16 *Williams (MPA)*

First, each of the three molecules was optimized by ab initio quantum mechanics using HF-631g** wavefunctions (Frisch et al., 1995). The conformations of IV and V seemed straightforward. For molecule VI , a model with the two rings coplanar to the SO2 bisector was obtained.

Intermolecular energy minimization was done by off-ridge eigenvector minimization (Williams, 1972b), steepest descents, or Newton-Raphson as internally selected by the MPA program (Williams,1972b; Williams, 1992; Williams, 1996). Crystal structure prediction was carried out automatically in two stages. In the first stage, the starting molecule was initially placed in a large orthogonal cell, e.g. 24x24x24A, avoiding close proximity to symmetry operators, and rotated to a Lattman grid point (Williams,1973). While holding the rotational position of the molecule and cell angles, the three cell edge lengths were optimized.

In the second stage all crystal structure variables consistent with the space group were included and optimized. This procedure was repeated for a Lattman grid of 536 points with spacing of about 29 degrees, and for each space group. Often, several starting grid points led to the same minimum, but still there were many subsidiary energy minima.

Intermolecular force field W99 was used (Williams, 2001). This force field uses (exp-6-1) terms based on foreshortened X-H distances (Starr & Williams, 1977) and extra charge sites. Atomic and extra charge sites were obtained using program Pdm97 (Williams, 1997). Extra charge sites were placed on CH2 groups (Williams, 1994; Williams & Abraha, 1999) and bent digonal nitrogen (Williams & Weller, 1983). For molecule V the bromine atom force field was transferred from krypton (Williams, 1972a). For molecule VI the sulfur atom force field was taken from a study of Sn molecules (Abraha & Williams, 1999).

Molecule IV. The molecular structure had error 0.049A rms with maximum error 0.104. Although none of the three lowest energy structures were correct, the rank 4 prediction was successful. When the starting molecular structure was replaced by the observed molecular structure, no better results were obtained.

Molecule V. The molecular structure had error 0.106A rms with maximum error 0.315. The rank 3 prediction was successful. When the starting molecular structure was replaced by the observed molecular structure, the rank 1 prediction was successful. This suggests that the original rank 3 placement is an artifact of the slightly incorrect molecular structure.

Molecule VI . The starting molecular structure was completely wrong, and needed adjustment about three significant torsion angles. However, predictions were based on allowing only two torsion angles, and all failed. When the starting molecular structure was replaced by the observed molecular structure, no better results were obtained.

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EXPERIMENTAL STRUCTURES (CIF – FORMAT)

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of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc.
and is
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 not relevant to the choice of reflections for refinement.  R-factors
based
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and R-
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In this refinement, all H atoms were located from the difference
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planes)
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N1 H1 0.873(15) . ?
C1 O1 1.2199(14) . ?
C1 C2 1.5025(15) . ?
C2 C3 1.5151(18) . ?
C2 C8 1.5379(17) . ?
C2 H2 1.009(14) . ?
C3 C4 1.5231(18) . ?
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C3 H3A 1.001(15) . ?
C3 H3B 1.004(14) . ?
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C4 H4 0.929(17) . ?
C5 O2 1.2133(13) . ?
C6 C7 1.516(2) . ?
C6 H6A 1.038(16) . ?
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C7 C8 1.5215(18) . ?
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O1 C1 C2 123.22(10) . . ?
N1 C1 C2 117.41(10) . . ?
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C3 C2 H2 111.8(8) . . ?
C8 C2 H2 108.5(8) . . ?
C2 C3 C4 108.16(10) . . ?
C2 C3 H3A 110.8(8) . . ?
C4 C3 H3A 108.7(8) . . ?
C2 C3 H3B 111.3(8) . . ?
C4 C3 H3B 111.6(8) . . ?
H3A C3 H3B 106.3(12) . . ?
C5 C4 C3 110.09(10) . . ?
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C6 C4 H4 109.2(10) . . ?
O2 C5 N1 119.32(10) . . ?
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C7 C6 H6A 109.9(8) . . ?
C4 C6 H6A 104.7(9) . . ?
C7 C6 H6B 112.5(9) . . ?
C4 C6 H6B 107.0(9) . . ?
H6A C6 H6B 109.7(12) . . ?
C6 C7 C8 112.53(11) . . ?
C6 C7 H7A 109.3(8) . . ?
C8 C7 H7A 107.0(8) . . ?
C6 C7 H7B 110.3(10) . . ?
C8 C7 H7B 109.2(10) . . ?
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# Experimental coordinates Molecule V  (Fronczek)
data_Gabriel45

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 Refinement of F^2^ against ALL reflections.  The weighted R-factor
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based
 on F, with F set to zero for negative F^2^. The threshold expression
of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc.
and is
 not relevant to the choice of reflections for refinement.  R-factors
based
 on F^2^ are statistically about twice as large as those based on F,
and R-
 factors based on ALL data will be even larger.
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P=(Fo^2^+2Fc^2^)/3'
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S S 0.53225(19) 0.45051(10) 0.30589(7) 0.0622(3) Uani 1 1 d . . .
O1 O 0.6825(7) 0.3659(4) 0.2999(3) 0.0865(12) Uani 1 1 d . . .
O2 O 0.5099(10) 0.5173(5) 0.3830(3) 0.1043(17) Uani 1 1 d . . .
N N 0.5533(5) 0.5566(3) 0.2262(2) 0.0523(8) Uani 1 1 d . . .
C1 C 0.3829(7) 0.5989(4) 0.0899(3) 0.0557(10) Uani 1 1 d . . .
H1 H 0.3270 0.6792 0.1064 0.067 Uiso 1 1 calc R . .
C2 C 0.4345(5) 0.5295(3) 0.1694(2) 0.0462(8) Uani 1 1 d . . .
C3 C 0.3080(6) 0.4175(4) 0.1775(3) 0.0559(10) Uani 1 1 d . . .
C4 C 0.3776(9) 0.3256(4) 0.1077(4) 0.0745(15) Uani 1 1 d . . .
H4A H 0.5101 0.3151 0.1108 0.089 Uiso 1 1 calc R . .
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H5B H 0.2332 0.3397 -0.0077 0.103 Uiso 1 1 calc R . .
C6 C 0.2327(8) 0.5144(4) 0.0527(3) 0.0667(13) Uani 1 1 d . . .
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C7 C 0.3199(8) 0.3770(5) 0.2696(4) 0.0685(12) Uani 1 1 d . . .
H7A H 0.3266 0.2862 0.2744 0.082 Uiso 1 1 calc R . .
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C8 C 0.1301(6) 0.4733(4) 0.1372(4) 0.0654(12) Uani 1 1 d . . .
C9 C 0.0480(7) 0.5805(5) 0.1894(5) 0.0823(17) Uani 1 1 d . . .
H9A H -0.0494 0.6195 0.1575 0.123 Uiso 1 1 calc R . .
H9B H 0.1419 0.6415 0.2015 0.123 Uiso 1 1 calc R . .
H9C H -0.0001 0.5480 0.2422 0.123 Uiso 1 1 calc R . .
C10 C -0.0240(10) 0.3749(6) 0.1239(6) 0.105(3) Uani 1 1 d . . .
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O1 0.086(2) 0.072(2) 0.101(3) 0.030(2) -0.017(2) 0.006(2)
O2 0.169(5) 0.092(3) 0.0521(19) -0.0027(19) 0.011(3) -0.031(3)
N 0.0623(19) 0.0404(14) 0.0540(18) 0.0081(13) 0.0009(15) -0.0051(15)
C1 0.066(2) 0.0450(18) 0.057(2) 0.0058(17) -0.0018(19) 0.0077(17)
C2 0.0517(18) 0.0362(14) 0.0507(19) 0.0020(14) 0.0037(16) 0.0042(15)
C3 0.060(2) 0.0390(18) 0.069(3) -0.0031(17) -0.001(2) -0.0045(17)
C4 0.088(3) 0.043(2) 0.093(4) -0.015(2) -0.006(3) 0.014(2)
C5 0.126(5) 0.055(3) 0.077(3) -0.027(3) -0.009(3) 0.014(3)
C6 0.085(3) 0.050(2) 0.065(3) -0.014(2) -0.022(2) 0.015(2)
C7 0.078(3) 0.049(2) 0.078(3) 0.014(2) 0.012(3) -0.011(2)
C8 0.055(2) 0.0415(18) 0.100(4) -0.014(2) -0.009(2) -0.0058(17)
C9 0.055(2) 0.063(3) 0.129(5) -0.024(3) 0.004(3) 0.006(2)
C10 0.076(3) 0.079(4) 0.159(7) -0.022(4) -0.029(4) -0.020(3)

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;
 All esds (except the esd in the dihedral angle between two l.s.
planes)
 are estimated using the full covariance matrix.  The cell esds are
taken
 into account individually in the estimation of esds in distances,
angles
 and torsion angles; correlations between esds in cell parameters are
only
 used when they are defined by crystal symmetry.  An approximate
(isotropic)
 treatment of cell esds is used for estimating esds involving l.s.
planes.
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S N 1.687(3) . ?
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N C2 1.271(6) . ?
C1 C2 1.494(6) . ?
C1 C6 1.529(7) . ?
C1 H1 0.9800 . ?
C2 C3 1.510(5) . ?
C3 C7 1.505(7) . ?
C3 C4 1.550(7) . ?
C3 C8 1.556(7) . ?
C4 C5 1.539(9) . ?
C4 H4A 0.9700 . ?
C4 H4B 0.9700 . ?
C5 C6 1.532(7) . ?
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C6 C8 1.578(9) . ?
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C7 H7A 0.9700 . ?
C7 H7B 0.9700 . ?
C8 C9 1.524(7) . ?
C8 C10 1.547(7) . ?
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C9 H9B 0.9600 . ?
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O1 S C7 111.1(2) . . ?
N S C7 97.7(2) . . ?
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C2 C1 Br 113.2(3) . . ?
C6 C1 Br 116.1(3) . . ?
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C6 C1 H1 108.4 . . ?
Br C1 H1 108.4 . . ?
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N C2 C3 122.2(4) . . ?
C1 C2 C3 107.9(4) . . ?
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C2 C3 C4 103.9(4) . . ?
C7 C3 C8 123.0(5) . . ?
C2 C3 C8 99.8(3) . . ?
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C3 C4 H4A 111.1 . . ?
C5 C4 H4B 111.1 . . ?
C3 C4 H4B 111.1 . . ?
H4A C4 H4B 109.1 . . ?
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C6 C5 H5B 110.9 . . ?
C4 C5 H5B 110.9 . . ?
H5A C5 H5B 108.9 . . ?
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C1 C6 C8 100.5(4) . . ?
C5 C6 C8 101.8(4) . . ?
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C9 C8 C6 115.2(4) . . ?
C10 C8 C6 114.7(6) . . ?
C3 C8 C6 93.0(4) . . ?
C8 C9 H9A 109.5 . . ?
C8 C9 H9B 109.5 . . ?
H9A C9 H9B 109.5 . . ?
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H9B C9 H9C 109.5 . . ?
C8 C10 H10A 109.5 . . ?
C8 C10 H10B 109.5 . . ?
H10A C10 H10B 109.5 . . ?
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H10B C10 H10C 109.5 . . ?

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O1 S N C2 105.3(3) . . . . ?
C7 S N C2 -9.8(3) . . . . ?
S N C2 C1 173.9(3) . . . . ?
S N C2 C3 -1.6(5) . . . . ?
C6 C1 C2 N -179.8(4) . . . . ?
Br C1 C2 N 54.8(5) . . . . ?
C6 C1 C2 C3 -3.7(4) . . . . ?
Br C1 C2 C3 -129.1(3) . . . . ?
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O2 S C7 C3 130.3(4) . . . . ?
O1 S C7 C3 -95.2(4) . . . . ?
N S C7 C3 17.4(3) . . . . ?
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C7 C3 C8 C10 -71.8(7) . . . . ?
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C4 C3 C8 C10 65.2(7) . . . . ?
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 Refinement of F^2^ against ALL reflections.  The weighted R-factor
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of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc.
and is
 not relevant to the choice of reflections for refinement.  R-factors
based
 on F^2^ are statistically about twice as large as those based on F,
and R-
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C13 0.060(12) 0.054(4) 0.074(4) -0.016(4) 0.000(7) -0.005(5)
N12 0.041(7) 0.033(3) 0.058(3) 0.005(2) -0.009(3) -0.006(3)
N13 0.036(6) 0.036(3) 0.044(3) 0.000(2) -0.010(4) 0.001(3)
N14 0.075(8) 0.034(3) 0.071(3) 0.010(3) -0.011(4) 0.000(3)
O11 0.055(6) 0.040(3) 0.076(2) 0.014(2) -0.027(3) -0.008(3)
O12 0.041(5) 0.046(2) 0.065(2) -0.012(2) -0.001(3) 0.004(2)
S11 0.034(2) 0.0354(9) 0.0597(9) 0.0005(7) -0.0105(11) -0.0003(9)

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planes)
 are estimated using the full covariance matrix.  The cell esds are
taken
 into account individually in the estimation of esds in distances,
angles
 and torsion angles; correlations between esds in cell parameters are
only
 used when they are defined by crystal symmetry.  An approximate
(isotropic)
 treatment of cell esds is used for estimating esds involving l.s.
planes.
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ALL PARTICIPANTS – SUBMITTED STRUCTURES

LISTS
of crystal structures of the test molecules IV, V, VI
submitted by the participants of CSP2001

CONTENTS

I. Ab initio submission

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TITL Ammon IV 1
CELL   10.158564    7.926620    9.899114   90.000000   76.987421   90.000000
SPACEGROUP P21/c
ATOM  C1      0.624759      0.837068      0.785428
ATOM  C2      0.805525      1.055741      0.753368
ATOM  C3      0.861977      0.763570      0.643003
ATOM  C4      0.916249      0.920354      0.704331
ATOM  C5      0.730929      0.696159      0.737203
ATOM  C6      0.685749      0.978626      0.858136
ATOM  C7      0.575891      0.907231      0.661988
ATOM  C8      0.758361      1.127984      0.629622
ATOM  H1      0.535302      0.781695      0.854439
ATOM  H2      0.843915      0.794220      0.540523
ATOM  H3      0.955518      0.883736      0.794780
ATOM  H4      0.753510      0.639372      0.830597
ATOM  H5      0.720375      0.927266      0.947146
ATOM  H6      0.849790      1.162149      0.798676
ATOM  H7      0.939155      0.664066      0.625399
ATOM  H8      1.000765      0.976139      0.628525
ATOM  H9      0.686907      0.596457      0.684178
ATOM  Ha      0.609542      1.075256      0.898378
ATOM  Hb      0.615480      1.094088      0.514622
ATOM  O1      0.813128      1.245045      0.559388
ATOM  O2      0.483858      0.846704      0.617775
ATOM  N1      0.646363      1.048027      0.597803
ENERGY -24.09 kcal/mol with distributed multipole electrostatics.
COMMENT d = 1.310 g/cc.  Lowest E and highest density structure.
COMMENT Volume additivity calcns suggest d = 1.349 g/cc.
COMMENT This structure is essentially the same as that obtained
COMMENT with atom-centered monopoles.  N-H..O = 1.885 Angs is
COMMENT reasonable for the expected strong intermolecular contact.

TITL Ammon IV 2
CELL    7.623809   12.255159    8.340882   90.000000   90.000000   90.000000
SPACEGROUP P212121
ATOM  C1      0.915423      0.518840      0.157254
ATOM  C2      1.114238      0.621518      0.340433
ATOM  C3      1.063854      0.693754      0.054865
ATOM  C4      1.191295      0.686902      0.197587
ATOM  C5      0.987452      0.581640      0.009791
ATOM  C6      1.059378      0.506900      0.285022
ATOM  C7      0.757056      0.578169      0.226762
ATOM  C8      0.957761      0.681817      0.411678
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ATOM  H1      0.866658      0.438946      0.117763
ATOM  H2      0.956642      0.750264      0.083692
ATOM  H3      1.312396      0.645621      0.160193
ATOM  H4      1.090228      0.530896     -0.044478
ATOM  H5      1.172800      0.463839      0.234267
ATOM  H6      1.212575      0.617561      0.436444
ATOM  H7      1.131489      0.729019     -0.049149
ATOM  H8      1.228460      0.768988      0.237932
ATOM  H9      0.883260      0.590721     -0.080100
ATOM  Ha      1.012220      0.458175      0.386744
ATOM  Hb      0.689590      0.693253      0.394845
ATOM  O1      0.969480      0.752340      0.513745
ATOM  O2      0.607310      0.565322      0.180084
ATOM  N1      0.794017      0.652546      0.349424
ENERGY -23.17 kcal/mol with distributed multipole electrostatics.
COMMENT d = 1.287 g/cc. N-H..O = 1.96 Angs is very reasonable
COMMENT for the expected strong intermolecular contact.
COMMENT This structure is essentially the same as that obtained
COMMENT with atom-centered monopoles (E = -23.62 kcal/mol, d =
COMMENT 1.308 g/cc.

TITL Ammon IV 3
CELL    7.306599    5.834670   10.233157   76.803283   95.125085  111.483947
SPACEGROUP P-1
ATOM  C1      0.071529      0.105811      0.696283
ATOM  C2      0.326638      0.292311      0.858950
ATOM  C3      0.316465      0.557822      0.622427
ATOM  C4      0.445785      0.506001      0.744394
ATOM  C5      0.184238      0.314792      0.577631
ATOM  C6      0.217013      0.051141      0.805893
ATOM  C7     -0.075844      0.185456      0.753537
ATOM  C8      0.181691      0.373721      0.917735
ATOM  H1     -0.016248     -0.063610      0.658329
ATOM  H2      0.224916      0.655261      0.646719
ATOM  H3      0.559722      0.447945      0.713998
ATOM  H4      0.274655      0.239533      0.532226
ATOM  H5      0.322352     -0.006788      0.764050
ATOM  H6      0.427582      0.260864      0.941319
ATOM  H7      0.410101      0.687825      0.538687
ATOM  H8      0.521960      0.678136      0.782899
ATOM  H9      0.079034      0.354310      0.500473
ATOM  Ha      0.139540     -0.104627      0.887534
ATOM  Hb     -0.103149      0.364089      0.897971
ATOM  O1      0.222512      0.491816      1.006700
ATOM  O2     -0.242188      0.152091      0.710406
ATOM  N1     -0.006724      0.307873      0.860482
ENERGY -23.17 kcal/mol with distributed multipole electrostatics.
COMMENT d = 1.287 g/cc.
COMMENT Volume additivity calcns suggest d = 1.349 g/cc.
COMMENT N-H..O = 1.866 Angs is reasonable for the expected
COMMENT strong intermolecular contact.
COMMENT This structure is essentially the same as that obtained
COMMENT with atom-centered monopoles (E = -23.63 kcal/mol &
COMMENT d = 1.326 g/cc).


TITL Dzyabchenko IV 1
SPACEGROUP P21/c
CELL 8.980 7.840 13.047 90.00 126.11 90.00
ATOM O1   0.54827  0.21851 0.50752
ATOM O2   0.17854 -0.10842 0.16440
ATOM N1   0.36075  0.06322 0.33146
ATOM H1   0.39372 -0.03836 0.38740
ATOM C3   0.39405  0.37006 0.30859
ATOM C5   0.18753  0.18745 0.11693
ATOM C8   0.44325  0.21390 0.39296
ATOM C9   0.23904  0.03333 0.20344
ATOM C1   0.04095  0.36366 0.20739
ATOM C4   1.34846  1.31074 1.18247
ATOM C2   0.22155  0.45939 0.28583
ATOM C6   0.01538  0.27709 0.09449
ATOM H11  0.51103  0.45526 0.35612
ATOM H12  0.15779  0.14291 0.02830
ATOM H2   0.02981  0.27299 0.26488
ATOM H10 -0.07075  0.45259 0.17384
ATOM H5   0.31313  0.42038 0.12204
ATOM H6   0.46773  0.25439 0.19470
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ATOM H4   0.25174  0.49278 0.37661
ATOM H7  -0.09562  0.18563 0.05424
ATOM H3   0.20703  0.57924 0.23994
ATOM H8  -0.02894  0.37059 0.02094
ENERGY -29.52 kcal/mol
COMMENT Density 1.371 g/cm3
COMMENT Confidence level 5 (1-10), by energy

TITL Dzyabchenko IV 2
SPACEGROUP P21/c
CELL 9.232 8.550 12.156 90.00 127.69 90.00
ATOM O1  0.21776 0.02842 0.60089
ATOM O2 -0.18637 0.33081 0.23464
ATOM N1  0.02398 0.18399 0.41851
ATOM H1 -0.07888 0.12963 0.40928
ATOM C3  0.35508 0.21487 0.54038
ATOM C5  0.12934 0.38378 0.33580
ATOM C8  0.19673 0.13280 0.52514
ATOM C9 -0.02648 0.29982 0.32285
ATOM C1  0.28388 0.49357 0.58608
ATOM C4  1.28815 1.27088 1.39805
ATOM C2  0.41694 0.35882 0.63876
ATOM C6  0.19158 0.52744 0.43453
ATOM H11 0.46586 0.13213 0.58321
ATOM H12 0.07975 0.42104 0.23328
ATOM H2  0.18399 0.47221 0.60345
ATOM H10 0.35742 0.59662 0.64644
ATOM H5  0.39922 0.32937 0.40785
ATOM H6  0.25121 0.17312 0.32920
ATOM H4  0.45477 0.31890 0.73750
ATOM H7  0.07509 0.60300 0.39340
ATOM H3  0.54227 0.40023 0.65993
ATOM H8  0.28434 0.59323 0.42617
ENERGY -29.33 kcal/mol
COMMENT
Density 1.340 g/cm3
COMMENT Confidence level 3 (1-10), by energy

TITL Dzyabchenko IV 3
SPACEGROUP P-1
CELL 5.667 6.450 10.918 86.77 81.74 79.16
ATOM O1   0.61970 -0.12624 0.16138
ATOM O2   0.22141  0.14121 0.51947
ATOM N1   0.40975  0.01368 0.33683
ATOM H1   0.54389 -0.06331 0.38153
ATOM C3   0.23639  0.10234 0.14197
ATOM C5   0.01391  0.25173 0.34198
ATOM C8   0.44000 -0.01441 0.21136
ATOM C9   0.22002  0.13331 0.40914
ATOM C1   0.28049  0.48186 0.19762
ATOM C4   1.00105  1.12765 1.23004
ATOM C2   0.29044  0.32530 0.09825
ATOM C6   0.06834  0.47444 0.29793
ATOM H11  0.22814  0.01035 0.06355
ATOM H12 -0.15238  0.26587 0.40567
ATOM H2   0.44903  0.45704 0.23625
ATOM H10  0.26272  0.63889 0.15588
ATOM H5  -0.14405  0.21047 0.18180
ATOM H6  -0.04604 -0.02431 0.25801
ATOM H4   0.46478  0.30613 0.04109
ATOM H7   0.09058  0.55740 0.37751
ATOM H3   0.15936  0.38974 0.03703
ATOM H8  -0.09484  0.56043 0.26558
ENERGY -29.23 kcal/mol
COMMENT Density 1.312 g/cm3
COMMENT Confidence level 1 (1-10), by energy

TITL ERK IV/1
CELL   9.0960   8.1460  10.6500  90.0000  97.1230  90.0000
SPACEGROUP P21/n
ATOM C1     0.54858    0.21472    0.11625
ATOM C2     0.58420    0.36661    0.19322
ATOM C3     0.66831    0.31816    0.32532
ATOM C4     0.56832    0.18893    0.38270
ATOM C5     0.53669    0.05039    0.29145
ATOM H6     0.50609   -0.02354    0.11457
ATOM H7     0.65466    0.44394    0.14217
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ATOM C8     0.44209    0.46429    0.21622
ATOM H9     0.77609    0.26387    0.31387
ATOM H10    0.68963    0.42507    0.38737
ATOM C11    0.42298    0.27575    0.41162
ATOM H12    0.62704    0.13950    0.47024
ATOM N13    0.52773    0.06988    0.16747
ATOM O14    0.53422    0.20990   -0.00128
ATOM O15    0.51854   -0.09416    0.32313
ATOM C16    0.33893    0.36655    0.29558
ATOM H17    0.27625    0.27665    0.23424
ATOM H18    0.25917    0.45082    0.32916
ATOM H19    0.37988    0.49805    0.12541
ATOM H20    0.47503    0.57895    0.26538
ATOM H21    0.45097    0.36380    0.48805
ATOM H22    0.34828    0.18599    0.44631
END

TITL ERK IV/2
CELL   10.0650   8.0210  10.1460  90.0000 104.7850  90.0000
SPACEGROUP P21/a
ATOM C1      0.12750   -0.11587    0.25252
ATOM C2      0.24488   -0.05982    0.19763
ATOM C3      0.35856    0.01996    0.31519
ATOM C4      0.28603    0.16000    0.37817
ATOM C5      0.16617    0.08698    0.41988
ATOM H6      0.01845   -0.08002    0.38755
ATOM H7      0.28656   -0.16962    0.15892
ATOM C8      0.20120    0.07398    0.08220
ATOM H9      0.40259   -0.07357    0.39230
ATOM H10     0.44324    0.06881    0.27734
ATOM C11     0.24207    0.30166    0.26971
ATOM H12     0.35786    0.20886    0.46901
ATOM N13     0.09425   -0.04042    0.35596
ATOM O14     0.05061   -0.23442    0.20522
ATOM O15     0.12273    0.13772    0.51691
ATOM C16     0.14699    0.23769    0.13286
ATOM H17     0.04414    0.21523    0.14609
ATOM H18     0.13680    0.33449    0.05543
ATOM H19     0.12247    0.02252   -0.00273
ATOM H20     0.28965    0.10456    0.04250
ATOM H21     0.33401    0.35706    0.24913
ATOM H22     0.19003    0.40118    0.31051
END

TITL ERK IV/3
CELL   12.0309  11.5265  11.7185  90.0000  90.0000  90.0000
SPACEGROUP Pbca
ATOM C1      0.12619    0.47362    0.23764
ATOM C2      0.19958    0.38396    0.29109
ATOM C3      0.16391    0.26129    0.24722
ATOM C4      0.16948    0.26694    0.11396
ATOM C5      0.10038    0.36619    0.07294
ATOM H6      0.03832    0.52112    0.10321
ATOM H7      0.18859    0.38894    0.38335
ATOM C8      0.32527    0.40145    0.26110
ATOM H9      0.07905    0.24095    0.27482
ATOM H10     0.21801    0.19328    0.28123
ATOM C11     0.29389    0.28057    0.07738
ATOM H12     0.13482    0.18729    0.07836
ATOM N13     0.08363    0.46112    0.13411
ATOM O14     0.09765    0.56494    0.28588
ATOM O15     0.05387    0.36891   -0.02167
ATOM C16     0.35048    0.38892    0.13126
ATOM H17     0.32169    0.46668    0.08683
ATOM H18     0.44016    0.38344    0.11792
ATOM H19     0.35285    0.48676    0.29028
ATOM H20     0.37437    0.33684    0.30734
ATOM H21     0.34009    0.20325    0.10315
ATOM H22     0.30010    0.28665   -0.01545
END

TITL Hofmann IV 1
SPACEGROUP P-1
CELL   6.946   6.801   8.124     87.407  89.492  85.143
ATOM C1  -0.49306   -0.19726    0.25086
ATOM C2  -0.36358   -0.38129    0.19983
ATOM C3  -0.27807   -0.34967    0.02901
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ATOM N4  -0.10370   -0.27364    0.00807
ATOM C5   0.00091   -0.22250    0.13829
ATOM C6  -0.07298   -0.24898    0.31370
ATOM C7  -0.19383   -0.06107    0.36810
ATOM C8  -0.19979   -0.42389    0.32595
ATOM O9  -0.36602   -0.39274   -0.09105
ATOM O10  0.15535   -0.15456    0.11326
ATOM H11 -0.56332   -0.22988    0.37138
ATOM H12 -0.61008   -0.16239    0.15868
ATOM H13 -0.45132   -0.51061    0.19760
ATOM H14 -0.04946   -0.25316   -0.11067
ATOM H15  0.05410   -0.28049    0.39604
ATOM H16 -0.23479   -0.08034    0.50009
ATOM H17 -0.10481    0.06760    0.35670
ATOM H18 -0.25903   -0.44351    0.45287
ATOM H19 -0.11195   -0.56316    0.29735
ATOM C20 -0.37834   -0.01477    0.26497
ATOM H21 -0.33924    0.04202    0.13973
ATOM H22 -0.47155    0.10437    0.32258
ENERGY -74.48
COMMENT d=1.332g/cc. Lowest energy structure.

TITL Hofmann IV 2
SPACEGROUP P-1
CELL    6.819   5.937  10.416   90.463  92.421  62.810
ATOM C1  -0.19653   -0.23802    0.37529
ATOM C2  -0.02889   -0.18945    0.29936
ATOM C3  -0.00595   -0.29785    0.16515
ATOM N4  -0.13590   -0.15505    0.06426
ATOM C5  -0.29143    0.08935    0.07904
ATOM C6  -0.32612    0.21392    0.20969
ATOM C7  -0.50253    0.17730    0.28296
ATOM C8  -0.10763    0.09775    0.29035
ATOM O9   0.13022   -0.51506    0.14711
ATOM O10 -0.40388    0.20870   -0.01381
ATOM H11 -0.19858   -0.17145    0.47554
ATOM H12 -0.14377   -0.44518    0.38030
ATOM H13  0.13618   -0.28232    0.35010
ATOM H14 -0.11655   -0.23529   -0.02641
ATOM H15 -0.38098    0.41966    0.19436
ATOM H16 -0.53457    0.28455    0.37416
ATOM H17 -0.66053    0.25620    0.22441
ATOM H18 -0.13019    0.18253    0.38771
ATOM H19  0.01783    0.13629    0.24310
ATOM C20 -0.43172   -0.10316    0.31389
ATOM H21 -0.44084   -0.20180    0.22439
ATOM H22 -0.54925   -0.11599    0.38061
ENERGY  -71.19
COMMENT d=1.358g/cc.

TITL Hofmann IV 3
SPACEGROUP P-1
CELL     6.892   6.423  10.368  77.203  82.764  61.310
ATOM C1   -0.45097    0.40178   -0.28905
ATOM C2   -0.23977    0.27744   -0.20578
ATOM C3   -0.27153    0.13815   -0.07321
ATOM N4   -0.21949   -0.09899   -0.05840
ATOM C5   -0.13770   -0.22093   -0.16104
ATOM C6   -0.10023   -0.09656   -0.29727
ATOM C7   -0.30726    0.01669   -0.38323
ATOM C8   -0.04662    0.10387   -0.28345
ATOM O9   -0.34429    0.23908    0.02128
ATOM O10  -0.09456   -0.43210   -0.14302
ATOM H11  -0.42736    0.51480   -0.38138
ATOM H12  -0.59321    0.52442   -0.23278
ATOM H13  -0.20035    0.41646   -0.18639
ATOM H14  -0.24394   -0.18901    0.03365
ATOM H15   0.04248   -0.23394   -0.34581
ATOM H16  -0.26959    0.09199   -0.48479
ATOM H17  -0.35053   -0.12585   -0.39185
ATOM H18  -0.35053   -0.12585   -0.39185
ATOM H19   0.11015    0.02386   -0.22894
ATOM C20  -0.50858    0.21851   -0.32556
ATOM H21  -0.57398    0.13762   -0.23635
ATOM H22  -0.64228    0.31435   -0.39917
ENERGY   -70.11
COMMENT d=1.296g/cc.
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TITL Leusen IV 1
SPACEGROUP  P21/a  (P 1 21/a 1)
CELL    9.958  7.596 10.474 90.000 105.163 90.000
ATOM  C1     0.74440   0.06093   0.68707
ATOM  C2     0.69721  -0.08075   0.57623
ATOM  C3     0.63841  -0.25061   0.62359
ATOM  C4     0.73156  -0.32077   0.75634
ATOM  C5     0.77825  -0.17512   0.86393
ATOM  C6     0.85698  -0.02912   0.80392
ATOM  C7     0.62214   0.13395   0.74094
ATOM  N8     0.58827   0.05018   0.84073
ATOM  C9     0.65375  -0.08898   0.90777
ATOM O10     0.61649  -0.14602   1.00273
ATOM O11     0.55819   0.26653   0.69341
ATOM H12     0.79216   0.17326   0.64827
ATOM H13     0.61979  -0.02488   0.49017
ATOM H14     0.78782  -0.11537   0.53823
ATOM H15     0.53229  -0.22427   0.63354
ATOM H16     0.62396  -0.35389   0.54676
ATOM H17     0.67832  -0.42942   0.79370
ATOM H18     0.82551  -0.38208   0.73773
ATOM H19     0.85111  -0.23169   0.95209
ATOM H20     0.94214  -0.08655   0.76788
ATOM H21     0.90568   0.06875   0.88013
ATOM H22     0.50935   0.10338   0.87419
ENERGY  -19.65 kcal/mol asymmetric unit
DENSITY 1.331 g/(cm^3)
COMMENT Lowest energy structure according to CVFF950 force field.
COMMENT 0 dimensional dimer hydrogen bonding motif.
COMMENT Sampling difficult in this space group and small energy gap,
COMMENT indicating that this polymorph would be difficult to crystallize.

TITL Leusen IV 2
SPACEGROUP  P212121
CELL   11.538  5.955 11.346 90.000 90.000 90.000
ATOM  C1     0.25358   0.39036   0.61940
ATOM  C2     0.13573   0.30127   0.66774
ATOM  C3     0.10786   0.05601   0.63244
ATOM  C4     0.13525   0.00065   0.50230
ATOM  C5     0.25333   0.09475   0.45823
ATOM  C6     0.25207   0.35667   0.48079
ATOM  C7     0.36133   0.26556   0.67366
ATOM  N8     0.40089   0.07912   0.62150
ATOM  C9     0.36122  -0.01237   0.52162
ATOM O10     0.41005  -0.17725   0.48036
ATOM O11     0.40994   0.33771   0.76212
ATOM H12     0.26175   0.57110   0.64014
ATOM H13     0.13313   0.31666   0.76486
ATOM H14     0.06586   0.41297   0.63529
ATOM H15     0.15679  -0.06115   0.68922
ATOM H16     0.01571   0.01940   0.65073
ATOM H17     0.13088  -0.18319   0.48896
ATOM H18     0.06571   0.06839   0.44538
ATOM H19     0.26089   0.06124   0.36295
ATOM H20     0.17495   0.43632   0.44070
ATOM H21     0.32876   0.43641   0.43999
ATOM H22     0.47125   0.00241   0.65933
ENERGY  -19.60 kcal/mol asymmetric unit
DENSITY 1.305 g/(cm^3)
COMMENT Second lowest energy structure according to CVFF950 force field.
COMMENT 1 dimensional spiral hydrogen bonding motif.
COMMENT Good sampling in this space group, but hampered by small energy gap.
COMMENT This polymorph might be easier to crystallize than the other two.

TITL Leusen IV 3
SPACEGROUP  P21/a  (P 1 21/a 1)
CELL    8.024 10.509  9.182 90.000 83.015 90.000
ATOM  C1     0.16420   0.44371   0.80552
ATOM  C2     0.11871   0.47805   0.65000
ATOM  C3     0.25731   0.55442   0.55565
ATOM  C4     0.33032   0.66484   0.63976
ATOM  C5     0.36700   0.62927   0.79784
ATOM  C6     0.20000   0.57342   0.88293
ATOM  C7     0.32093   0.35331   0.80167
ATOM  N8     0.47455   0.40424   0.79868
ATOM  C9     0.51162   0.52859   0.80013
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ATOM O10     0.65745   0.56220   0.80346
ATOM O11     0.30281   0.23742   0.79994
ATOM H12     0.05616   0.39564   0.86838
ATOM H13     0.08904   0.39093   0.59053
ATOM H14     0.00053   0.53388   0.66350
ATOM H15     0.35896   0.48809   0.51394
ATOM H16     0.20879   0.59182   0.45628
ATOM H17     0.44484   0.70260   0.57465
ATOM H18     0.24015   0.74500   0.64800
ATOM H19     0.40225   0.71602   0.85458
ATOM H20     0.09447   0.64057   0.88145
ATOM H21     0.21493   0.55735   0.99962
ATOM H22     0.57420   0.34332   0.79798
ENERGY  -19.54 kcal/mol asymmetric unit
DENSITY 1.324 g/(cm^3)
COMMENT Third lowest energy structure according to CVFF950 force field.
COMMENT 1 dimensional zig-zag hydrogen bonding motif.
COMMENT Sampling difficult in this space group and small energy gap,
COMMENT indicating that this polymorph would be difficult to crystallize.


TITL LOMMERSE IV-1
SPACEGROUP P212121
CELL    8.091    9.500    9.998   90.000   90.000   90.000
ATOM    C1    0.38543    0.34916    0.26124
ATOM    C2    0.27432    0.46093    0.19622
ATOM    C3    0.17848    0.40286    0.07568
ATOM    C4    0.09190    0.26147    0.10664
ATOM    C5    0.21793    0.15348    0.15708
ATOM    C6    0.29333    0.20920    0.28725
ATOM    C7    0.15898    0.22993    0.38996
ATOM    C8   -0.04148    0.28195    0.21022
ATOM    N1    0.00368    0.26284    0.34211
ATOM    O1    0.18258    0.22063    0.50996
ATOM    O2   -0.18271    0.31542    0.18244
ATOM    H1    0.43643    0.38843    0.35395
ATOM    H2    0.48872    0.32604    0.19579
ATOM    H3    0.34903    0.54938    0.16477
ATOM    H4    0.18847    0.50207    0.26967
ATOM    H5    0.08823    0.47879    0.04174
ATOM    H6    0.26287    0.38465   -0.00672
ATOM    H7    0.03036    0.22467    0.01763
ATOM    H8    0.15955    0.05239    0.17330
ATOM    H9    0.31369    0.13807    0.08312
ATOM   H10    0.37853    0.13432    0.32981
ATOM   H11   -0.08470    0.27617    0.41014
COMM Ranked[43] [010214206237] P212121  -42.369    0.000
COMM Chain structure, to be expected
COMM Bad H..H contact (2.2 A).
END

TITL LOMMERSE IV-2
SPACEGROUP Pbca
CELL   11.579   11.785   11.145   90.000   90.000   90.000
ATOM    C1    0.43728    0.30935    0.29629
ATOM    C2    0.38080    0.35706    0.41030
ATOM    C3    0.25044    0.33348    0.41482
ATOM    C4    0.22090    0.20824    0.38717
ATOM    C5    0.27108    0.17373    0.26535
ATOM    C6    0.40275    0.18475    0.27181
ATOM    C7    0.44903    0.10819    0.36901
ATOM    C8    0.26806    0.13157    0.48382
ATOM    N1    0.37712    0.08761    0.46536
ATOM    O1    0.54520    0.06637    0.36617
ATOM    O2    0.21542    0.10896    0.57539
ATOM    H1    0.53023    0.31596    0.30213
ATOM    H2    0.41052    0.35899    0.21928
ATOM    H3    0.39564    0.44758    0.41494
ATOM    H4    0.42220    0.32127    0.48887
ATOM    H5    0.21587    0.35656    0.50155
ATOM    H6    0.20662    0.38532    0.34863
ATOM    H7    0.12842    0.19775    0.38889
ATOM    H8    0.24640    0.08772    0.24293
ATOM    H9    0.23739    0.22822    0.19562
ATOM   H10    0.44275    0.15716    0.18948
ATOM   H11    0.40785    0.03689    0.52919
COMM Ranked[19] [010227045947] Pbca  -44.949    0.000
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COMM Dimer, which is not to be expected
COMM Nice layered structure
END

TITL LOMMERSE IV-3
SPACEGROUP P21/c
CELL    6.567   10.529   12.407   90.000   77.425   90.000
ATOM    C1   -0.00189    0.25958    0.28686
ATOM    C2    0.06064    0.37850    0.34361
ATOM    C3    0.29832    0.39256    0.32627
ATOM    C4    0.41152    0.37636    0.20404
ATOM    C5    0.35474    0.24836    0.15978
ATOM    C6    0.11932    0.24693    0.16568
ATOM    C7    0.06268    0.35373    0.09666
ATOM    C8    0.35347    0.48253    0.13483
ATOM    N1    0.18607    0.46106    0.08654
ATOM    O1   -0.08512    0.34923    0.05208
ATOM    O2    0.44477    0.58395    0.12165
ATOM    H1   -0.16769    0.26003    0.28998
ATOM    H2    0.03086    0.17542    0.33046
ATOM    H3   -0.00798    0.37440    0.43110
ATOM    H4   -0.00425    0.46225    0.31295
ATOM    H5    0.33742    0.48376    0.35630
ATOM    H6    0.35849    0.32055    0.37347
ATOM    H7    0.57740    0.38420    0.19768
ATOM    H8    0.44056    0.23386    0.07576
ATOM    H9    0.39644    0.17182    0.20889
ATOM   H10    0.07233    0.16048    0.13138
ATOM   H11    0.14848    0.53121    0.04077
COMM Ranked[3] [010129113879] P21/c  -48.252    0.000
COMM Dimer, which is not to be expected
END

TITL Mooy-IV-1
SPACEGROUP  P21/c
CELL   10.247  7.706  9.962 90.000 76.334 90.000
ATOM  C1     0.36742   0.74740   0.63996
ATOM  C2     0.23423   0.81851   0.73157
ATOM  C3     0.12706   0.67423   0.77710
ATOM  C4     0.18530   0.52952   0.85276
ATOM  C5     0.30415   0.44541   0.74817
ATOM  C6     0.41718   0.58248   0.70221
ATOM  C7     0.08541   0.59574   0.65822
ATOM  N8     0.15148   0.45751   0.59104
ATOM  C9     0.25509   0.37951   0.62948
ATOM O10    -0.01223   0.65525   0.61784
ATOM O11     0.30933   0.25186   0.56087
ATOM H12     0.35254   0.71599   0.53773
ATOM H13     0.44408   0.84802   0.62649
ATOM H14     0.25528   0.87819   0.82359
ATOM H15     0.19464   0.91970   0.67564
ATOM H16     0.03931   0.72846   0.84801
ATOM H17     0.22002   0.58335   0.93915
ATOM H18     0.10837   0.43321   0.89424
ATOM H19     0.34166   0.33692   0.79817
ATOM H20     0.45531   0.61980   0.79161
ATOM H21     0.50029   0.52524   0.62611
ATOM H22     0.12188   0.41111   0.51230
ENERGY  -9.57 kcal/mol
COMMENT Density 1.331 g/cc
COMMENT Lowest-energy structure in Dreiding+Multipole force field
COMMENT Good confidence in the energy function used
COMMENT Confidence (1-3) : 2

TITL Mooy-IV-2
SPACEGROUP  P21/c
CELL    9.229 10.406  7.963 90.000 83.870 90.000
ATOM  C1    -0.06033   0.45132   0.73833
ATOM  C2    -0.15164   0.52637   0.88062
ATOM  C3    -0.30683   0.55827   0.83536
ATOM  C4    -0.38478   0.43183   0.79787
ATOM  C5    -0.30326   0.37229   0.63719
ATOM  C6    -0.14458   0.33759   0.66868
ATOM  C7    -0.30257   0.64324   0.68588
ATOM  N8    -0.30331   0.59394   0.52859
ATOM  C9    -0.30630   0.46613   0.49822
ATOM O10    -0.29571   0.76249   0.70317
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ATOM O11    -0.31031   0.42869   0.34956
ATOM H12    -0.02776   0.51826   0.63600
ATOM H13     0.03870   0.41488   0.78484
ATOM H14    -0.16135   0.46885   0.99589
ATOM H15    -0.09520   0.61537   0.90567
ATOM H16    -0.36787   0.60560   0.94238
ATOM H17    -0.38339   0.36547   0.90350
ATOM H18    -0.49846   0.45043   0.77956
ATOM H19    -0.36027   0.28524   0.60621
ATOM H20    -0.14837   0.25896   0.75924
ATOM H21    -0.08487   0.30348   0.55143
ATOM H22    -0.30201   0.65224   0.43261
ENERGY  -9.53 kcal/mol
COMMENT Density 1.338 g/cc
COMMENT 2nd lowest-energy structure in Dreiding+Multipole force field

TITL Mooy-IV-3
SPACEGROUP  Pbca
CELL   11.974 11.366 11.560 90.000 90.000 90.000
ATOM  C1     0.84875   0.39797   0.87335
ATOM  C2     0.79364   0.28751   0.92742
ATOM  C3     0.67013   0.27152   0.88951
ATOM  C4     0.66220   0.26870   0.75612
ATOM  C5     0.70110   0.38962   0.71006
ATOM  C6     0.82585   0.40861   0.74165
ATOM  C7     0.59992   0.36913   0.93223
ATOM  N8     0.58384   0.46662   0.86736
ATOM  C9     0.62858   0.48125   0.76100
ATOM O10     0.55379   0.36239   1.02902
ATOM O11     0.60570   0.57318   0.70633
ATOM H12     0.81648   0.47618   0.91690
ATOM H13     0.93857   0.39464   0.88858
ATOM H14     0.84087   0.20994   0.90142
ATOM H15     0.79848   0.29445   1.02141
ATOM H16     0.63767   0.18883   0.92351
ATOM H17     0.71554   0.19939   0.72166
ATOM H18     0.57648   0.25017   0.72891
ATOM H19     0.69184   0.39133   0.61630
ATOM H20     0.87551   0.34260   0.69630
ATOM H21     0.85277   0.49512   0.71177
ATOM H22     0.53681   0.52887   0.89815
ENERGY  -9.34 kcal/mol
COMMENT Density 1.294 g/cc
COMMENT 3rd lowest-energy structure in Dreiding+Multipole force field


TITL Motherwell IV  1
SPACEGROUP P212121
CELL       8.037   6.527  14.097  90.000  90.000  90.000
ATOM O1          0.65252   0.11763   0.14765
ATOM O2          0.28386  -0.25834  -0.02090
ATOM N1          0.46766  -0.06525   0.06169
ATOM C1          0.17136   0.04357   0.05242
ATOM C2          0.24621   0.25529   0.06767
ATOM C3          0.37288   0.25083   0.14733
ATOM C4          0.28552   0.18579   0.24014
ATOM C5          0.18776  -0.01524   0.23581
ATOM C6          0.08341  -0.02731   0.14422
ATOM C11         0.51037   0.10050   0.12146
ATOM C12         0.30836  -0.10616   0.02758
ATOM H1N1        0.55976  -0.16150   0.04220
ATOM H1C1        0.08181   0.04978  -0.00492
ATOM H1C2        0.14795   0.36196   0.08566
ATOM H2C2        0.30667   0.30468   0.00293
ATOM H1C3        0.42713   0.40107   0.15761
ATOM H1C4        0.19972   0.30644   0.25985
ATOM H2C4        0.37990   0.17012   0.29449
ATOM H1C5        0.10556  -0.02413   0.29654
ATOM H2C5        0.27417  -0.14250   0.23745
ATOM H1C6       -0.02593   0.06736   0.15395
ATOM H2C6        0.04587  -0.18526   0.13449
ENERGY -47.2 Kcal/mole
COMMENT Lowest energy globally.  Low volume. Good scoring functions.
COMMENT Found several times in P212121 runs.
COMMENT Good planar H-bonding motif, via screw axis.
COMMENT ID=182359
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TITL Motherwell IV 2
SPACEGROUP P21
CELL       6.288   7.926   7.668  90.000 100.706  90.000
ATOM O1          0.17961   0.38245   0.27341
ATOM O2          0.48884  -0.00356  -0.03512
ATOM N1          0.32812   0.18872   0.11623
ATOM C1          0.21942  -0.11302   0.11927
ATOM C2          0.00755  -0.03743   0.15159
ATOM C3          0.05003   0.09823   0.29316
ATOM C4          0.16747   0.01882   0.46876
ATOM C5          0.37462  -0.07904   0.45848
ATOM C6          0.34234  -0.19307   0.29280
ATOM C11         0.18750   0.23621   0.23168
ATOM C12         0.35682   0.02456   0.05976
ATOM H1N1        0.41450   0.28092   0.07118
ATOM H1C1        0.18571  -0.20904   0.01739
ATOM H1C2       -0.09017  -0.13609   0.19458
ATOM H2C2       -0.07849   0.01744   0.02929
ATOM H1C3       -0.10063   0.15296   0.31503
ATOM H1C4        0.05592  -0.06716   0.51479
ATOM H2C4        0.20922   0.11953   0.56445
ATOM H1C5        0.41753  -0.15661   0.57603
ATOM H2C5        0.50402   0.00958   0.45201
ATOM H1C6        0.25299  -0.30362   0.32050
ATOM H2C6        0.50077  -0.23078   0.27075
ENERGY  -46.5  kcal/mole
COMMENT   Good energy, volume, scoring functions
COMMENT   Good planar screw axis chain motif for H-bonds.
COMMENT ID=155622

TITL  Motherwell IV 3
SPACEGROUP Pbca
CELL      11.748  11.638  11.152  90.000  90.000  90.000
ATOM O1          0.07154   0.13135  -0.04701
ATOM O2          0.11985  -0.07831   0.29055
ATOM N1          0.09415   0.02921   0.12352
ATOM C1          0.21676   0.10342   0.28819
ATOM C2          0.18184   0.21936   0.23674
ATOM C3          0.19265   0.21930   0.10128
ATOM C4          0.31814   0.19744   0.06689
ATOM C5          0.37251   0.08978   0.12104
ATOM C6          0.34201   0.07824   0.25494
ATOM C11         0.11583   0.12595   0.05037
ATOM C12         0.14102   0.01055   0.23664
ATOM H1N1        0.04053  -0.03108   0.09131
ATOM H1C1        0.20803   0.10506   0.38485
ATOM H1C2        0.23636   0.28559   0.27355
ATOM H2C2        0.09428   0.23687   0.26099
ATOM H1C3        0.16688   0.30146   0.06464
ATOM H1C4        0.36747   0.27104   0.09573
ATOM H2C4        0.32262   0.18997  -0.02980
ATOM H1C5        0.46412   0.09546   0.11190
ATOM H2C5        0.34189   0.01479   0.07343
ATOM H1C6        0.39524   0.13742   0.30466
ATOM H2C6        0.36099  -0.00898   0.28226
ENERGY -46.5 kcal/mole
COMMENT Lowest energy in Pbca. Witnin top 5 globally. Low volume.
COMMENT Good score functions.
COMMENT Dimer H-bond motif.  Chosen as best energy structure showing dimer.
COMMENT ID=182944

TITL Price IV 1
SPACEGROUP P21/c
CELL   11.1287  6.1423  15.5307  90.0000  134.3100  90.0000
ATOM  N1      0.610273      0.728550      0.577910
ATOM  C1      0.669765      1.037122      0.730627
ATOM  C2      0.912024      0.669736      0.861676
ATOM  C3      0.959058      0.889316      0.845492
ATOM  C4      0.764790      0.691417      0.850658
ATOM  C5      0.805521      1.006572      0.730180
ATOM  C6      0.615253      0.812755      0.735228
ATOM  C7      0.737611      0.876145      0.621167
ATOM  C8      0.544742      0.679699      0.626276
ATOM  O1      0.789897      0.891209      0.573392
ATOM  O2      0.440218      0.535018      0.582669
ATOM  H1      0.565995      0.637625      0.506187
ATOM  H2      1.020473      0.601298      0.949365
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ATOM  H3      0.879930      0.554230      0.794691
ATOM  H4      0.804785      0.783416      0.927393
ATOM  H5      1.012489      0.995004      0.921882
ATOM  H6      0.723500      0.531551      0.852184
ATOM  H7      1.054411      0.868635      0.843411
ATOM  H8      0.514204      0.824964      0.731853
ATOM  H9      0.845298      1.162224      0.723067
ATOM  H10     0.719156      1.132935      0.808953
ATOM  H11     0.562747      1.126040      0.650567
ENERGY -138.96 kJ/mol
COMMENT Global minimum found in search.
COMMENT High confidence in the dimer structure, as found in all low energy
COMMENT structures. Fairly low confidence in packing of dimers because
COMMENT there are 13 other local minima found within 5 kJ/mol. However,
COMMENT several of these higher energy structures have similar packing
COMMENT to the global minimum.

TITL Price IV 2
SPACEGROUP P21/c
CELL    6.1439  7.0935  18.1478  90.0000  87.3960  90.0000
ATOM  N1      0.776880      0.047310      0.954100
ATOM  C1      0.520430      0.332670      0.906140
ATOM  C2      0.887840      0.245440      0.799360
ATOM  C3      0.655180      0.178920      0.787530
ATOM  C4      0.890910      0.416760      0.850500
ATOM  C5      0.523850      0.150930      0.860980
ATOM  C6      0.754730      0.383870      0.922670
ATOM  C7      0.623080     -0.007830      0.903970
ATOM  C8      0.857100      0.228280      0.966490
ATOM  O1      0.579100     -0.174750      0.895760
ATOM  O2      1.003380      0.253340      1.009110
ATOM  H1      0.847130     -0.058350      0.982230
ATOM  H2      0.968840      0.280260      0.746330
ATOM  H3      0.981890      0.130690      0.822460
ATOM  H4      0.822380      0.538710      0.822840
ATOM  H5      0.570350      0.284420      0.755500
ATOM  H6      1.057630      0.452750      0.863420
ATOM  H7      0.656120      0.047620      0.756150
ATOM  H8      0.761120      0.509930      0.956950
ATOM  H9      0.359390      0.104590      0.849620
ATOM  H10     0.446930      0.446240      0.875070
ATOM  H11     0.421930      0.314780      0.957310
ENERGY 138.22 kJ/mol
COMMENT Second lowest energy structure. Relative E = +0.74 kJ/mol
COMMENT A similar motif to structure 1, but a distinct packing with
COMMENT no low energy transformation to the global minimum.

TITL Price IV 3
SPACEGROUP Pbca
CELL   11.5256  11.8586  11.4818  90.0000  90.0000  90.0000
ATOM  N1      0.051909      0.956228      0.128658
ATOM  C1      0.123920      0.770529      0.249488
ATOM  C2      0.319030      0.886996      0.130335
ATOM  C3      0.297382      0.899298      0.261154
ATOM  C4      0.265368      0.778526      0.082397
ATOM  C5      0.168342      0.884589      0.292265
ATOM  C6      0.136968      0.766308      0.117179
ATOM  C7      0.098521      0.979319      0.238406
ATOM  C8      0.066708      0.859417      0.060940
ATOM  O1      0.084093      1.071599      0.284104
ATOM  O2      0.026456      0.854236     -0.037659
ATOM  H1      0.006699      1.019887      0.090938
ATOM  H2      0.412180      0.887536      0.113123
ATOM  H3      0.283270      0.959796      0.084325
ATOM  H4      0.312129      0.705627      0.117107
ATOM  H5      0.346362      0.834748      0.308233
ATOM  H6      0.272877      0.775535     -0.012312
ATOM  H7      0.327443      0.981258      0.292182
ATOM  H8      0.102957      0.687668      0.081561
ATOM  H9      0.157533      0.893490      0.386215
ATOM  H10     0.174001      0.702530      0.289438
ATOM  H11     0.033290      0.758510      0.274509
ENERGY 136.827 kJ/mol
COMMENT Fifth lowest energy structure, but #3 and #4 are very similar
COMMENT to the global minimum in structure, so not included. This crystal
COMMENT also has much greater attachment energies for it's dominant faces,
COMMENT so may be favoured by growth rate.
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TITL Scheraga IV 1
SPACEGROUP P21/c
CELL  10.112  7.918  9.697  90.00  77.04  90.00
ATOM C1      -.26798   .13153   .37728
ATOM C2      -.31338   .06158   .24975
ATOM O3      -.32669   .24085   .45096
ATOM C4      -.19075  -.00433   .14067
ATOM C5      -.41828  -.08080   .29533
ATOM H6      -.36155   .16587   .20793
ATOM C7      -.12382  -.14408   .21012
ATOM H8      -.22293  -.05365   .04904
ATOM H9      -.11924   .09702   .10339
ATOM C10     -.07778  -.07418   .33729
ATOM C11     -.22349  -.29209   .25491
ATOM H12     -.03296  -.19097   .13913
ATOM N13     -.15279   .05920   .40641
ATOM O14      .01599  -.12927   .37874
ATOM H15     -.12352   .10411   .49124
ATOM H16     -.45614  -.11634   .20297
ATOM C17     -.35748  -.23617   .35270
ATOM H18     -.50410  -.03311   .37357
ATOM H19     -.17552  -.38942   .30545
ATOM H20     -.24375  -.34697   .15898
ATOM H21     -.42975  -.33952   .36620
ATOM H22     -.34129  -.20906   .45752
ENERGY 28.09 kcal/mol
COMMENT Lowest energy structure.
COMMENT The packing seems reasonable.
COMMENT Confidence level (1-10): 8, by energy

TITL Scheraga IV 2
SPACEGROUP Pbca
CELL 12.0030  11.1960  11.3790  90.0000  90.0000  90.0000
ATOM C1       .40998   .37197   .07671
ATOM C2       .34037   .27061   .12609
ATOM O3       .45048   .37051  -.01896
ATOM C4       .34998   .26807   .26013
ATOM C5       .21746   .28491   .08891
ATOM H6       .37356   .18985   .08720
ATOM C7       .30764   .38750   .30782
ATOM H8       .30068   .19525   .29558
ATOM H9       .43566   .25268   .28690
ATOM C10      .37748   .48892   .25897
ATOM C11      .18387   .40523   .27551
ATOM H12      .31663   .39245   .40237
ATOM N13      .42371   .46996   .14925
ATOM O14      .39219   .58098   .30934
ATOM H15      .46870   .53729   .11635
ATOM H16      .17323   .20533   .11755
ATOM C17      .16268   .39595   .14284
ATOM H18      .21176   .28773  -.00616
ATOM H19      .15516   .49071   .30856
ATOM H20      .13648   .33664   .32105
ATOM H21      .07364   .39374   .12640
ATOM H22      .19346   .47571   .09919
ENERGY 27.69 kcal/mol
COMMENT Relative E=+0.40 kcal/mol.
COMMENT Confidence level (1-10): 5, by energy

TITL Scheraga IV 3
SPACEGROUP P-1
CELL  9.9760   7.1730   5.7070 109.9000 104.1200  83.9200
ATOM C1       .47380  -.09028  -.15681
ATOM C2       .39428  -.27405  -.20719
ATOM O3       .58277  -.09527  -.21024
ATOM C4       .30477  -.23411  -.01152
ATOM C5       .30349  -.33671  -.48098
ATOM H6       .47179  -.38924  -.19035
ATOM C7       .20373  -.06250  -.03721
ATOM H8       .24833  -.36571  -.04644
ATOM H9       .36862  -.19852   .18103
ATOM C10      .28306   .12166   .01426
ATOM C11      .10779  -.11902  -.30644
ATOM H12      .14119  -.02262   .10412
ATOM N13      .41161   .08923  -.04562
ATOM O14      .23947   .28635   .09841
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ATOM H15      .46333   .21052  -.01457
ATOM H16      .25832  -.47758  -.51504
ATOM C17      .18802  -.18373  -.52008
ATOM H18      .36780  -.36281  -.61783
ATOM H19      .03777   .00447  -.32338
ATOM H20      .04475  -.24009  -.32493
ATOM H21      .11724  -.24546  -.70321
ATOM H22      .23166  -.05495  -.53036
ENERGY 27.33 kcal/mol
COMMENT Releative E=+0.76 kcal/mol
COMMENT Confidence level (1-10): 4, by energy.

TITL  Dunitz/Schweizer  IV   1
SPACEGROUP  P21/c
CELL     8.43380   6.54250  15.77380  90.00000  88.44550  90.00000
ATOM H1      0.0987   -0.1865   -0.1698
ATOM C2      0.1549   -0.0443   -0.1526
ATOM C3      0.3336    0.1346   -0.0548
ATOM C4      0.3348    0.2406   -0.2111
ATOM C5      0.4309    0.2251   -0.1302
ATOM C6      0.2473    0.0411   -0.2306
ATOM C7      0.2665   -0.0740   -0.0786
ATOM C8      0.2000    0.2783   -0.0288
ATOM H9      0.2501    0.3652   -0.2050
ATOM H10      0.5327    0.1259   -0.1416
ATOM H11      0.3324   -0.0748   -0.2510
ATOM H12      0.3620   -0.1773   -0.0970
ATOM C13      0.0209    0.0992   -0.1267
ATOM H14      0.4087    0.1238   -0.0004
ATOM H15      0.4133    0.2801   -0.2644
ATOM H16      0.4767    0.3738   -0.1130
ATOM H17      0.1670    0.0637   -0.2823
ATOM H18      0.2037   -0.1429   -0.0248
ATOM O19     -0.1073    0.0935   -0.1565
ATOM N20      0.0558    0.2432   -0.0658
ATOM O21      0.2151    0.4165    0.0198
ATOM H22     -0.0318    0.3394   -0.0495
ENERGY  -111.1 kcal/mol
COMMENT lowest energy structure found in P21/c with UNI FF + ES charges

TITL  Dunitz Schweizer IV 2
SPACEGROUP  P21/c
CELL     6.19860  15.10100  10.35160  90.00000 116.91800  90.00000
ATOM H1     -0.4232   -0.0907    0.1754
ATOM C2     -0.2400   -0.1027    0.1923
ATOM C3      0.1250   -0.1976    0.3039
ATOM C4      0.0142   -0.1263    0.0574
ATOM C5      0.1368   -0.2048    0.1585
ATOM C6     -0.2383   -0.1072    0.0438
ATOM C7     -0.1376   -0.1882    0.2772
ATOM C8      0.2724   -0.1191    0.3902
ATOM H9      0.1270   -0.0679    0.0966
ATOM H10      0.0470   -0.2661    0.1068
ATOM H11     -0.3622   -0.1595   -0.0183
ATOM H12     -0.2432   -0.2445    0.2159
ATOM C13     -0.0932   -0.0239    0.2783
ATOM H14      0.2098   -0.2554    0.3689
ATOM H15      0.0004   -0.1399   -0.0490
ATOM H16      0.3238   -0.2104    0.1787
ATOM H17     -0.3086   -0.0459   -0.0148
ATOM H18     -0.1484   -0.1871    0.3791
ATOM O19     -0.1742    0.0489    0.2676
ATOM N20      0.1472   -0.0406    0.3714
ATOM O21      0.4841   -0.1224    0.4690
ATOM H22      0.2448    0.0115    0.4268
ENERGY  -106.0 kcal/mol
COMMENT another dimeric structure in P21/c

TITL  Dunitz/Schweizer IV 3
SPACEGROUP  C2/c
CELL    11.29500  12.27080  12.96470  90.00000  81.74900  90.00000
ATOM H1     -0.1967   -0.1979   -0.2873
ATOM C2     -0.2185   -0.1346   -0.2296
ATOM C3     -0.2137    0.0625   -0.1881
ATOM C4     -0.3928   -0.0517   -0.1064
ATOM C5     -0.3481    0.0615   -0.1444
ATOM C6     -0.3532   -0.1410   -0.1871
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ATOM C7     -0.1871   -0.0216   -0.2755
ATOM C8     -0.1395    0.0384   -0.1021
ATOM H9     -0.3603   -0.0707   -0.0336
ATOM H10     -0.3967    0.0885   -0.2063
ATOM H11     -0.4020   -0.1324   -0.2529
ATOM H12     -0.2397   -0.0041   -0.3372
ATOM C13     -0.1442   -0.1590   -0.1438
ATOM H14     -0.1884    0.1436   -0.2153
ATOM H15     -0.4896   -0.0511   -0.0889
ATOM H16     -0.3660    0.1206   -0.0817
ATOM H17     -0.3742   -0.2208   -0.1536
ATOM H18     -0.0935   -0.0180   -0.3099
ATOM O19     -0.1170   -0.2488   -0.1209
ATOM N20     -0.1097   -0.0696   -0.0902
ATOM O21     -0.1085    0.1064   -0.0461
ATOM H22     -0.0622   -0.0858   -0.0326
ENERGY  -106.48 kcal/mol
COMMENT best structure in C2/c (dimeric)

TITL Schmidt IV 1
SPACEGROUP P21/c
CELL  10.0865   7.4148   9.7931  90.000 103.627  90.000
ATOM        C1   0.31206  -0.05042   0.24659
ATOM        C2   0.26766  -0.13370   0.37082
ATOM        N3   0.15734  -0.05741   0.41368
ATOM        C4   0.08525   0.09176   0.34704
ATOM        C5   0.12899   0.17587   0.22272
ATOM        C6   0.23265   0.32507   0.27336
ATOM        C7   0.36691   0.25524   0.36153
ATOM        C8   0.42072   0.09260   0.29788
ATOM        C9   0.19019   0.03291   0.14469
ATOM       O10   0.32662  -0.26614   0.43528
ATOM       O11  -0.01161   0.15193   0.39118
ATOM       H12   0.35341  -0.15364   0.19784
ATOM       H13   0.04214   0.23111   0.15725
ATOM       H14   0.19176   0.41834   0.33138
ATOM       H15   0.24973   0.39131   0.18546
ATOM       H16   0.35490   0.22202   0.46109
ATOM       H17   0.43905   0.35793   0.37463
ATOM       H18   0.45842   0.13335   0.21267
ATOM       H19   0.50117   0.03590   0.37172
ATOM       H20   0.22140   0.09151   0.06097
ATOM       H21   0.11806  -0.06546   0.10445
ATOM       H22   0.12800  -0.11306   0.49600
ENERGY -98.21 kJ/mol
COMMENT  Relatively small unit cell volume (V=178.0 A3/mol).
COMMENT  Good van der Waals packing (vdW energy = -74.5 kJ/mol)
COMMENT  Hydrogen bonds less favorable than in prediction 2 and 3
COMMENT  (Distance O...H =1.81 Angstroem).
COMMENT  Confidence level (1-10): 3, by energy
COMMENT  Confidence level for all predictions of IV is relatively low,
COMMENT  because the force field is not designed for H bridges.

TITL Schmidt IV 2
SPACEGROUP Pbca
CELL  11.3928  11.6958  10.9476  90.000  90.000  90.000
ATOM        C1   0.30354   0.30874   0.11763
ATOM        C2   0.25407   0.38027   0.01343
ATOM        N3   0.14190   0.42726   0.02601
ATOM        C4   0.07308   0.41202   0.13048
ATOM        C5   0.12188   0.34059   0.23510
ATOM        C6   0.08606   0.21600   0.21958
ATOM        C7   0.14224   0.15988   0.10935
ATOM        C8   0.27269   0.18327   0.09889
ATOM        C9   0.25489   0.35024   0.23908
ATOM       O10   0.30989   0.39757  -0.08212
ATOM       O11  -0.02574   0.45643   0.13492
ATOM       H12   0.39429   0.31815   0.11558
ATOM       H13   0.08542   0.37232   0.31532
ATOM       H14  -0.00478   0.21086   0.21205
ATOM       H15   0.11041   0.17211   0.29823
ATOM       H16   0.10041   0.18821   0.03053
ATOM       H17   0.12891   0.07203   0.11422
ATOM       H18   0.31749   0.13580   0.16431
ATOM       H19   0.30224   0.15702   0.01350
ATOM       H20   0.28783   0.30020   0.30973
ATOM       H21   0.27996   0.43443   0.25502
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ATOM       H22   0.10936   0.47479  -0.04317
ENERGY -97.60 kJ/mol
COMMENT  Larger unit cell volume (V=182.4 A3/mol).
COMMENT  Worse van der Waals packing (vdW energy = -70.8 kJ/mol).
COMMENT  Hydrogen bonds better than in prediction 1 (O...H =1.60 Angstroem).
COMMENT  Confidence level (1-10): 2.5, by energy and chemical intuition
COMMENT  (good hydrogen bonds)

TITL Schmidt IV 3
SPACEGROUP P21/c
CELL   9.2842   8.5413  11.7212  90.000 128.088  90.000
ATOM        C1   0.84705   0.20151   0.02738
ATOM        C2   0.69115   0.12363   0.01609
ATOM        N3   0.51329   0.18014  -0.08613
ATOM        C4   0.47175   0.30477  -0.17927
ATOM        C5   0.62685   0.38332  -0.16871
ATOM        C6   0.70280   0.51992  -0.06285
ATOM        C7   0.79807   0.46859   0.09228
ATOM        C8   0.92902   0.33315   0.13860
ATOM        C9   0.77801   0.26577  -0.11938
ATOM       O10   0.71728   0.01248   0.09505
ATOM       O11   0.31045   0.34837  -0.26723
ATOM       H12   0.94621   0.11627   0.06193
ATOM       H13   0.57181   0.42539  -0.27146
ATOM       H14   0.59692   0.59641  -0.09435
ATOM       H15   0.79490   0.58022  -0.06928
ATOM       H16   0.70026   0.43709   0.10472
ATOM       H17   0.86988   0.56306   0.16098
ATOM       H18   1.04592   0.37297   0.15424
ATOM       H19   0.96907   0.28915   0.23704
ATOM       H20   0.88451   0.32050  -0.11064
ATOM       H21   0.72911   0.17552  -0.19444
ATOM       H22   0.41012   0.12814  -0.09350
ENERGY -96.35 kJ/mol
COMMENT  Larger unit cell volume (V=182.9 A3/mol).
COMMENT  Worse van der Waals packing (vdW energy = -71.1 kJ/mol)
COMMENT  Hydrogen bonds better than in prediction 1 (O...H =1.68 Angstroem).
COMMENT  Confidence level (1-10): 1.5, by energy
COMMENT  There are 6 further packings with energies < -95 kJ/mol.

TITL  Van Eijck IV 1
SPACEGROUP P21/c
CELL   10.26230   7.53718   9.82555    90.000   104.517    90.000
ATOM C1            .304299   .029929   .856145
ATOM H2            .267959   .088740   .940561
ATOM H3            .379294  -.068752   .903737
ATOM C4            .367176   .172683   .782473
ATOM H5            .453551   .227189   .858423
ATOM C6            .187240  -.056367   .749131
ATOM H7            .146738  -.163095   .800757
ATOM C8            .263510   .320525   .733005
ATOM H9            .304974   .419458   .674753
ATOM H10           .245821   .388525   .824642
ATOM C11           .077325   .083906   .698700
ATOM H12           .034494   .119422   .785984
ATOM H13          -.004407   .026849   .617699
ATOM C14           .128189   .253478   .642233
ATOM H15           .136867   .228989   .535557
ATOM H16           .053518   .357933   .634306
ATOM C17           .415189   .092442   .660599
ATOM O18           .509970   .145106   .621381
ATOM C19           .236059  -.136310   .627846
ATOM O20           .187754  -.264826   .563100
ATOM N21           .344120  -.052618   .594675
ATOM H22           .376767  -.105332   .515500
ENERGY   -210.913 kJ/mol
COMMENT The lowest energy in the empirical as well as ab initio force field.
COMMENT Second best are 1.5 and 0.9 kJ/mol higher, respectively.
COMMENT This is not much, but there are at least two indications.

TITL  Van Eijck IV 2
SPACEGROUP P212121
CELL   11.23151  11.29203   5.91571    90.000    90.000    90.000
ATOM C1            .500569   .738352   .606806
ATOM H2            .579875   .700027   .683335
ATOM H3            .423689   .696835   .685916
ATOM C4            .499699   .713787   .353029
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ATOM H5            .496112   .618401   .327239
ATOM C6            .498375   .872317   .645969
ATOM H7            .493465   .889110   .827164
ATOM C8            .615634   .759991   .249823
ATOM H9            .610388   .753437   .066357
ATOM H10           .688187   .702003   .300907
ATOM C11           .614220   .925688   .555568
ATOM H12           .686621   .901653   .669226
ATOM H13           .607460  1.021823   .561008
ATOM C14           .647367   .887813   .314204
ATOM H15           .605192   .947577   .194011
ATOM H16           .742845   .899493   .293334
ATOM C17           .390231   .770003   .243194
ATOM O18           .341262   .731343   .079893
ATOM C19           .389486   .928231   .533644
ATOM O20           .340553  1.015818   .600768
ATOM N21           .347074   .871882   .342735
ATOM H22           .275777   .908971   .267401
ENERGY   -209.397 kJ/mol
COMMENT The best free energy if we discard a structure with six imaginary
COMMENT    frequencies. It is also the second best in energy.
COMMENT But it is very bad (#22) in the ab-initio force field.

TITL  Van Eijck IV 3
SPACEGROUP P21/c
CELL    9.07146   7.84339  12.59642    90.000    56.006    90.000
ATOM C1            .161777   .660894   .678929
ATOM H2            .200331   .546768   .619710
ATOM H3            .044934   .714080   .686741
ATOM C4            .312819   .791405   .616765
ATOM H5            .340013   .826449   .523597
ATOM C6            .116999   .615954   .812206
ATOM H7            .003821   .529210   .858461
ATOM C8            .481315   .712927   .596899
ATOM H9            .578665   .813545   .571340
ATOM H10           .540870   .627691   .514784
ATOM C11           .276071   .524377   .797887
ATOM H12           .286263   .397379   .759231
ATOM H13           .251096   .506100   .892471
ATOM C14           .454680   .616103   .712223
ATOM H15           .472381   .704713   .770918
ATOM H16           .560314   .521864   .676358
ATOM C17           .257217   .951139   .699738
ATOM O18           .305354  1.092440   .659723
ATOM C19           .066507   .776423   .894548
ATOM O20          -.032345   .779441  1.009027
ATOM N21           .141680   .927253   .829994
ATOM H22           .107314  1.033353   .883755
ENERGY   -209.270 kJ/mol
COMMENT The third energy and also the third free energy.
COMMENT But it is only fifth in the ab-initio force field.


TITL Verwer IV 1
SPACEGROUP P21/n
CELL  9.1319   8.1080  10.6618  90.0000  96.9903  90.0000
ATOM C1   0.16369  0.36176 0.70817
ATOM C2   0.07926  0.27486 0.59064
ATOM C3  -0.06819  0.19208 0.61671
ATOM C4  -0.16533  0.32045 0.67754
ATOM C5  -0.08171  0.36903 0.80892
ATOM C6   0.06263  0.46201 0.78791
ATOM C7  -0.03947  0.05164 0.70642
ATOM N8  -0.02964  0.06996 0.83077
ATOM C9  -0.04836  0.21518 0.88383
ATOM O10 -0.02312 -0.09332 0.67324
ATOM O11 -0.03139  0.20920 1.00124
ATOM H12  0.22245  0.26850 0.76885
ATOM H13  0.24607  0.44417 0.67641
ATOM H14  0.05458  0.36579 0.51563
ATOM H15  0.15185  0.18297 0.55568
ATOM H16 -0.12808  0.14767 0.52815
ATOM H17 -0.18664  0.42857 0.61668
ATOM H18 -0.27215  0.26553 0.68954
ATOM H19 -0.15123  0.44922 0.85891
ATOM H20  0.03296  0.57820 0.73942
ATOM H21  0.12441  0.49278 0.87920
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ATOM H22 -0.00878 -0.02487 0.88317
ENERGY -136.13 kcal/mol
COMMENT d=1.298 g/cc
COMMENT structure ranked nr. 1 by energy

TITL Verwer IV 2
SPACEGROUP P21/c
CELL 10.1714   7.9904  10.0337  90.0000  75.8960  90.0000
ATOM   C1  0.36442  0.73535  0.64622
ATOM   C2  0.22895  0.79920  0.74152
ATOM   C3  0.12248  0.65708  0.78820
ATOM   C4  0.18678  0.51578  0.85852
ATOM   C5  0.30438  0.43704  0.74664
ATOM   C6  0.41734  0.57205  0.70054
ATOM   C7  0.08014  0.58284  0.66872
ATOM   N8  0.14438  0.45541  0.59650
ATOM   C9  0.24871  0.38048  0.62961
ATOM  O10 -0.01677  0.63443  0.62480
ATOM  O11  0.29746  0.26355  0.55148
ATOM  H12  0.34921  0.71134  0.54392
ATOM  H13  0.44087  0.83344  0.63496
ATOM  H14  0.25102  0.85647  0.83258
ATOM  H15  0.18620  0.89718  0.68896
ATOM  H16  0.03379  0.70602  0.86179
ATOM  H17  0.22448  0.56493  0.94366
ATOM  H18  0.11044  0.42180  0.90139
ATOM  H19  0.34503  0.32894  0.78958
ATOM  H20  0.45851  0.60431  0.78826
ATOM  H21  0.50076  0.52019  0.62164
ATOM  H22  0.11277  0.41575  0.51977
ENERGY -135.88 kcal/mol
COMMENT d= 1.2865 g/cc
COMMENT structure ranked nr. 2 by energy

TITL Verwer IV 3
SPACEGROUP P21/c
CELL 6.2259  10.9005  12.4816  90.0000  76.8224  90.0000
ATOM   C1  0.91058  0.12214  0.65813
ATOM   C2  0.66670  0.07967  0.67234
ATOM   C3  0.53210  0.08196  0.79437
ATOM   C4  0.54628  0.21282  0.84297
ATOM   C5  0.79211  0.23637  0.84559
ATOM   C6  0.93381  0.24010  0.72524
ATOM   C7  0.62262 -0.00645  0.86405
ATOM   N8  0.78425  0.02221  0.91288
ATOM   C9  0.86656  0.13478  0.90858
ATOM  O10  0.55533 -0.11349  0.88194
ATOM  O11  1.02001  0.14487  0.95664
ATOM  H12  1.00483  0.04810  0.68474
ATOM  H13  0.98331  0.13801  0.57101
ATOM  H14  0.58577  0.13996  0.62360
ATOM  H15  0.66470 -0.01265  0.63850
ATOM  H16  0.36016  0.05905  0.79693
ATOM  H17  0.48708  0.28190  0.79355
ATOM  H18  0.44236  0.21907  0.92610
ATOM  H19  0.80553  0.32384  0.88645
ATOM  H20  0.88333  0.31948  0.68340
ATOM  H21  1.10705  0.25292  0.72654
ATOM  H22  0.84053 -0.03858  0.95432
ATOM  END  0.00000  0.00000  0.00000
ENERGY -135.75 kcal/mol
COMMENT d=1.2336 g/cc
COMMENT structure ranked nr. 3 by energy


TITL IV 1 Williams
SPACEGROUP P21/c
CELL         10.42    7.48    9.91     90.00     77.05     90.00
ATOM H5           0.37342   0.43035   0.11048
ATOM H6           0.27756   0.57219   0.06608
ATOM C4           0.30662   0.52229   0.14634
ATOM H3           0.15142   0.33996   0.20738
ATOM H7           0.44385   0.72252   0.16103
ATOM O2           0.18125   0.24061   0.43891
ATOM C3           0.18946   0.44059   0.24887
ATOM C8           0.23456   0.36296   0.37192
ATOM H13          0.36844   0.39935   0.47910
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ATOM N1           0.34249   0.44416   0.40534
ATOM C7           0.41026   0.59265   0.34405
ATOM O1           0.49782   0.65444   0.38867
ATOM C5           0.36486   0.67001   0.22108
ATOM H2           0.04818   0.61900   0.21615
ATOM H10          0.24359   0.87463   0.18528
ATOM C2           0.08187   0.58285   0.29763
ATOM C6           0.26220   0.81870   0.26913
ATOM H1           0.00760   0.52929   0.36462
ATOM H9           0.30025   0.91204   0.31836
ATOM C1           0.13381   0.74747   0.36077
ATOM H12          0.14795   0.71755   0.45339
ATOM H11          0.06651   0.84232   0.37556
ENERGY -87.76

TITL IV 2 Williams
SPACEGROUP P21/n
CELL          6.37   12.16   10.18     90.00    102.02     90.00
ATOM H5           0.89318   0.43648   0.39277
ATOM H6           0.94969   0.31401   0.44108
ATOM C4           0.84442   0.35948   0.37968
ATOM H3           0.61843   0.37200   0.50248
ATOM H7           0.97010   0.33450   0.20712
ATOM O2           0.30190   0.45325   0.34635
ATOM C3           0.62137   0.34585   0.41152
ATOM C8           0.45986   0.41640   0.31739
ATOM H13          0.40667   0.47647   0.13567
ATOM N1           0.50344   0.43558   0.19195
ATOM C7           0.67113   0.39395   0.14002
ATOM O1           0.68257   0.41281   0.02678
ATOM C5           0.83228   0.32339   0.23437
ATOM H2           0.65177   0.18273   0.46925
ATOM H10          0.88662   0.15769   0.27181
ATOM C2           0.55230   0.22400   0.39907
ATOM C6           0.76903   0.20092   0.21690
ATOM H1           0.40772   0.21637   0.41839
ATOM H9           0.75945   0.17891   0.12276
ATOM C1           0.55771   0.17552   0.26070
ATOM H12          0.43577   0.20439   0.19337
ATOM H11          0.53675   0.09526   0.26244
ENERGY -86.29

TITL IV 3 Williams
SPACEGROUP C2/c
CELL         22.28   10.29    6.89     90.00     96.19     90.00
ATOM H5           0.12853   0.23765   0.35313
ATOM H6           0.15778   0.36134   0.26334
ATOM C4           0.13681   0.27880   0.22944
ATOM H3           0.21407   0.16734   0.19806
ATOM H7           0.04981   0.35676   0.16708
ATOM O2           0.16996  -0.03622   0.04613
ATOM C3           0.17654   0.19104   0.11754
ATOM C8           0.14431   0.06375   0.06650
ATOM H13          0.06285  -0.00610   0.00908
ATOM N1           0.08195   0.06904   0.04124
ATOM C7           0.04564   0.17748   0.04801
ATOM O1          -0.00781   0.16870   0.01285
ATOM C5           0.07801   0.30462   0.09898
ATOM H2           0.21742   0.33607  -0.02859
ATOM H10          0.10764   0.46257  -0.04939
ATOM C2           0.19242   0.25961  -0.06946
ATOM C6           0.09112   0.37632  -0.08860
ATOM H1           0.21746   0.20176  -0.14128
ATOM H9           0.05306   0.39118  -0.17235
ATOM C1           0.13622   0.30314  -0.20182
ATOM H12          0.11632   0.22679  -0.26727
ATOM H11          0.14843   0.35899  -0.30692
ENERGY -84.78

TITL Ammon V 1
SPACEGROUP P21/n
CELL    9.1367    7.5432   19.6806   90.0000  118.0947   90.0000
ATOM  H1     -0.12113   0.15094  -0.29590
ATOM  C2     -0.10837   0.17125  -0.23810
ATOM  C3      0.01100   0.32775  -0.19533
ATOM  C4     -0.02274   0.01003  -0.18579
ATOM  H5     -0.23352   0.19184  -0.24489
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ATOM  C6     -0.03503   0.02941  -0.11028
ATOM  C7      0.15592   0.23634  -0.12441
ATOM  H8      0.05914   0.39190  -0.23084
ATOM  H9     -0.04756   0.43146  -0.17720
ATOM  H10    -0.06654  -0.11934  -0.21359
ATOM  C11     0.16714   0.04904  -0.15672
ATOM  H12     0.00780  -0.08925  -0.07378
ATOM  C13     0.28652  -0.08050  -0.09494
ATOM  C14     0.21539   0.05396  -0.22175
ATOM  C15     0.30684   0.34836  -0.07495
ATOM  C16     0.08092   0.18379  -0.07224
ATOM  BR17   -0.25991   0.06768  -0.12252
ATOM  H18     0.26665  -0.21583  -0.11814
ATOM  H19     0.27441  -0.08340  -0.04203
ATOM  H20     0.41586  -0.04556  -0.07795
ATOM  H21     0.20432  -0.07907  -0.24634
ATOM  H22     0.34535   0.09516  -0.19887
ATOM  H23     0.13929   0.14426  -0.26909
ATOM  H24     0.42385   0.27384  -0.05013
ATOM  H25     0.31892   0.47064  -0.10218
ATOM  S26     0.27260   0.41543   0.00759
ATOM  N27     0.12108   0.25633  -0.00751
ATOM  O28     0.41907   0.37571   0.08063
ATOM  O29     0.19472   0.59056  -0.00700
ENERGY -33.41 kcal/mol based on atom-centered charges for electrostatics.
COMMENT d = 1.622 g/cc.  Next to lowest E structure.
COMMENT Previously, we had depended too much on the highest density
COMMENT to identify the best structure.  Volume additivity calcns
COMMENT suggest d = 1.651 g/cc.  Lowest E structure (-34.34 kcal/mol)
COMMENT had too low a density (d = 1.596 g/cc) for our tastes.  This
COMMENT is a compromise.

TITL Ammon V 2
SPACEGROUP P21/n
CELL    7.0990   15.8103   10.7066   90.0000  100.6034   90.0000
ATOM  H1      0.21881   0.50481  -0.08133
ATOM  C2      0.11248   0.46583  -0.14333
ATOM  C3      0.07294   0.38124  -0.07811
ATOM  C4      0.19083   0.43636  -0.26170
ATOM  H5     -0.01729   0.50439  -0.17020
ATOM  C6      0.02534   0.39537  -0.35695
ATOM  C7      0.14093   0.31246  -0.16452
ATOM  H8      0.15577   0.37608   0.01886
ATOM  H9     -0.07862   0.37269  -0.07210
ATOM  H10     0.26692   0.48542  -0.30541
ATOM  C11     0.31452   0.35642  -0.21083
ATOM  H12     0.06556   0.38092  -0.44887
ATOM  C13     0.39342   0.30646  -0.31355
ATOM  C14     0.48496   0.37684  -0.10414
ATOM  C15     0.14597   0.22159  -0.11872
ATOM  C16    -0.00773   0.31476  -0.28775
ATOM  BR17   -0.20848   0.46449  -0.40455
ATOM  H18     0.48921   0.34664  -0.35753
ATOM  H19     0.28266   0.28140  -0.38980
ATOM  H20     0.47843   0.25222  -0.27101
ATOM  H21     0.59137   0.41476  -0.14186
ATOM  H22     0.55618   0.31819  -0.06606
ATOM  H23     0.44550   0.41187  -0.02422
ATOM  H24     0.26228   0.18407  -0.14575
ATOM  H25     0.14398   0.21366  -0.01709
ATOM  S26    -0.08159   0.17589  -0.20766
ATOM  N27    -0.12652   0.25540  -0.32282
ATOM  O28    -0.04382   0.09731  -0.27054
ATOM  O29    -0.23031   0.18001  -0.12964
ENERGY -32.33 kcal/mol
COMMENT d = 1.643 g/cc.  Close to lowest E structure and with a
COMMENT good density in comparison to volume additivity calcns of
COMMENT d = 1.651 g/cc.

TITL Ammon V 3
SPACEGROUP Cc
CELL    7.1513   16.0805   13.7236   90.0000  130.3932   90.0000
ATOM  H1      0.16372   0.25162   0.11935
ATOM  C2     -0.00247   0.21322   0.05807
ATOM  C3      0.02394   0.13045   0.12505
ATOM  C4     -0.04352   0.18350  -0.06175
ATOM  H5     -0.15683   0.25127   0.03165
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ATOM  C6     -0.30100   0.14310  -0.15608
ATOM  C7      0.00466   0.06227   0.03797
ATOM  H8      0.20204   0.12568   0.22225
ATOM  H9     -0.11889   0.12239   0.13247
ATOM  H10    -0.01253   0.23138  -0.10698
ATOM  C11     0.12887   0.10491  -0.01066
ATOM  H12    -0.35318   0.12836  -0.24901
ATOM  C13     0.10401   0.05512  -0.11447
ATOM  C14     0.40266   0.12514   0.09539
ATOM  C15     0.05549  -0.02685   0.08504
ATOM  C16    -0.26429   0.06426  -0.08516
ATOM  BR17   -0.57830   0.21130  -0.20283
ATOM  H18     0.15414   0.09422  -0.16005
ATOM  H19    -0.08080   0.03035  -0.19025
ATOM  H20     0.23007   0.00183  -0.07171
ATOM  H21     0.46946   0.16203   0.05604
ATOM  H22     0.51073   0.06753   0.13378
ATOM  H23     0.44357   0.16006   0.17601
ATOM  H24     0.14287  -0.06412   0.05717
ATOM  H25     0.15495  -0.03416   0.18769
ATOM  S26    -0.25663  -0.07174  -0.00235
ATOM  N27    -0.41581   0.00596  -0.11898
ATOM  O28    -0.28208  -0.14939  -0.06532
ATOM  O29    -0.32487  -0.06701   0.07759
ENERGY -31.72 kcal/mol
COMMENT d = 1.615 g/cc. There really was no obvious choice for
COMMENT guess # 3.  This was a compromise between E and d.
COMMENT A better guess in C2 has E = -32.58 kcal/mol, but d =
COMMENT 1.558 g/cc.


COMMENT – AMMON WAS ALLOWED A SECOND SUBMISSION SELECTING ONLY SOHNKE SPACEGPS
TITL Ammon V 1   (second submission)
SPACEGROUP P212121
CELL   10.3943   16.3540    7.1279   90.0000   90.0000   90.0000
ATOM  H1     -0.17877  -0.50079   0.19626
ATOM  C2     -0.11790  -0.46774   0.29676
ATOM  C3     -0.17851  -0.38437   0.35483
ATOM  C4      0.01095  -0.44261   0.20483
ATOM  H5     -0.10222  -0.50842   0.41716
ATOM  C6      0.10244  -0.41005   0.35927
ATOM  C7     -0.07902  -0.32028   0.28224
ATOM  H8     -0.27214  -0.37396   0.28765
ATOM  H9     -0.19306  -0.37874   0.50686
ATOM  H10     0.05539  -0.49020   0.11760
ATOM  C11    -0.02547  -0.36121   0.09854
ATOM  H12     0.20040  -0.39906   0.30741
ATOM  C13     0.08947  -0.31570   0.01065
ATOM  C14    -0.12629  -0.37341  -0.05684
ATOM  C15    -0.11641  -0.23081   0.29397
ATOM  C16     0.03775  -0.33025   0.41108
ATOM  Br17    0.12990  -0.48295   0.57636
ATOM  H18     0.13627  -0.35438  -0.09517
ATOM  H19     0.16326  -0.29670   0.11189
ATOM  H20     0.05660  -0.26016  -0.06138
ATOM  H21    -0.08502  -0.40945  -0.17201
ATOM  H22    -0.15498  -0.31404  -0.11537
ATOM  H23    -0.21399  -0.40471  -0.00978
ATOM  H24    -0.07788  -0.19355   0.17881
ATOM  H25    -0.21971  -0.21913   0.31182
ATOM  S26    -0.03469  -0.19462   0.51135
ATOM  N27     0.07236  -0.27669   0.53014
ATOM  O28     0.03986  -0.12072   0.47324
ATOM  O29    -0.12402  -0.19828   0.66980
ENERGY -31.64 kcal/mol
COMMENT d = 1.602 g/cc.  Overall, the second lowest E
COMMENT acentric structure without a glide plane.
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COMMENT The lowest E acentric  (C2, E = -32.58
COMMENT kcal/mol, d =1.558 g/cc) had too low a
COMMENT density to be acceptable (volume additivity
COMMENT predicted d = 1.651 g/cc).
COMMENT We consider this to be the first lowest E
COMMENT with an acceptable density.


TITL Ammon V 2  (second submission)
SPACEGROUP P212121
CELL   10.7988   12.8019    8.6079   90.0000   90.0000   90.0000
ATOM  H1      0.03299  -0.19442  -0.01270
ATOM  C2     -0.02338  -0.17218   0.08816
ATOM  C3      0.03451  -0.21153   0.24326
ATOM  C4     -0.15063  -0.22757   0.08357
ATOM  H5     -0.03390  -0.08689   0.08527
ATOM  C6     -0.23484  -0.17966   0.21063
ATOM  C7     -0.06489  -0.28886   0.30728
ATOM  H8      0.12228  -0.25298   0.22473
ATOM  H9      0.05284  -0.14825   0.32624
ATOM  H10    -0.19473  -0.22895  -0.03134
ATOM  C11    -0.12078  -0.33813   0.15536
ATOM  H12    -0.33083  -0.20756   0.20356
ATOM  C13    -0.23502  -0.40766   0.18369
ATOM  C14    -0.02813  -0.40223   0.05885
ATOM  C15    -0.03083  -0.35271   0.44933
ATOM  C16    -0.17312  -0.21927   0.35713
ATOM  Br17   -0.25301  -0.02624   0.20606
ATOM  H18    -0.28216  -0.42403   0.07333
ATOM  H19    -0.30344  -0.37397   0.26363
ATOM  H20    -0.20693  -0.48318   0.23282
ATOM  H21    -0.07030  -0.42498  -0.05217
ATOM  H22    -0.00375  -0.47445   0.12050
ATOM  H23     0.05838  -0.36072   0.03266
ATOM  H24    -0.07222  -0.43106   0.45048
ATOM  H25     0.06873  -0.35740   0.47432
ATOM  S26    -0.10388  -0.27974   0.61269
ATOM  N27    -0.20422  -0.20522   0.49806
ATOM  O28    -0.17853  -0.34997   0.70825
ATOM  O29    -0.01323  -0.20934   0.68345
ENERGY -31.42 kcal/mol
COMMENT d = 1.631 g/cc.  Second lowest E soltuion
COMMENT with an acceptable density.


TITL Ammon V 3  (second submission)
SPACEGROUP P212121
CELL   10.5948   11.5236    9.8832   90.0000   90.0000   90.0000
ATOM  H1     -0.02926  -0.36291   0.27538
ATOM  C2      0.04658  -0.31489   0.32637
ATOM  C3      0.06016  -0.18929   0.26987
ATOM  C4      0.17648  -0.37018   0.29563
ATOM  H5      0.02598  -0.31622   0.43523
ATOM  C6      0.27694  -0.31370   0.38853
ATOM  C7      0.19563  -0.18840   0.20787
ATOM  H8     -0.00962  -0.17027   0.19079
ATOM  H9      0.05000  -0.12234   0.34817
ATOM  H10     0.17784  -0.46537   0.29993
ATOM  C11     0.21140  -0.31595   0.15392
ATOM  H12     0.36902  -0.35708   0.38236
ATOM  C13     0.34552  -0.34463   0.10381
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ATOM  C14      0.11910  -0.34930   0.04031
ATOM  C15      0.23431  -0.08224   0.12732
ATOM  C16      0.28436  -0.19248   0.33004
ATOM  Br17     0.23945  -0.31537   0.58419
ATOM  H18      0.35618  -0.43873   0.09069
ATOM  H19      0.42119  -0.31486   0.17131
ATOM  H20      0.36260  -0.30454   0.00469
ATOM  H21      0.12732  -0.44229   0.01775
ATOM  H22      0.14249  -0.30196  -0.05279
ATOM  H23      0.01977  -0.33143   0.06413
ATOM  H24      0.29790  -0.10175   0.04260
ATOM  H25      0.15607  -0.02707   0.09308
ATOM  S26      0.32843   0.00461   0.25027
ATOM  N27      0.35391  -0.10792   0.36578
ATOM  O28      0.45006   0.03688   0.19163
ATOM  O29      0.24778   0.09158   0.31484
ENERGY -30.75 kcal/mol
COMMENT d = 1.608 g/cc.  Third lowest E solution
COMMENT with an acceptable density.
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TITL Dzyabchenko V 1
SPACEGROUP P212121
CELL 12.959 10.440 8.360 90.00 90.00 90.00
ATOM S1     0.45506   0.37632   0.87990
ATOM BR1    0.72742   0.47376   0.47134
ATOM O3     0.39318   0.46436   0.96857
ATOM O4     0.50961   0.28058   0.96841
ATOM N5     0.54041   0.46341   0.77409
ATOM C6     0.38454   0.30667   0.71503
ATOM C7     0.44954   0.34002   0.57044
ATOM C8     0.52760   0.43652   0.62675
ATOM C9     0.57574   0.49881   0.48202
ATOM C10    0.51342   0.43071   0.34771
ATOM C11    0.55335   0.29035   0.33670
ATOM C12    0.51124   0.22827   0.49154
ATOM C13    0.40626   0.41421   0.42286
ATOM C14    0.35153   0.53837   0.46551
ATOM C15    0.33108   0.33552   0.32377
ATOM H18    0.30762   0.34385   0.69722
ATOM H19    0.37521   0.20394   0.71991
ATOM H20    0.55727   0.59968   0.48159
ATOM H21    0.51619   0.48113   0.23499
ATOM H22    0.52616   0.24199   0.23056
ATOM H23    0.63648   0.28536   0.32977
ATOM H24    0.46347   0.14582   0.46701
ATOM H25    0.57230   0.19288   0.56755
ATOM H26    0.38915   0.59272   0.55839
ATOM H27    0.27262   0.51831   0.50409
ATOM H28    0.34653   0.59839   0.35890
ATOM H29    0.35893   0.24150   0.29407
ATOM H30    0.31544   0.38689   0.21221
ATOM H31    0.25779   0.32579   0.38656
ENERGY -122.90 kcal/mol COMMENT
Density = 1.716 g/cm3
COMMENT Confidence level 5 (1-10), by energy
COMMENT There is one more minimum slightly less deep in energy
COMMENT (-122.78 kcal/mol) with nearly the same unit cell constants
COMMENT and the molecule position/orientation but one methyl group
COMMENT rotated by 10 degrees with respect to the present structure.
COMMENT At non-zero temperature the two minima probably collapse into
COMMENT a single free-energy minimum with average parameters. Therefore
COMMENT we submit here only one of them.
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TITL Dzyabchenko V 2
SPACEGROUP P212121
CELL 7.906 8.931 15.959 90.00 90.00 90.00
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ATOM S1     0.20690   0.61325   0.55040
ATOM BR1    0.14709   0.10476   0.42029
ATOM O3     0.34714   0.67219   0.59605
ATOM O4     0.04387   0.62267   0.58892
ATOM N5     0.25045   0.43250   0.52983
ATOM C6     0.20175   0.68233   0.44403
ATOM C7     0.20430   0.54115   0.39155
ATOM C8     0.24632   0.41538   0.45059
ATOM C9     0.29548   0.28014   0.39945
ATOM C10    0.28217   0.34804   0.30995
ATOM C11    0.09079   0.36643   0.28941
ATOM C12    0.03594   0.49739   0.34675
ATOM C13    0.34026   0.51030   0.32276
ATOM C14    0.52133   0.52798   0.35321
ATOM C15    0.32112   0.61022   0.24624
ATOM H18    0.30762   0.75170   0.42610
ATOM H19    0.09097   0.74677   0.42767
ATOM H20    0.42580   0.25187   0.41216
ATOM H21    0.35030   0.28401   0.26352
ATOM H22    0.06892   0.39050   0.22398
ATOM H23    0.01959   0.26560   0.30174
ATOM H24   -0.01769   0.58922   0.31164
ATOM H25   -0.06176   0.46469   0.39037
ATOM H26    0.54071   0.48805   0.41610
ATOM H27    0.55734   0.64617   0.35102
ATOM H28    0.60658   0.46770   0.31152
ATOM H29    0.20292   0.59757   0.21422
ATOM H30    0.42353   0.58601   0.20216
ATOM H31    0.33499   0.72709   0.26520
ENERGY -122.81 kcal/mol
COMMENT Density=1.722 g/cm3
COMMENT Confidence level 3 (1-10), by energy


TITL Dzyabchenko V 3
SPACEGROUP P212121
CELL 13.351 8.524 10.083 90.00 90.00 90.00
ATOM S1    0.39207  -0.10985   0.21608
ATOM BR1   0.03313   0.05487   0.26285
ATOM O3    0.43936  -0.18286   0.10515
ATOM O4    0.40415  -0.18318   0.34269
ATOM N5    0.26907  -0.09756   0.18105
ATOM C6    0.41983   0.09736   0.22424
ATOM C7    0.31748   0.17380   0.22275
ATOM C8    0.24434   0.04667   0.18676
ATOM C9    0.14634   0.12245   0.14874
ATOM C10   0.17614   0.29805   0.16273
ATOM C11   0.18408   0.33492   0.31358
ATOM C12   0.28027   0.24690   0.35582
ATOM C13   0.28599   0.29949   0.11817
ATOM C14   0.30356   0.24939  -0.02462
ATOM C15   0.33916   0.45566   0.13658
ATOM H18   0.46317   0.14301   0.14244
ATOM H19   0.45929   0.13494   0.31218
ATOM H20   0.13029   0.09739   0.04592
ATOM H21   0.12617   0.37603   0.11029
ATOM H22   0.18889   0.45927   0.33310
ATOM H23   0.11911   0.29571   0.36811
ATOM H24   0.33493   0.32443   0.39982
ATOM H25   0.26558   0.15924   0.43068
ATOM H26   0.30126   0.12287  -0.03654
ATOM H27   0.37483   0.29113  -0.06241
ATOM H28   0.24460   0.29915  -0.08709
ATOM H29   0.33836   0.49763   0.23741
ATOM H30   0.30342   0.54415   0.07399
ATOM H31   0.41691   0.44602   0.10447
ENERGY -122.47 kcal/mol
COMMENT Density 1.691 g/cm3
COMMENT Confidence level 1 (1-10), by energy

TITL ERK V/1
CELL   8.0400  10.5080   7.4460  90.0000 104.4450  90.0000
SPACEGROUP P21
ATOM S1     -0.03605    0.14424    0.41973
ATOM BR2     0.33041   -0.02216    0.02197
ATOM O3     -0.00713    0.12910    0.61560
ATOM O4     -0.20128    0.10907    0.30749
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ATOM N5      0.11527    0.05856    0.35356
ATOM C6      0.02601    0.30062    0.35930
ATOM C7      0.15601    0.27332    0.24812
ATOM C8      0.19866    0.13421    0.27459
ATOM C9      0.35913    0.10873    0.21012
ATOM C10     0.39928    0.24618    0.15586
ATOM C11     0.26534    0.28050   -0.02771
ATOM C12     0.09687    0.29674    0.03466
ATOM C13     0.34205    0.32866    0.29954
ATOM C14     0.44116    0.30464    0.50430
ATOM C15     0.34773    0.47154    0.26650
ATOM H16    -0.08627    0.35239    0.28073
ATOM H17     0.08312    0.35267    0.48627
ATOM H18     0.46053    0.07469    0.32662
ATOM H19     0.53275    0.25945    0.14977
ATOM H20     0.30150    0.36751   -0.08905
ATOM H21     0.25377    0.20744   -0.13487
ATOM H22     0.04128    0.39147    0.00183
ATOM H23    -0.00086    0.22730   -0.03289
ATOM H24     0.42633    0.21043    0.55933
ATOM H25     0.40102    0.37114    0.59811
ATOM H26     0.57836    0.31961    0.51918
ATOM H27     0.29178    0.52322    0.36443
ATOM H28     0.28143    0.50646    0.13034
ATOM H29     0.48118    0.50229    0.28930
END

TITL ERK V/2
CELL   0.0000  14.3190  11.0080   7.5710  90.0000  90.0000  90.0000
SPACEGROUP P212121
ATOM S1       0.09572    0.48564    0.65581
ATOM BR2     -0.12466    0.30051    0.22269
ATOM O3       0.09570    0.46859    0.84271
ATOM O4       0.09579    0.60792    0.59191
ATOM N5       0.00123    0.41323    0.57587
ATOM C6       0.18499    0.39580    0.54918
ATOM C7       0.13094    0.31968    0.41770
ATOM C8       0.02953    0.33503    0.46390
ATOM C9      -0.02557    0.23748    0.37047
ATOM C10      0.05571    0.16809    0.27889
ATOM C11      0.09103    0.24859    0.12357
ATOM C12      0.14126    0.35440    0.21878
ATOM C13      0.13543    0.17803    0.41346
ATOM C14      0.11592    0.11709    0.59501
ATOM C15      0.22911    0.12950    0.34912
ATOM H16      0.23652    0.45498    0.48711
ATOM H17      0.21948    0.33972    0.64822
ATOM H18     -0.05967    0.17940    0.46798
ATOM H19      0.03733    0.07541    0.23986
ATOM H20      0.13809    0.19789    0.03696
ATOM H21      0.03464    0.28083    0.03800
ATOM H22      0.21446    0.36176    0.17897
ATOM H23      0.10800    0.44213    0.19040
ATOM H24      0.05912    0.15599    0.67222
ATOM H25      0.17716    0.12141    0.68076
ATOM H26      0.09967    0.02111    0.57512
ATOM H27      0.28377    0.14895    0.44567
ATOM H28      0.25511    0.16429    0.22438
ATOM H29      0.22506    0.03090    0.33435
END

TITL ERK V/3
CELL   0.0000   7.4630  14.7160  10.9600  90.0000  90.0000  90.0000
SPACEGROUP P212121
ATOM S1      0.37947   -0.54747    0.03372
ATOM BR2     0.21516   -0.81840    0.28302
ATOM O3      0.31600   -0.45676    0.04988
ATOM O4      0.36405   -0.58617   -0.08553
ATOM N5      0.26781   -0.61340    0.13353
ATOM C6      0.60270   -0.56202    0.09442
ATOM C7      0.58153   -0.63854    0.18561
ATOM C8      0.38329   -0.65219    0.20152
ATOM C9      0.35313   -0.70941    0.31386
ATOM C10     0.55037   -0.72084    0.35700
ATOM C11     0.64329   -0.78851    0.26800
ATOM C12     0.66169   -0.73265    0.14908
ATOM C13     0.63619   -0.62966    0.32256
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ATOM C14     0.55483   -0.54529    0.38756
ATOM C15     0.83830   -0.62516    0.34146
ATOM H16     0.69624   -0.57802    0.02103
ATOM H17     0.64409   -0.49901    0.13837
ATOM H18     0.27647   -0.67051    0.38075
ATOM H19     0.56244   -0.73972    0.45321
ATOM H20     0.77323   -0.81053    0.30333
ATOM H21     0.56648   -0.85100    0.25399
ATOM H22     0.80127   -0.72712    0.11961
ATOM H23     0.58627   -0.76347    0.07366
ATOM H24     0.41519   -0.53034    0.36674
ATOM H25     0.62832   -0.48347    0.36438
ATOM H26     0.56462   -0.55404    0.48629
ATOM H27     0.89152   -0.56142    0.30550
ATOM H28     0.91834   -0.67834    0.29987
ATOM H29     0.86823   -0.62710    0.43900
END

TITL Gavezzotti Compound V first structure
SPACEGROUP P212121
CELL   11.8582    7.0154   13.1776   90.0000   90.0000   90.0000
ATOM    C1   -0.2103    0.0631   -0.1481
ATOM    C2   -0.1445   -0.0886   -0.2025
ATOM    S3   -0.0398   -0.1578   -0.1102
ATOM    O4    0.0658   -0.0671   -0.1296
ATOM    O5   -0.0389   -0.3597   -0.0952
ATOM    N6   -0.0988   -0.0574   -0.0078
ATOM    C7   -0.1813    0.0441   -0.0375
ATOM    C8   -0.2678    0.1537    0.0219
ATOM   BR9   -0.1977    0.3652    0.0879
ATOM   C10   -0.3443    0.2258   -0.0642
ATOM   C11   -0.2785    0.3846   -0.1186
ATOM   C12   -0.1857    0.2760   -0.1736
ATOM   C13   -0.3417    0.0595   -0.1414
ATOM   C14   -0.3978    0.0995   -0.2436
ATOM   C15   -0.3878   -0.1285   -0.1004
ATOM   H16   -0.1990   -0.2085   -0.2179
ATOM   H17   -0.1029   -0.0263   -0.2675
ATOM   H18   -0.3147    0.0577    0.0702
ATOM   H19   -0.4278    0.2663   -0.0401
ATOM   H20   -0.3327    0.4522   -0.1735
ATOM   H21   -0.2411    0.4776   -0.0625
ATOM   H22   -0.1951    0.2974   -0.2543
ATOM   H23   -0.1051    0.3152   -0.1416
ATOM   H24   -0.4881    0.1097   -0.2335
ATOM   H25   -0.3660    0.2323   -0.2740
ATOM   H26   -0.3788   -0.0149   -0.2958
ATOM   H27   -0.4782   -0.1171   -0.0908
ATOM   H28   -0.3492   -0.1591   -0.0281
ATOM   H29   -0.3691   -0.2418   -0.1532
ENERGY -110.0 kJ/mol
COMMENT Plausible under all crystal stability criteria
COMMENT Energy ordering irrelevant, 14 structures within 2 kJ/mol
COMMENT If science is not wishful thinking, zero confidence level

TITL   Gavezzotti Compound V second structure
SPACEGROUP P21
CELL    6.9771   12.0004    7.4216   90.0000  116.1241   90.0000
ATOM    C1    0.2110   -0.0023    0.3017
ATOM    C2    0.2757    0.0799    0.4713
ATOM    S3    0.0354    0.1595    0.4073
ATOM    O4   -0.0777    0.1216    0.5161
ATOM    O5    0.0750    0.2766    0.4097
ATOM    N6   -0.0979    0.1195    0.1675
ATOM    C7    0.0074    0.0413    0.1365
ATOM    C8   -0.0294   -0.0196   -0.0524
ATOM   BR9   -0.2798   -0.1095   -0.1377
ATOM   C10    0.1698   -0.0944    0.0237
ATOM   C11    0.1347   -0.1863    0.1505
ATOM   C12    0.1571   -0.1239    0.3372
ATOM   C13    0.3446   -0.0205    0.1821
ATOM   C14    0.5576   -0.0781    0.3073
ATOM   C15    0.3892    0.0874    0.0982
ATOM   H16    0.3983    0.1339    0.4689
ATOM   H17    0.3151    0.0354    0.6097
ATOM   H18   -0.0254    0.0387   -0.1620
ATOM   H19    0.2087   -0.1250   -0.0928
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ATOM   H20    0.2610   -0.2471    0.1919
ATOM   H21   -0.0263   -0.2180    0.0719
ATOM   H22    0.2905   -0.1579    0.4666
ATOM   H23    0.0051   -0.1243    0.3432
ATOM   H24    0.6361   -0.0964    0.2137
ATOM   H25    0.5294   -0.1551    0.3680
ATOM   H26    0.6578   -0.0241    0.4287
ATOM   H27    0.4686    0.0684    0.0056
ATOM   H28    0.2404    0.1297    0.0093
ATOM   H29    0.4901    0.1407    0.2207
ENERGY -109.3 kJ/mol
COMMENT See comments to first structure

TITL Gavezzotti Compound V third structure
SPACEGROUP P212121
CELL   11.7203    9.3684   10.0578   90.0000   90.0000   90.0000
ATOM    C1    0.2910    0.2176    0.1912
ATOM    C2    0.3916    0.1234    0.2210
ATOM    S3    0.4834    0.2380    0.3172
ATOM    O4    0.5721    0.2977    0.2369
ATOM    O5    0.5167    0.1717    0.4395
ATOM    N6    0.3885    0.3660    0.3528
ATOM    C7    0.2984    0.3418    0.2858
ATOM    C8    0.1848    0.4154    0.2858
ATOM   BR9    0.2004    0.6027    0.2127
ATOM   C10    0.1179    0.3202    0.1887
ATOM   C11    0.1637    0.3538    0.0491
ATOM   C12    0.2824    0.2876    0.0510
ATOM   C13    0.1656    0.1692    0.2176
ATOM   C14    0.1269    0.0520    0.1223
ATOM   C15    0.1460    0.1176    0.3596
ATOM   H16    0.3640    0.0351    0.2821
ATOM   H17    0.4338    0.0957    0.1291
ATOM   H18    0.1472    0.4091    0.3836
ATOM   H19    0.0263    0.3288    0.1979
ATOM   H20    0.1119    0.2994   -0.0239
ATOM   H21    0.1713    0.4678    0.0375
ATOM   H22    0.2867    0.2051   -0.0238
ATOM   H23    0.3452    0.3716    0.0434
ATOM   H24    0.0374    0.0300    0.1377
ATOM   H25    0.1401    0.0866    0.0209
ATOM   H26    0.1757   -0.0438    0.1404
ATOM   H27    0.0564    0.0954    0.3743
ATOM   H28    0.1730    0.1993    0.4287
ATOM   H29    0.1950    0.0217    0.3766
ENERGY -109.9 kJ/mol
COMMENT See comments to first structure

TITL Hofmann V 1
SPACEGROUP P-1
CELL      6.874   9.962   8.441  95.459  80.576 100.305
ATOM C1    0.04175  -0.15800   0.13489
ATOM C2    0.00917  -0.09641   0.31110
ATOM C3   -0.21492  -0.15323   0.37029
ATOM C4   -0.34635  -0.07894   0.28422
ATOM C5   -0.30431  -0.14307   0.11717
ATOM C6   -0.16479  -0.24519   0.11821
ATOM C7   -0.23985  -0.29955   0.28621
ATOM C8   -0.45861  -0.37776   0.31034
ATOM C9   -0.11162  -0.39491   0.34064
ATOM C10  -0.17241  -0.34529  -0.03136
ATOM S11  -0.34575  -0.28114  -0.13086
ATOM N12  -0.41463  -0.14903   0.00674
ATOM O13  -0.26907  -0.21050  -0.28979
ATOM O14  -0.54738  -0.37322  -0.15180
ATOM Br15 -0.28232   0.12014   0.29634
ATOM H16   0.08179  -0.07654   0.04732
ATOM H17   0.16213  -0.22162   0.11472
ATOM H18   0.10812  -0.13040   0.38562
ATOM H19   0.04338   0.01739   0.31871
ATOM H20  -0.25623  -0.14876   0.50347
ATOM H21  -0.50722  -0.10707   0.33295
ATOM H22  -0.46567  -0.48481   0.25798
ATOM H23  -0.51770  -0.38107   0.44073
ATOM H24  -0.56387  -0.33417   0.25148
ATOM H25  -0.12884  -0.49500   0.26986
ATOM H26   0.05049  -0.35527   0.32634
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ATOM H27  -0.16165  -0.41362   0.46975
ATOM H28  -0.02594  -0.33888  -0.11066
ATOM H29  -0.23225  -0.45212  -0.00123
ENERGY   -105.73
COMMENT d=1.734g/cc.

TITL Hofmann V 2
SPACEGROUP P21/c
CELL   10.876   9.285  15.602    90.000  49.937  90.000
ATOM C1   -0.28059  -0.17633   0.37700
ATOM C2   -0.42310  -0.13320   0.38227
ATOM C3   -0.37148  -0.19273   0.26979
ATOM C4   -0.23036  -0.09732   0.17234
ATOM C5   -0.10064  -0.14475   0.17431
ATOM C6   -0.16934  -0.25867   0.26465
ATOM C7   -0.28637  -0.33588   0.25586
ATOM C8   -0.20600  -0.41365   0.14258
ATOM C9   -0.39778  -0.44932   0.34818
ATOM C10  -0.03252  -0.34469   0.24479
ATOM S11   0.14037  -0.25663   0.12207
ATOM N12   0.05109  -0.13208   0.09286
ATOM O13   0.24871  -0.16342   0.13170
ATOM O14   0.25305  -0.34378   0.01230
ATOM Br15 -0.26814   0.10990   0.19105
ATOM H16  -0.21911  -0.07975   0.37677
ATOM H17  -0.32044  -0.24583   0.44889
ATOM H18  -0.53774  -0.18305   0.45509
ATOM H19  -0.44419  -0.01474   0.39172
ATOM H20  -0.47203  -0.20416   0.26845
ATOM H21  -0.19872  -0.12746   0.09138
ATOM H22  -0.15727  -0.52003   0.14036
ATOM H23  -0.29576  -0.43226   0.13137
ATOM H24  -0.10235  -0.35546   0.06786
ATOM H25  -0.32751  -0.54546   0.33629
ATOM H26  -0.46089  -0.41160   0.43458
ATOM H27  -0.49093  -0.48445   0.34348
ATOM H28  -0.03015  -0.33298   0.31446
ATOM H29  -0.03325  -0.45979   0.22642
ENERGY   -104.60
COMMENT d=1.610g/cc.

TITL Hofmann V 3
SPACEGROUP P21/c
CELL      10.718   9.285  16.000  90.000  49.226  90.000
ATOM C1   -0.28690  -0.12907   0.36435
ATOM C2   -0.42307  -0.08594   0.36070
ATOM C3   -0.35591  -0.14547   0.24677
ATOM C4   -0.20620  -0.05005   0.15426
ATOM C5   -0.08335  -0.09748   0.16465
ATOM C6   -0.16315  -0.21141   0.25439
ATOM C7   -0.27284  -0.28861   0.23772
ATOM C8   -0.17827  -0.36639   0.12481
ATOM C9   -0.39352  -0.40205   0.32679
ATOM C10  -0.03004  -0.29742   0.24248
ATOM S11   0.15391  -0.20936   0.12567
ATOM N12   0.07385  -0.08482   0.08949
ATOM O13   0.25523  -0.11615   0.14267
ATOM O14   0.27860  -0.29651   0.01849
ATOM Br15 -0.24509   0.15717   0.17134
ATOM H16  -0.22849  -0.03248   0.36806
ATOM H17  -0.33633  -0.19857   0.43672
ATOM H18  -0.54365  -0.13578   0.42924
ATOM H19  -0.44461   0.03252   0.36919
ATOM H20  -0.45116  -0.15689   0.23892
ATOM H21  -0.16310  -0.08019   0.07191
ATOM H22  -0.13164  -0.47276   0.12562
ATOM H23  -0.26168  -0.38500   0.10736
ATOM H24  -0.06780  -0.30820   0.05358
ATOM H25  -0.32488  -0.49819   0.3189
ATOM H26  -0.46738  -0.36433   0.41279
ATOM H27  -0.48121  -0.43719   0.31591
ATOM H28  -0.03902  -0.28571   0.31525
ATOM H29  -0.02777  -0.41252   0.22329
ENERGY   -101.39
COMMENT d=1.610g/cc.

TITL Leusen V 1
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SPACEGROUP  P212121
CELL    7.336 12.110 13.343 90.000 90.000 90.000
ATOM  C1     0.79054   0.76005   0.07866
ATOM  C2     0.84135   0.71322   0.18476
ATOM  C3     0.75645   0.80108   0.25825
ATOM  C4     0.87205   0.90509   0.24778
ATOM  C5     0.82514   0.96048   0.14952
ATOM  C6     0.68692   0.87153   0.10634
ATOM  C7     0.57262   0.83531   0.20603
ATOM  C8     0.46117   0.93025   0.25385
ATOM  C9     0.42901   0.74419   0.18890
ATOM C10     0.76544   0.77133   0.36802
ATOM S11     0.97279   0.83780   0.40655
ATOM N12     0.98270   0.93502   0.31515
ATOM Br13    1.03560   0.98235   0.06413
ATOM O14     0.96088   0.89090   0.51494
ATOM O15     1.14120   0.75600   0.39882
ATOM H16     0.91161   0.77354   0.03131
ATOM H17     0.70024   0.70288   0.03759
ATOM H18     0.77997   0.63077   0.19629
ATOM H19     0.99034   0.70369   0.19450
ATOM H20     0.75870   1.04128   0.16103
ATOM H21     0.60161   0.90298   0.04460
ATOM H22     0.54137   1.00246   0.27744
ATOM H23     0.35642   0.96173   0.20150
ATOM H24     0.38887   0.90262   0.32216
ATOM H25     0.47757   0.67107   0.14786
ATOM H26     0.37547   0.71288   0.26091
ATOM H27     0.31105   0.77546   0.14576
ATOM H28     0.65234   0.80687   0.41178
ATOM H29     0.76829   0.68210   0.38357
ENERGY  8.96 kcal/mol asymmetric unit
DENSITY 1.637 g/(cm^3)
COMMENT Lowest energy structure according to CVFF950 force field.
COMMENT Good sampling and good energy separation.
COMMENT Confidence level: high.

TITL Leusen V 2
SPACEGROUP  P212121
CELL   12.391  6.924 13.628 90.000 90.000 90.000
ATOM  C1     0.77544   0.40200   0.62850
ATOM  C2     0.68884   0.27839   0.68451
ATOM  C3     0.71538   0.06539   0.65106
ATOM  C4     0.68049   0.05089   0.54409
ATOM  C5     0.76045   0.15996   0.48160
ATOM  C6     0.83621   0.24268   0.56546
ATOM  C7     0.84176   0.06257   0.64331
ATOM  C8     0.89739  -0.11861   0.60032
ATOM  C9     0.90712   0.10356   0.73750
ATOM C10     0.65196  -0.08929   0.70370
ATOM S11     0.53897  -0.12158   0.62305
ATOM N12     0.59745  -0.04227   0.51818
ATOM Br13    0.69185   0.36085   0.40466
ATOM O14     0.49997  -0.33953   0.61708
ATOM O15     0.44371   0.02032   0.65247
ATOM H16     0.73915   0.51763   0.58346
ATOM H17     0.83189   0.47080   0.68067
ATOM H18     0.69829   0.29493   0.76480
ATOM H19     0.60546   0.32253   0.66589
ATOM H20     0.80492   0.06293   0.43178
ATOM H21     0.91576   0.29058   0.53849
ATOM H22     0.85861  -0.18164   0.53494
ATOM H23     0.98173  -0.08686   0.57905
ATOM H24     0.90094  -0.23689   0.65439
ATOM H25     0.88064   0.22917   0.78091
ATOM H26     0.90445  -0.01989   0.78895
ATOM H27     0.99300   0.12987   0.72014
ATOM H28     0.69516  -0.22784   0.70956
ATOM H29     0.62478  -0.04992   0.77777
ENERGY  9.13 kcal/mol asymmetric unit
DENSITY 1.660 g/(cm^3)
COMMENT Second lowest energy structure according to CVFF950 force field.
COMMENT Good sampling and good energy separation.
COMMENT Confidence level: high.

TITL Leusen V 3
SPACEGROUP  P21
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CELL    7.158 10.485  8.247 90.000 76.096 90.000
ATOM  C1    -0.04270   0.13263   0.24450
ATOM  C2     0.03912   0.14802   0.40413
ATOM  C3     0.26040   0.11805   0.33670
ATOM  C4     0.27625  -0.02473   0.30081
ATOM  C5     0.20554  -0.05132   0.14607
ATOM  C6     0.14234   0.08813   0.10836
ATOM  C7     0.31059   0.17636   0.15537
ATOM  C8     0.51400   0.15201   0.04228
ATOM  C9     0.28261   0.32114   0.13768
ATOM C10     0.38268   0.14304   0.45948
ATOM S11     0.41758  -0.01373   0.53474
ATOM N12     0.34737  -0.10155   0.38774
ATOM Br13   -0.00361  -0.17290   0.18746
ATOM O14     0.63660  -0.03990   0.53031
ATOM O15     0.28480  -0.04199   0.71496
ATOM H16    -0.16228   0.06364   0.26226
ATOM H17    -0.09679   0.22457   0.20829
ATOM H18     0.01631   0.24635   0.45371
ATOM H19    -0.03174   0.08296   0.50611
ATOM H20     0.32112  -0.08725   0.04272
ATOM H21     0.12777   0.10031  -0.02079
ATOM H22     0.56614   0.05317   0.04083
ATOM H23     0.52059   0.17712  -0.08938
ATOM H24     0.62412   0.20982   0.08215
ATOM H25     0.14574   0.36030   0.21189
ATOM H26     0.39587   0.37615   0.17666
ATOM H27     0.28910   0.34720   0.00657
ATOM H28     0.52495   0.18337   0.40077
ATOM H29     0.31574   0.20675   0.56337
ENERGY  9.78 kcal/mol asymmetric unit
DENSITY 1.615 g/(cm^3)
COMMENT Third lowest energy structure according to CVFF950 force field.
COMMENT Good sampling; this structure is considerably higher in energy
COMMENT than the first two; unlikely to be stable.

TITL  LOMMERSE IV-1
SPACEGROUP P21
CELL    7.711   10.744    8.160   90.000   97.706   90.000
ATOM    C1    0.23340   -0.15228    0.09700
ATOM    C2    0.36740   -0.08012    0.22072
ATOM    C3    0.25223    0.01822    0.29512
ATOM    C4    0.19941    0.10937    0.15477
ATOM    C5    0.06578    0.04626    0.03150
ATOM    C6    0.05916   -0.08442    0.10892
ATOM    C7    0.07439   -0.05157    0.29802
ATOM    C8    0.08583   -0.16601    0.41126
ATOM    C9   -0.07342    0.03179    0.34506
ATOM   C10    0.33908    0.09190    0.44167
ATOM    N1    0.25497    0.21972    0.15354
ATOM   Br1    0.11788    0.05328   -0.19892
ATOM    S1    0.40041    0.24266    0.34740
ATOM    O1    0.33043    0.36016    0.45047
ATOM    O2    0.60668    0.23341    0.31379
ATOM    H1    0.26716   -0.15066   -0.02665
ATOM    H2    0.22449   -0.24867    0.13160
ATOM    H3    0.43081   -0.13950    0.31738
ATOM    H4    0.46904   -0.03619    0.16224
ATOM    H5   -0.05706    0.09407    0.02409
ATOM    H6   -0.05607   -0.13604    0.06042
ATOM    H7   -0.03796   -0.21499    0.39490
ATOM    H8    0.18612   -0.23124    0.38927
ATOM    H9    0.11120   -0.13753    0.53954
ATOM   H10   -0.19859   -0.01312    0.31044
ATOM   H11   -0.05826    0.04609    0.47742
ATOM   H12   -0.07952    0.12278    0.28845
ATOM   H13    0.25320    0.11923    0.52861
ATOM   H14    0.45963    0.05339    0.50127
COMM [2] [010126222072] P21  -39.984    0.000
COMM Ranked 2nd, with N..H contact
END

TITL  LOMMERSE IV-2
SPACEGROUP P212121
CELL    9.486   11.243   11.584   90.000   90.000   90.000
ATOM    C1    0.16664    0.36956    0.35596
ATOM    C2    0.12888    0.24617    0.30449
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ATOM    C3    0.26423    0.21139    0.23671
ATOM    C4    0.26666    0.29519    0.13372
ATOM    C5    0.30611    0.41657    0.17713
ATOM    C6    0.31578    0.39384    0.30828
ATOM    C7    0.38533    0.26698    0.31106
ATOM    C8    0.39875    0.21459    0.43279
ATOM    C9    0.53149    0.26007    0.25397
ATOM   C10    0.27122    0.08548    0.19088
ATOM    N1    0.24619    0.26207    0.03107
ATOM   Br1    0.17753    0.54488    0.12709
ATOM    S1    0.21773    0.10124    0.03531
ATOM    O1    0.33418    0.03387   -0.04749
ATOM    O2    0.04754    0.07175    0.02461
ATOM    H1    0.09286    0.43732    0.33066
ATOM    H2    0.16794    0.36774    0.44900
ATOM    H3    0.10755    0.18103    0.37067
ATOM    H4    0.03808    0.24886    0.24840
ATOM    H5    0.40502    0.44349    0.14077
ATOM    H6    0.37314    0.46221    0.35335
ATOM    H7    0.47572    0.26473    0.48167
ATOM    H8    0.30177    0.21470    0.48103
ATOM    H9    0.43583    0.12363    0.42817
ATOM   H10    0.60312    0.32114    0.29609
ATOM   H11    0.57507    0.17170    0.26342
ATOM   H12    0.53175    0.28027    0.16286
ATOM   H13    0.37545    0.04835    0.18708
ATOM   H14    0.19643    0.02514    0.22821
COMM [14] [010314206685] P212121  -37.493    0.000
COMM Ranked 14th, P212121 seems less popular
END

TITL LOMMERSE IV-3
SPACEGROUP P21
CELL    7.481    9.233    9.095   90.000   97.139   90.000
ATOM    C1    0.54376    0.05040    0.21100
ATOM    C2    0.50395    0.00576    0.36820
ATOM    C3    0.29540   -0.00988    0.34940
ATOM    C4    0.22525    0.14432    0.32940
ATOM    C5    0.25569    0.19356    0.17711
ATOM    C6    0.35470    0.06137    0.12201
ATOM    C7    0.25092   -0.06706    0.18687
ATOM    C8    0.32972   -0.21669    0.16002
ATOM    C9    0.04819   -0.07259    0.13164
ATOM   C10    0.21370   -0.07602    0.47793
ATOM    N1    0.14722    0.21059    0.42459
ATOM   Br1    0.37924    0.38238    0.17256
ATOM    S1    0.13655    0.08547    0.57917
ATOM    O1   -0.07457    0.06217    0.60820
ATOM    O2    0.29465    0.12638    0.71638
ATOM    H1    0.61606    0.15111    0.21167
ATOM    H2    0.62361   -0.02990    0.16301
ATOM    H3    0.56634   -0.09601    0.40314
ATOM    H4    0.54907    0.08504    0.45187
ATOM    H5    0.12909    0.21362    0.11122
ATOM    H6    0.35372    0.06019    0.00352
ATOM    H7    0.30691   -0.24235    0.04306
ATOM    H8    0.47212   -0.22541    0.19511
ATOM    H9    0.26268   -0.29901    0.21796
ATOM   H10    0.02791   -0.08190    0.01211
ATOM   H11   -0.01248   -0.16678    0.17592
ATOM   H12   -0.02659    0.02055    0.16176
ATOM   H13    0.09279   -0.13728    0.44702
ATOM   H14    0.30720   -0.13203    0.55716
COMM [XX] [010122215223] P21  -34.339    0.000
COMM Derived/optimised from ROLBOJ.
END

TITL Mooy-V-1
SPACEGROUP  P212121
CELL   13.144  7.228 11.939 90.000 90.000 90.000
ATOM  C1     0.41762   0.16891   0.76436
ATOM  C2     0.31132   0.11966   0.71814
ATOM  C3     0.24096   0.20079   0.81036
ATOM  C4     0.25566   0.08392   0.90761
ATOM  C5     0.35173   0.12108   0.96123
ATOM  C6     0.39142   0.26828   0.87640
ATOM  C7     0.29410   0.38242   0.84826
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ATOM  C8     0.12612   0.19946   0.78416
ATOM  S9     0.08938  -0.01516   0.84844
ATOM N10     0.18529  -0.02855   0.93609
ATOM C11     0.24322   0.48309   0.94965
ATOM C12     0.30774   0.53281   0.75596
ATOM B13     0.43655  -0.09535   0.97869
ATOM O14    -0.01551  -0.00767   0.91412
ATOM O15     0.09757  -0.18263   0.76279
ATOM H16     0.45793   0.26032   0.70719
ATOM H17     0.46334   0.04547   0.77752
ATOM H18     0.29834   0.18655   0.63747
ATOM H19     0.30207  -0.02978   0.70878
ATOM H20     0.34030   0.18240   1.04365
ATOM H21     0.45441   0.35037   0.90869
ATOM H22     0.11015   0.19965   0.69475
ATOM H23     0.08668   0.31337   0.82529
ATOM H24     0.21747   0.38701   1.01383
ATOM H25     0.29732   0.57864   0.98747
ATOM H26     0.17714   0.56149   0.92157
ATOM H27     0.23326   0.57920   0.72744
ATOM H28     0.34962   0.48302   0.68346
ATOM H29     0.34881   0.65082   0.79039
ENERGY  37.94 kcal/mol
COMMENT Density 1.31 g/cc
COMMENT Lowest-energy structure in Dreiding+Multipole force field
COMMENT First three structures span 1 kcal/mol in energy, increasing the
COMMENT confidence in the prediction for this compound
COMMENT Confidence (1-3) : 3

TITL Mooy-V-2
SPACEGROUP  P21
CELL    7.096 10.549  8.545 90.000 112.826 90.000
ATOM  C1     0.09045  -0.10802   0.58952
ATOM  C2     0.23434  -0.16101   0.76348
ATOM  C3     0.21683  -0.05911   0.88860
ATOM  C4     0.32132   0.05240   0.86444
ATOM  C5     0.21031   0.11143   0.70339
ATOM  C6     0.02334   0.02005   0.64130
ATOM  C7    -0.00907  -0.01334   0.80692
ATOM  C8     0.31591  -0.09493   1.07856
ATOM  S9     0.54248   0.00161   1.15187
ATOM N10     0.48345   0.09206   0.98365
ATOM C11    -0.06599   0.10244   0.89382
ATOM C12    -0.17569  -0.11580   0.78662
ATOM B13     0.36270   0.12259   0.55939
ATOM O14     0.55853   0.08748   1.30901
ATOM O15     0.74576  -0.07458   1.17814
ATOM H16    -0.04118  -0.16977   0.53065
ATOM H17     0.16858  -0.09610   0.50291
ATOM H18     0.18071  -0.25333   0.78655
ATOM H19     0.39070  -0.17015   0.77051
ATOM H20     0.16357   0.20646   0.72242
ATOM H21    -0.11024   0.06121   0.54182
ATOM H22     0.35741  -0.19477   1.09691
ATOM H23     0.21881  -0.06982   1.14631
ATOM H24     0.04484   0.17916   0.92238
ATOM H25    -0.21406   0.13911   0.80953
ATOM H26    -0.07605   0.07335   1.01271
ATOM H27    -0.18916  -0.13155   0.90785
ATOM H28    -0.14257  -0.20673   0.74295
ATOM H29    -0.32266  -0.08281   0.69501
ENERGY  38.60 kcal/mol
COMMENT Density 1.26 g/cc
COMMENT 2nd-lowest energy structure in Dreiding+Multipole force field

TITL Mooy-V-3
SPACEGROUP  P212121
CELL   10.746  9.982 10.848 90.000 90.000 90.000
ATOM  C1     0.20320   0.59055   0.43236
ATOM  C2     0.19207   0.53767   0.56595
ATOM  C3     0.06159   0.47032   0.56368
ATOM  C4    -0.02716   0.57916   0.55860
ATOM  C5    -0.02626   0.64289   0.43988
ATOM  C6     0.07421   0.55316   0.37728
ATOM  C7     0.04832   0.41117   0.43159
ATOM  C8     0.02766   0.38439   0.67682
ATOM  S9    -0.07080   0.49602   0.76230
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ATOM N10    -0.09775   0.60301   0.65073
ATOM C11    -0.08209   0.35111   0.39890
ATOM C12     0.14489   0.30069   0.39660
ATOM B13     0.01164   0.83173   0.44824
ATOM O14    -0.19594   0.42380   0.80216
ATOM O15     0.00116   0.56721   0.87214
ATOM H16     0.27784   0.53931   0.38360
ATOM H17     0.22094   0.69810   0.43003
ATOM H18     0.26553   0.46533   0.58579
ATOM H19     0.19682   0.61971   0.63260
ATOM H20    -0.11591   0.63043   0.39527
ATOM H21     0.07161   0.55759   0.27678
ATOM H22     0.10835   0.35310   0.73024
ATOM H23    -0.02705   0.29767   0.65011
ATOM H24    -0.15868   0.41118   0.43442
ATOM H25    -0.09216   0.34442   0.29919
ATOM H26    -0.09101   0.25078   0.43756
ATOM H27     0.12608   0.20939   0.44861
ATOM H28     0.24046   0.33002   0.41531
ATOM H29     0.13761   0.27818   0.29863
ENERGY  38.93 kcal/mol
COMMENT Density 1.27 g/cc
COMMENT 3rd-lowest energy structure in Dreiding+Multipole force field

TITL Motherwell V 1
SPACEGROUP P212121
CELL       7.955   8.485  16.424  90.000  90.000  90.000
ATOM S1         0.22749  -0.07362   0.57650
ATOM O1         0.06945  -0.05910   0.61717
ATOM O2         0.36235  -0.14485   0.62092
ATOM N1         0.29074   0.10560   0.54652
ATOM C1         0.27466   0.11334   0.46953
ATOM C2         0.32289   0.24061   0.41052
ATOM C3         0.27793   0.16124   0.32924
ATOM C4         0.32099  -0.01406   0.34473
ATOM C5         0.08512   0.16133   0.32372
ATOM C6         0.03417   0.04001   0.38737
ATOM C7         0.20474  -0.02220   0.42117
ATOM C8         0.20316  -0.16196   0.47738
ATOM C9         0.26686  -0.12888   0.27799
ATOM C10        0.50568  -0.04459   0.36442
ATOM H3         0.33334   0.22179   0.27777
ATOM H4         0.02523   0.27373   0.33534
ATOM H5         0.04937   0.11868   0.26404
ATOM H6        -0.04371   0.08323   0.43663
ATOM H7        -0.02938  -0.06247   0.36293
ATOM H8         0.30976  -0.23543   0.46183
ATOM H9         0.08229  -0.22069   0.47742
ATOM H10        0.14282  -0.10920   0.25279
ATOM H11        0.28399  -0.24764   0.30069
ATOM H12        0.33792  -0.09200   0.22507
ATOM H13        0.52996  -0.16725   0.37835
ATOM H14        0.58349  -0.02325   0.31144
ATOM H15        0.55729   0.02689   0.41299
ATOM Br1        0.19278   0.43120   0.42787
ATOM H1C2       0.45231   0.27914   0.41517
ENERGY -54.4 kcal/mole
COMMENT  Global lowest E. Global Lowest Volume.
COMMENT  Reasonable atom contacts, but perhaps too closely
COMMENT  packed. Br shows two O contacts at 3.2, not seen in SO2...Br in CSD.
COMMENT  E(HH) reasonably low.
COOMENT  Not the best contact-score function.
COMMENT  ID=171329

TITL Motherwell V 2
SPACEGROUP P212121
CELL       7.602  14.106  10.353  90.000  90.000  90.000
ATOM S1         0.24644  -0.15954   0.13847
ATOM O1         0.29324  -0.19329   0.26399
ATOM O2         0.28992  -0.21860   0.03067
ATOM N1         0.34045  -0.05349   0.11496
ATOM C1         0.22037   0.00925   0.12019
ATOM C2         0.22755   0.11421   0.09706
ATOM C3         0.03202   0.14024   0.11034
ATOM C4        -0.06300   0.05289   0.05284
ATOM C5        -0.01165   0.13435   0.25503
ATOM C6        -0.00762   0.02825   0.28160
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ATOM C7         0.03196  -0.01662   0.14717
ATOM C8         0.01966  -0.12245   0.13297
ATOM C9        -0.26278   0.05138   0.06915
ATOM C10       -0.02033   0.03380  -0.08888
ATOM H3         0.00401   0.21018   0.07243
ATOM H4         0.07778   0.17181   0.31847
ATOM H5        -0.14437   0.16023   0.26922
ATOM H6         0.08829   0.00474   0.35201
ATOM H7        -0.13267  -0.00135   0.31131
ATOM H8        -0.03927  -0.13713   0.03986
ATOM H9        -0.04490  -0.15487   0.21509
ATOM H10       -0.31113   0.07319   0.16295
ATOM H11       -0.30987  -0.01797   0.04054
ATOM H12       -0.30749   0.11282   0.01569
ATOM H13       -0.08294  -0.03005  -0.12439
ATOM H14       -0.07521   0.08877  -0.14980
ATOM H15        0.11850   0.03020  -0.11180
ATOM Br1        0.37029   0.17805   0.22590
ATOM H1C2       0.28646   0.13449   0.00591
ENERGY -52.6 kcal/mole
COMMENT Ranked 2 in energy globally. Good contact-score functions.
COMMENT Low volume, almost global lowest.
COMMENT Good Br...O contact, as often seen in CSD.
COMMENT ID=165306

TITL Motherwell V 3
SPACEGROUP P21
CELL       8.804  10.919   8.224  90.000  46.673  90.000
ATOM S1         0.13098   0.07039   0.53388
ATOM O1        -0.03170   0.00102   0.72863
ATOM O2         0.23239   0.16149   0.55647
ATOM N1         0.03490   0.13945   0.43857
ATOM C1         0.10857   0.08519   0.26010
ATOM C2         0.08718   0.11355   0.09801
ATOM C3         0.23110   0.01552  -0.08149
ATOM C4         0.40823   0.00453  -0.08447
ATOM C5         0.11493  -0.10704   0.01942
ATOM C6         0.12338  -0.13270   0.19501
ATOM C7         0.25143  -0.02350   0.17118
ATOM C8         0.31779  -0.02804   0.29763
ATOM C9         0.56307  -0.09990  -0.22599
ATOM C10        0.53162   0.12246  -0.14849
ATOM H3         0.26933   0.03500  -0.23522
ATOM H4        -0.04473  -0.10699   0.09329
ATOM H5         0.20388  -0.17654  -0.10940
ATOM H6        -0.02603  -0.13962   0.36576
ATOM H7         0.21023  -0.21418   0.16383
ATOM H8         0.47449   0.00885   0.18980
ATOM H9         0.29718  -0.11851   0.36431
ATOM H10        0.49518  -0.18654  -0.21240
ATOM H11        0.66094  -0.10745  -0.19094
ATOM H12        0.63566  -0.07796  -0.39463
ATOM H13        0.64818   0.11302  -0.13952
ATOM H14        0.62348   0.14439  -0.32264
ATOM H15        0.43829   0.20279  -0.05379
ATOM Br1       -0.19892   0.09457   0.23445
ATOM H1C2       0.12703   0.20673   0.03598
ENERGY -52.4 kcal/mole
COMMENT Lowest energy in P21 - rank 3 globally. Lowest Volume in P21.
COMMENT Reasonable contacts, but not best score function value.
COMMENT No Br...O close contacts.
COMMENT ID=165806

TITL PRICE V 1
SPACEGROUP P212121
CELL   16.222716   10.413043    7.177183   90.000000   90.000000   90.000000
ATOM  S1      0.943065      0.719405      0.242668
ATOM  O1      0.946974      0.631562      0.090042
ATOM  O2      0.869573      0.790736      0.276540
ATOM  N1      1.022748      0.822407      0.225920
ATOM  C1      1.077264      0.789474      0.339707
ATOM  C2      1.157527      0.854245      0.389556
ATOM  C3      1.190179      0.762299      0.541573
ATOM  C4      1.108780      0.726760      0.647219
ATOM  C5      1.214671      0.633792      0.450515
ATOM  C6      1.130566      0.574233      0.394365
ATOM  C7      1.067333      0.674142      0.466623
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ATOM  C8      0.976440      0.639747      0.453524
ATOM  C9      1.120816      0.626594      0.801643
ATOM  C10     1.063749      0.841740      0.735390
ATOM  Br1     1.229295      0.883351      0.176834
ATOM  H1      1.145742      0.949238      0.442602
ATOM  H2      1.237970      0.805394      0.626235
ATOM  H3      1.254942      0.647537      0.332466
ATOM  H4      1.247292      0.573784      0.548994
ATOM  H5      1.124677      0.559784      0.245462
ATOM  H6      1.120153      0.482085      0.460339
ATOM  H7      0.940162      0.679230      0.566178
ATOM  H8      0.963888      0.538389      0.438365
ATOM  H9      1.152251      0.540564      0.756689
ATOM  H10     1.061492      0.597973      0.857969
ATOM  H11     1.156224      0.667970      0.915117
ATOM  H12     1.009974      0.809294      0.811825
ATOM  H13     1.103944      0.889675      0.834332
ATOM  H14     1.042567      0.913043      0.636519
ENERGY AQ26 -110.1 kJ/mol
COMMENT Global minumum in search by 1.7 kJ/mol
COMMENT This should be the observed structure on
COMMENT lattice energy assumption, unless there is
COMMENT a problem with my search or potential.

TITL PRICE V 2
SPACEGROUP P21
CELL    7.218408   10.703313    8.628916   90.000000   67.553694   90.000000
ATOM  S1      0.072110      0.966357      0.852437
ATOM  O1      0.221125      0.879426      0.854883
ATOM  O2      0.105626      1.040964      0.707337
ATOM  N1      0.014430      1.060919      1.020343
ATOM  C1     -0.148855      1.026184      1.129490
ATOM  C2     -0.273041      1.084125      1.296485
ATOM  C3     -0.453730      0.993854      1.357857
ATOM  C4     -0.483502      0.965732      1.190630
ATOM  C5     -0.384653      0.866535      1.399884
ATOM  C6     -0.250688      0.813867      1.225366
ATOM  C7     -0.265075      0.915866      1.102879
ATOM  C8     -0.167912      0.888497      0.916138
ATOM  C9     -0.647490      0.868898      1.209617
ATOM  C10    -0.530643      1.081288      1.106051
ATOM  Br1    -0.127752      1.105719      1.443496
ATOM  H1     -0.315738      1.177690      1.278213
ATOM  H2     -0.582425      1.033219      1.457693
ATOM  H3     -0.304424      0.876147      1.482242
ATOM  H4     -0.512284      0.806842      1.462919
ATOM  H5     -0.096935      0.798951      1.212188
ATOM  H6     -0.306013      0.725585      1.198998
ATOM  H7     -0.246895      0.930284      0.845015
ATOM  H8     -0.140429      0.790713      0.884673
ATOM  H9     -0.631059      0.782772      1.268363
ATOM  H10    -0.648599      0.845593      1.087550
ATOM  H11    -0.793433      0.907678      1.284261
ATOM  H12    -0.556852      1.054043      0.995066
ATOM  H13    -0.666595      1.125993      1.190766
ATOM  H14    -0.413270      1.151167      1.066921
ENERGY AH3 -108.4 kJ/mol
COMMENT Second lowest energy, but very easily found in search
COMMENT from a range structures. Hence may be favoured by topology
COMMENT of potential energy surface.

TITL PRICE V 3
SPACEGROUP P212121
CELL   10.859691   12.906902    8.562079   90.000000   90.000000   90.000000
ATOM  S1      0.897032      0.719946      0.884391
ATOM  O1      0.984404      0.789716      0.817354
ATOM  O2      0.827711      0.652181      0.786624
ATOM  N1      0.798922      0.788332      0.996547
ATOM  C1      0.828304      0.776424      1.136768
ATOM  C2      0.765447      0.814386      1.283218
ATOM  C3      0.850513      0.767896      1.409788
ATOM  C4      0.882120      0.659641      1.337220
ATOM  C5      0.975650      0.824159      1.405360
ATOM  C6      1.033633      0.786321      1.249808
ATOM  C7      0.936157      0.709414      1.186047
ATOM  C8      0.969089      0.647733      1.040670
ATOM  C9      0.974939      0.596724      1.433440
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ATOM  C10     0.769933      0.589276      1.308921
ATOM  Br1     0.742231      0.963664      1.288622
ATOM  H1      0.673264      0.783873      1.289203
ATOM  H2      0.807614      0.765816      1.523859
ATOM  H3      0.965073      0.907276      1.409101
ATOM  H4      1.031226      0.802463      1.504992
ATOM  H5      1.050553      0.848791      1.168047
ATOM  H6      1.120531      0.746937      1.268009
ATOM  H7      0.928789      0.571140      1.039363
ATOM  H8      1.066503      0.643138      1.015995
ATOM  H9      1.058427      0.638242      1.461449
ATOM  H10     1.000989      0.527090      1.370489
ATOM  H11     0.933039      0.572515      1.542642
ATOM  H12     0.799256      0.514582      1.264427
ATOM  H13     0.722059      0.575273      1.418227
ATOM  H14     0.703583      0.619808      1.226472
ENERGY AQ2 -106.0 kJ/mol  (4th in energy)
COMMENT Choice between 3 structures between -106.5 and -105.8 difficult.
COMMENT There is then an energy gap to -103.7 kJ/mol.
COMMENT This choice based on density, after consideration of
COMMENT elastic constants, attachment energies and structures
COMMENT did not provide any differentiation in top 5.

TITL Scheraga V 1
SPACEGROUP P21
CELL  7.2150  11.2660   8.8110  90.0000  60.3100  90.0000
ATOM C1       .09990   .18574  -.32455
ATOM C2       .04623   .11623  -.16128
ATOM H3       .02301   .27111  -.28969
ATOM C4      -.08090   .00800  -.15771
ATOM N5       .08082   .14042  -.03885
ATOM C6       .08352  -.07562  -.30078
ATOM C7      -.18748  -.03507   .03044
ATOM C8      -.20594   .06049  -.24445
ATOM C9       .13697  -.01046  -.47296
ATOM H10      .22207  -.08892  -.28551
ATOM H11      .01313  -.16209  -.29180
ATOM C12      .00357   .10416  -.40883
ATOM H13      .30516   .00805  -.55260
ATOM H14      .09055  -.06222  -.55212
ATOM H15     -.01857   .14924  -.50712
ATOM C16     -.33173  -.03114  -.28624
ATOM C17     -.36304   .16006  -.13852
ATOM H18     -.39931   .01086  -.35872
ATOM H19     -.23788  -.10588  -.36209
ATOM H20     -.46348  -.06568  -.16610
ATOM H21     -.40954   .20862  -.22076
ATOM H22     -.50725   .12287  -.03130
ATOM H23     -.30166   .22368  -.08223
ATOM Br24     .40054   .22299  -.46619
ATOM H25     -.34998  -.00436   .10813
ATOM H26     -.18039  -.12986   .04517
ATOM S27     -.03392   .03558   .11686
ATOM O28      .12798  -.04379   .10311
ATOM O29     -.17237   .09199   .27920
ENERGY 26.03 kcal/mol
COMMENT Lowest energy structure.
COMMENT The packing seems reasonable. Similar packings are found with
COMMENT slightly higer E.
COMMENT Confidence level (1-10): 6, by energy

TITL Scheraga V 2
SPACEGROUP P212121
CELL  9.9670  11.5280  10.7600  90.0000  90.0000  90.0000
ATOM C1       .14448   .06156   .02999
ATOM C2       .07821  -.05613   .03584
ATOM H3       .13443   .10482   .11817
ATOM C4      -.03847  -.05537  -.05459
ATOM N5       .10227  -.14083   .10512
ATOM C6       .02674  -.05986  -.18531
ATOM C7      -.12498  -.15771  -.01552
ATOM C8      -.08388   .07360  -.04271
ATOM C9       .09150   .06199  -.19844
ATOM H10      .09911  -.12967  -.19210
ATOM H11     -.04909  -.07547  -.25542
ATOM C12      .06014   .12028  -.07284
ATOM H13      .19798   .05750  -.21601
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ATOM H14      .04746   .11065  -.27409
ATOM H15      .07051   .21371  -.07301
ATOM C16     -.19095   .11118  -.13694
ATOM C17     -.13674   .10682   .08686
ATOM H18     -.20876   .20378  -.12900
ATOM H19     -.16510   .09318  -.23249
ATOM H20     -.28518   .06762  -.11739
ATOM H21     -.13946   .20053   .09633
ATOM H22     -.23853   .07558   .09910
ATOM H23     -.07832   .07266   .16343
ATOM Br24     .33650   .05484   .00245
ATOM H25     -.20793  -.13306   .04357
ATOM H26     -.16058  -.21089  -.09130
ATOM S27     -.01279  -.24484   .07818
ATOM O28      .04696  -.33270   .00270
ATOM O29     -.07533  -.27495   .19290
ENERGY 25.77 kcal/mol
COMMENT Releative E=+0.26 kcal/mol
COMMENT Confidence level (1-10): 5, by energy.

TITL Scheraga V 3
SPACEGROUP P21
CELL  7.3090  10.2360   8.4540  90.0000  78.0300  90.0000
ATOM C1      -.37932   .49802  -.26150
ATOM C2      -.27540   .53480  -.13111
ATOM H3      -.28213   .46305  -.36648
ATOM C4      -.29884   .68067  -.10272
ATOM N5      -.17489   .46639  -.06062
ATOM C6      -.50444   .69849  -.01177
ATOM C7      -.14568   .71768  -.01372
ATOM C8      -.30269   .72738  -.27757
ATOM C9      -.61778   .66749  -.14349
ATOM H10     -.53835   .63410   .09187
ATOM H11     -.52697   .79755   .03302
ATOM C12     -.46530   .63129  -.29203
ATOM H13     -.71654   .58904  -.10850
ATOM H14     -.69663   .75139  -.16941
ATOM H15     -.51094   .63437  -.40582
ATOM C16     -.35276   .87199  -.29090
ATOM C17     -.11927   .70357  -.40121
ATOM H18     -.36725   .89368  -.41340
ATOM H19     -.48088   .90114  -.21019
ATOM H20     -.24132   .93335  -.26521
ATOM H21     -.14356   .71215  -.52317
ATOM H22     -.01606   .77670  -.38808
ATOM H23     -.05585   .60913  -.39114
ATOM Br24    -.55292   .35444  -.20242
ATOM H25     -.02209   .75638  -.09269
ATOM H26     -.18985   .78214   .08820
ATOM S27     -.08007   .56304   .06226
ATOM O28     -.18079   .54464   .22452
ATOM O29      .11808   .54756   .02367
ENERGY 25.43kcal/mol
COMMENT Releative E=+0.60 kcal/mol.
COMMENT Confidence level (1-10): 4, by energy

TITL Schmidt V 1
SPACEGROUP P212121
CELL   8.9201  9.2143 13.3322 90.0000 90.0000 90.0000
ATOM   C1         0.23945  0.47667  0.16927
ATOM   C2         0.32824  0.34680  0.12106
ATOM   C3         0.22611  0.27888  0.04447
ATOM   C4         0.08260  0.37375  0.05444
ATOM   C5         0.00951  0.33965  0.15623
ATOM   C6         0.11625  0.40590  0.23392
ATOM   C7         0.15125  0.52876  0.07481
ATOM   C8         0.35524  0.56724  0.22110
ATOM   S9         0.52401  0.46401  0.22538
ATOM   N10        0.46505  0.33276  0.14634
ATOM   C11        0.03259  0.64482  0.09719
ATOM   C12        0.25005  0.58459 -0.01109
ATOM   O13        0.54593  0.41203  0.32538
ATOM   O14        0.64173  0.54972  0.18305
ATOM   Br15       0.19986  0.06809  0.05900
ATOM   H16        0.27222  0.29123 -0.02666
ATOM   H17        0.01158  0.36691 -0.00725
ATOM   H18       -0.00363  0.22862  0.16717
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ATOM   H19       -0.09642  0.38642  0.16023
ATOM   H20        0.06328  0.48366  0.27797
ATOM   H21        0.16086  0.32738  0.28135
ATOM   H22        0.37213  0.66425  0.18285
ATOM   H23        0.32098  0.59444  0.29325
ATOM   H24       -0.04050  0.61434  0.15420
ATOM   H25        0.08512  0.74056  0.11890
ATOM   H26       -0.03008  0.66499  0.03290
ATOM   H27        0.18814  0.58733 -0.07717
ATOM   H28        0.28703  0.68922  0.00450
ATOM   H29        0.34420  0.52026 -0.02293
ENERGY -99.23 kJ/mol
COMMENT  Best energy, smallest unit cell volume.
COMMENT  Confidence level (1-10): 5, by energy and volume.

TITL Schmidt V 2
SPACEGROUP P212121
CELL   6.7424 12.0180 13.6871 90.0000 90.0000 90.0000
ATOM   C1         0.15099  0.44190  0.28888
ATOM   C2         0.00685  0.34747  0.25308
ATOM   C3         0.05936  0.32364  0.14830
ATOM   C4         0.23058  0.40782  0.12973
ATOM   C5         0.14124  0.52556  0.12855
ATOM   C6         0.08342  0.54802  0.23510
ATOM   C7         0.34106  0.40734  0.23133
ATOM   C8         0.13787  0.44032  0.39805
ATOM   S9        -0.06909  0.35573  0.43022
ATOM   N10       -0.10595  0.30387  0.31704
ATOM   C11        0.51017  0.49243  0.23747
ATOM   C12        0.42524  0.29312  0.25932
ATOM   O13       -0.22789  0.42596  0.46175
ATOM   O14       -0.00279  0.27256  0.49742
ATOM   Br15      -0.16595  0.32897  0.05725
ATOM   H16        0.11217  0.24263  0.14230
ATOM   H17        0.31815  0.38777  0.06971
ATOM   H18        0.01920  0.53085  0.08231
ATOM   H19        0.24571  0.58270  0.10389
ATOM   H20        0.15579  0.61741  0.26321
ATOM   H21       -0.06845  0.56043  0.24276
ATOM   H22        0.26765  0.40873  0.42833
ATOM   H23        0.12015  0.52030  0.42572
ATOM   H24        0.46548  0.57234  0.21836
ATOM   H25        0.56458  0.49518  0.30854
ATOM   H26        0.62457  0.46874  0.19094
ATOM   H27        0.52212  0.26595  0.20522
ATOM   H28        0.50325  0.29874  0.32468
ATOM   H29        0.31549  0.23319  0.26835
ENERGY -98.46 kJ/mol
COMMENT  Energy rank 2
COMMENT  Confidence level (1-10): 4, by energy

TITL Schmidt V 3
SPACEGROUP P212121
CELL   7.2768  8.7081 17.4610 90.0000 90.0000 90.0000
ATOM   C1         0.27865 -0.03289  0.11899
ATOM   C2         0.20486  0.08637  0.17920
ATOM   C3         0.03878  0.16148  0.14410
ATOM   C4         0.02870  0.08135  0.06457
ATOM   C5         0.19190  0.13800  0.01625
ATOM   C6         0.36093  0.06418  0.05361
ATOM   C7         0.09151 -0.08724  0.08479
ATOM   C8         0.40498 -0.13630  0.16278
ATOM   S9         0.44609 -0.04894  0.25345
ATOM   N10        0.28180  0.08678  0.24466
ATOM   C11        0.11097 -0.19126  0.01435
ATOM   C12       -0.03567 -0.16805  0.14210
ATOM   O13        0.62746  0.01428  0.25390
ATOM   O14        0.40354 -0.15838  0.31188
ATOM   Br15       0.04511  0.38718  0.14399
ATOM   H16       -0.07718  0.13454  0.17621
ATOM   H17       -0.09932  0.09031  0.03847
ATOM   H18        0.20129  0.25717  0.01607
ATOM   H19        0.17694  0.10281 -0.04032
ATOM   H20        0.43242 -0.00549  0.01551
ATOM   H21        0.45162  0.14626  0.07468
ATOM   H22        0.34655 -0.24442  0.16969
ATOM   H23        0.52812 -0.15214  0.13360
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ATOM   H24        0.19400 -0.14357 -0.02789
ATOM   H25        0.16854 -0.29562  0.03059
ATOM   H26       -0.01802 -0.21193 -0.00915
ATOM   H27       -0.16880 -0.17077  0.12047
ATOM   H28        0.00781 -0.28046  0.15083
ATOM   H29       -0.03871 -0.11390  0.19517
ENERGY -97.81 kJ/mol
COMMENT  Energy rank 3
COMMENT  Confidence level (1-10): 3, by energy
COMMENT  There are 13 additional possible packings with energies < -95 kJ/mol
COMMENT  (10 packings in P212121, two in P21, one in C2).

TITL  Van Eijck V 1
SPACEGROUP P212121
CELL    9.98479  15.89078   7.11903    90.000    90.000    90.000
ATOM C1            .468909   .855063   .940382
ATOM C2            .596664   .811791  1.010379
ATOM H3            .668753   .798905   .899326
ATOM H4            .574063   .751646  1.077066
ATOM H5            .645764   .851712  1.114050
ATOM C6            .373298   .852212  1.108399
ATOM H7            .378771   .792207  1.182141
ATOM H8            .269260   .860358  1.067329
ATOM H9            .397525   .901836  1.208278
ATOM C10           .488498   .943963   .850116
ATOM H11           .533802   .989416   .945902
ATOM C12           .343985   .968076   .788518
ATOM H13           .342235  1.018370   .685238
ATOM H14           .283795   .987736   .908006
ATOM C15           .292692   .885576   .706184
ATOM H16           .198102   .866990   .770421
ATOM H17           .276873   .891497   .555457
ATOM C18           .406607   .821451   .751476
ATOM C19           .514890   .843431   .609149
ATOM C20           .576621   .924219   .674676
ATOM BR21          .587138  1.011535   .477122
ATOM H22           .679473   .912258   .718652
ATOM C23           .376850   .729933   .727366
ATOM H24           .386362   .696293   .859673
ATOM H25           .277454   .720013   .671032
ATOM N26           .553076   .788570   .488750
ATOM S27           .500100   .695550   .563970
ATOM O28           .439796   .650649   .411074
ATOM O29           .607513   .655757   .662157
ENERGY   -318.983 kJ/mol
COMMENT The best structure in free energy; the next one is 3.9 kJ/mol higher.
COMMENT It is the fourth one in energy.

TITL  Van Eijck V 2
SPACEGROUP P212121
CELL    7.94880  11.38622  12.39743    90.000    90.000    90.000
ATOM C1            .782094   .450193   .633773
ATOM C2            .929851   .502344   .696914
ATOM H3            .905111   .589854   .728480
ATOM H4           1.040584   .510214   .645514
ATOM H5            .963370   .445796   .764511
ATOM C6            .861689   .346940   .573505
ATOM H7            .960653   .377937   .519811
ATOM H8            .772263   .298027   .524694
ATOM H9            .918011   .285386   .630469
ATOM C10           .619923   .420355   .699718
ATOM H11           .641672   .355248   .762418
ATOM C12           .491797   .378240   .612956
ATOM H13           .361413   .386454   .638871
ATOM H14           .513810   .286972   .591479
ATOM C15           .531142   .460386   .519009
ATOM H16           .569187   .411113   .447676
ATOM H17           .421440   .512546   .497800
ATOM C18           .678361   .538319   .561751
ATOM C19           .596540   .618168   .645801
ATOM C20           .568681   .543220   .743549
ATOM BR21          .341363   .559110   .806051
ATOM H22           .655820   .569690   .806819
ATOM C23           .764680   .617566   .483052
ATOM H24           .894709   .591501   .469755
ATOM H25           .698291   .619516   .406682
ATOM N26           .605142   .730126   .635859
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ATOM S27           .754362   .758392   .545802
ATOM O28           .695036   .845470   .471523
ATOM O29           .907401   .785504   .601822
ENERGY   -320.070 kJ/mol
COMMENT The second best structure in free energy and also in energy.
COMMENT But the energy differences with next ones are extremely small.

TITL  Van Eijck V 3
SPACEGROUP P212121
CELL   14.65069   8.52371   8.71607    90.000    90.000    90.000
ATOM C1            .661322   .846078   .576590
ATOM C2            .765579   .844874   .561542
ATOM H3            .789768   .788295   .457383
ATOM H4            .796961   .782905   .657667
ATOM H5            .791590   .964549   .561200
ATOM C6            .644735   .929878   .729533
ATOM H7            .694945   .895190   .815536
ATOM H8            .577983   .904013   .777384
ATOM H9            .649395  1.056507   .714462
ATOM C10           .606860   .913433   .436936
ATOM H11           .624860  1.034288   .409401
ATOM C12           .505651   .893343   .487918
ATOM H13           .457695   .900330   .392772
ATOM H14           .486418   .982435   .571520
ATOM C15           .506610   .730024   .559448
ATOM H16           .479532   .732233   .675915
ATOM H17           .465295   .648732   .492165
ATOM C18           .609894   .684204   .558254
ATOM C19           .629432   .643066   .391278
ATOM C20           .630232   .795695   .306026
ATOM BR21          .550189   .796866   .123634
ATOM H22           .698832   .818697   .263558
ATOM C23           .637857   .543810   .649653
ATOM H24           .675228   .578796   .751233
ATOM H25           .579596   .472885   .682967
ATOM N26           .662918   .507848   .358689
ATOM S27           .709095   .439268   .518860
ATOM O28           .694361   .273279   .530179
ATOM O29           .801435   .492912   .523310
ENERGY   -320.391 kJ/mol
COMMENT The first structure in energy and the third one in free energy.
COMMENT But the energy differences with next ones are extremely small.

TITL Verwer V 1
SPACEGROUP P212121
CELL 7.1776  13.3227  12.2159  90.0000  90.0000  90.0000
ATOM   C1  0.40050  0.13422  0.77947
ATOM   C2  0.29263  0.18810  0.68638
ATOM   C3  0.08707  0.15417  0.70716
ATOM   C4  0.07779  0.04818  0.67899
ATOM   C5  0.17615 -0.01390  0.75606
ATOM   C6  0.24147  0.07217  0.83470
ATOM   C7  0.07231  0.14666  0.83515
ATOM   C8 -0.06410  0.20878  0.63810
ATOM   S9 -0.09298  0.12088  0.53162
ATOM  N10 -0.01529  0.01788  0.59723
ATOM  C11 -0.11370  0.10263  0.88334
ATOM  C12  0.10004  0.24700  0.90101
ATOM BR13  0.36892 -0.09447  0.68861
ATOM  O14 -0.28553  0.10724  0.50662
ATOM  O15  0.03555  0.14567  0.44647
ATOM  H16  0.46089  0.18764  0.83694
ATOM  H17  0.51349  0.08796  0.74777
ATOM  H18  0.30568  0.26943  0.69354
ATOM  H19  0.34338  0.16535  0.60561
ATOM  H20  0.07982 -0.06494  0.79682
ATOM  H21  0.27951  0.04483  0.91599
ATOM  H22 -0.02029  0.27901  0.60110
ATOM  H23 -0.19827  0.21632  0.67846
ATOM  H24 -0.16735  0.03768  0.83948
ATOM  H25 -0.09234  0.08023  0.96837
ATOM  H26 -0.22363  0.15871  0.88160
ATOM  H27 -0.02092  0.29585  0.89218
ATOM  H28  0.21942  0.29143  0.87572
ATOM  H29  0.11786  0.23003  0.98759
ENERGY -114.56 kcal/mol
COMMENT d= 1.6615 g/cc
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COMMENT structure ranked nr. 1 by energy

TITL Verwer V 2
SPACEGROUP P212121
CELL 12.8533   7.3814  12.3747  90.0000  90.0000  90.0000
ATOM   C1  0.41439  0.17170  0.76169
ATOM   C2  0.30341  0.12171  0.72291
ATOM   C3  0.23392  0.20572  0.81364
ATOM   C4  0.25261  0.10031  0.91126
ATOM   C5  0.35306  0.13828  0.95804
ATOM   C6  0.39077  0.27518  0.86949
ATOM   C7  0.29001  0.38756  0.84433
ATOM   C8  0.11496  0.20002  0.79317
ATOM   S9  0.08337 -0.00312  0.86023
ATOM  N10  0.18294 -0.00401  0.94869
ATOM  C11  0.24147  0.49599  0.94176
ATOM  C12  0.30035  0.53325  0.75255
ATOM BR13  0.43966 -0.07216  0.98164
ATOM  O14 -0.01167  0.01207  0.91913
ATOM  O15  0.09756 -0.14860  0.78547
ATOM  H16  0.45464  0.25692  0.70341
ATOM  H17  0.46186  0.05149  0.77361
ATOM  H18  0.28626  0.18302  0.64458
ATOM  H19  0.29359 -0.02498  0.71572
ATOM  H20  0.34400  0.20424  1.03655
ATOM  H21  0.45672  0.35737  0.89528
ATOM  H22  0.09226  0.18795  0.70906
ATOM  H23  0.07212  0.30739  0.83351
ATOM  H24  0.21146  0.40969  1.00569
ATOM  H25  0.30017  0.58496  0.97702
ATOM  H26  0.17610  0.57953  0.91549
ATOM  H27  0.22316  0.57784  0.72695
ATOM  H28  0.34019  0.48514  0.68090
ATOM  H29  0.34338  0.65087  0.78183
ATOM  END  0.00000  0.00000  0.00000
ENERGY -114.47 kcal/mol
COMMENT d= 1.6531 g/cc
COMMENT structure ranked nr. 2 by energy

TITL Verwer V 3
SPACEGROUP P212121
CELL 11.1706  10.6788  10.0135  90.0000  90.0000  90.0000
ATOM   C1 -0.06910  0.69951  0.08628
ATOM   C2  0.06079  0.68794  0.03198
ATOM   C3  0.06080  0.55328 -0.02986
ATOM   C4  0.05650  0.46626  0.08183
ATOM   C5 -0.05773  0.46774  0.14807
ATOM   C6 -0.12015  0.56631  0.05533
ATOM   C7 -0.06904  0.53579 -0.08709
ATOM   C8  0.17183  0.51827 -0.11508
ATOM   S9  0.25399  0.42639 -0.00154
ATOM  N10  0.14406  0.39502  0.10859
ATOM  C11 -0.10084  0.40213 -0.14370
ATOM  C12 -0.10658  0.62730 -0.20285
ATOM BR13 -0.04983  0.50724  0.33642
ATOM  O14  0.28922  0.31216 -0.06417
ATOM  O15  0.34166  0.50327  0.06233
ATOM  H16 -0.11978  0.77166  0.03431
ATOM  H17 -0.07058  0.72292  0.19209
ATOM  H18  0.07909  0.75916 -0.04353
ATOM  H19  0.12707  0.69797  0.11186
ATOM  H20 -0.09943  0.37596  0.13934
ATOM  H21 -0.21781  0.56260  0.06129
ATOM  H22  0.22676  0.59633 -0.14758
ATOM  H23  0.15039  0.45660 -0.19763
ATOM  H24 -0.06276  0.32538 -0.08615
ATOM  H25 -0.19773  0.38950 -0.14519
ATOM  H26 -0.06761  0.39056 -0.24540
ATOM  H27 -0.05759  0.60521 -0.29434
ATOM  H28 -0.08959  0.72551 -0.18236
ATOM  H29 -0.20207  0.61836 -0.22317
ENERGY -114.47mkcal/mol
COMMENT d=1.6248 g/cc
COMMENT structure ranked nr. 3 by energy
COMMENT Structure is nr. 4 in the clustered list. Structures nr. 2 and 3
COMMENT are identical, but have a different setting. The clustering
COMMENT does not recognize them as identical; this has been corrected later
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COMMENT on by hand.

TITL Williams V 1
SPACEGROUP Cc
CELL  6.91   15.97   10.53     90.00     81.26     90.00
ATOM C1          -0.13832   0.43982   0.34894
ATOM C2          -0.07283   0.37282   0.43995
ATOM C3          -0.11519   0.28911   0.37419
ATOM C4          -0.19409   0.31746   0.25185
ATOM C5          -0.02957   0.35788   0.15570
ATOM C6           0.00861   0.43690   0.22650
ATOM C7          -0.31279   0.39617   0.30127
ATOM C8          -0.14046   0.53095   0.39071
ATOM C9          -0.39487   0.44537   0.19545
ATOM C10         -0.48165   0.37606   0.41016
ATOM N1           0.12514   0.49575   0.19351
ATOM O1           0.05595   0.64886   0.24540
ATOM O2           0.23618   0.56495   0.38665
ATOM S1           0.08787   0.57140   0.30625
ATOM Br1          0.20221   0.28998   0.10526
ATOM H21         -0.15194   0.37827   0.52558
ATOM H22          0.06537   0.37950   0.45032
ATOM H31         -0.21649   0.25663   0.42888
ATOM H32          0.00111   0.25345   0.35505
ATOM H4          -0.26548   0.27397   0.21219
ATOM H5          -0.07570   0.37265   0.07503
ATOM H81         -0.14145   0.53970   0.48301
ATOM H82         -0.24600   0.56325   0.36115
ATOM H91         -0.28729   0.45860   0.12495
ATOM H92         -0.45525   0.49807   0.23182
ATOM H93         -0.49492   0.41113   0.16144
ATOM H101        -0.43026   0.34440   0.47872
ATOM H102        -0.58153   0.34195   0.37574
ATOM H103        -0.54186   0.42889   0.44613
ENERGY -128.95

TITL Williams V 2
SPACEGROUP P21
CELL    8.12   10.81    6.95     90.00     70.28     90.00
ATOM C1           0.12883   0.15139   0.76918
ATOM C2           0.27136   0.06179   0.78820
ATOM C3           0.44426   0.12715   0.66131
ATOM C4           0.38173   0.24770   0.58957
ATOM C5           0.30092   0.33592   0.77201
ATOM C6           0.13774   0.26582   0.89142
ATOM C7           0.21469   0.20274   0.55114
ATOM C8          -0.06101   0.11047   0.85515
ATOM C9           0.10871   0.30726   0.49755
ATOM C10          0.25310   0.10218   0.38463
ATOM N1           0.01780   0.29413   1.05323
ATOM O1          -0.30314   0.24495   1.13030
ATOM O2          -0.12170   0.10355   1.25498
ATOM S1          -0.14000   0.18557   1.10217
ATOM Br1          0.44848   0.37860   0.93106
ATOM H21          0.25865  -0.01893   0.72900
ATOM H22          0.26130   0.04779   0.93163
ATOM H31          0.50980   0.07724   0.54148
ATOM H32          0.52167   0.14260   0.74068
ATOM H4           0.47015   0.28837   0.47425
ATOM H5           0.26804   0.41526   0.72700
ATOM H81         -0.07840   0.02107   0.87673
ATOM H82         -0.13161   0.14190   0.77559
ATOM H91          0.08336   0.37241   0.60383
ATOM H92         -0.00257   0.27344   0.49110
ATOM H93          0.17710   0.34322   0.36323
ATOM H101         0.32126   0.03452   0.41778
ATOM H102         0.32121   0.13854   0.25052
ATOM H103         0.14155   0.06875   0.37839
ENERGY -128.55

TITL Williams V 3
SPACEGROUP P212121
CELL   10.66    6.93   15.58     90.00     90.00     90.00
ATOM C1           0.17521   0.93274   0.43578
ATOM C2           0.07944   0.86101   0.36819
ATOM C3           0.14133   0.91930   0.28175
ATOM C4           0.26637   1.01197   0.30930
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ATOM C5           0.35619   0.85783   0.34600
ATOM C6           0.28926   0.80341   0.42782
ATOM C7           0.22698   1.11658   0.39277
ATOM C8           0.13915   0.92134   0.52998
ATOM C9           0.33704   1.20837   0.44208
ATOM C10          0.12591   1.27155   0.37721
ATOM N1           0.32000   0.68686   0.48550
ATOM O1           0.28012   0.73546   0.64439
ATOM O2           0.12928   0.54420   0.55883
ATOM S1           0.21482   0.70212   0.56597
ATOM Br1          0.39245   0.63991   0.27182
ATOM H21         -0.00113   0.92763   0.37688
ATOM H22          0.06385   0.72151   0.37311
ATOM H31          0.09005   1.01548   0.25129
ATOM H32          0.15337   0.80925   0.24303
ATOM H4           0.30598   1.09214   0.26504
ATOM H5           0.43818   0.91341   0.36006
ATOM H81          0.04896   0.90905   0.54097
ATOM H82          0.17434   1.02758   0.56403
ATOM H91          0.40256   1.10975   0.45240
ATOM H92          0.30664   1.25896   0.49774
ATOM H93          0.37279   1.31549   0.40785
ATOM H101         0.05470   1.21385   0.34552
ATOM H102         0.16206   1.37854   0.34311
ATOM H103         0.09592   1.32202   0.43299
ENERGY -128.43

TITL Ammon VI 1
CELL   11.5082    6.6764    7.6139   85.8993   95.2965   81.1586
SPACEGROUP P-1
ATOM  H1     -0.47069  -0.28143  -0.31648
ATOM  C2     -0.48194  -0.12522  -0.28241
ATOM  C3     -0.38673  -0.05039  -0.19787
ATOM  C4     -0.59063   0.00261  -0.31935
ATOM  C5     -0.60354   0.20223  -0.27098
ATOM  C6     -0.39863   0.14794  -0.14765
ATOM  H7     -0.66528  -0.05376  -0.38477
ATOM  S8     -0.24670  -0.21477  -0.14792
ATOM  C9     -0.50788   0.27450  -0.18493
ATOM  H10    -0.68832   0.30084  -0.29946
ATOM  H11    -0.32345   0.19989  -0.07927
ATOM  O12    -0.17704  -0.12454  -0.01064
ATOM  O13    -0.27036  -0.42320  -0.11002
ATOM  N14    -0.19526  -0.19350  -0.34421
ATOM  H15    -0.51830   0.42879  -0.14611
ATOM  C16    -0.08091  -0.23680  -0.35710
ATOM  N17    -0.05303  -0.22274  -0.53176
ATOM  C18     0.01873  -0.29536  -0.22673
ATOM  C19     0.13055  -0.33369  -0.27904
ATOM  C20     0.05781  -0.25865  -0.58496
ATOM  H21    -0.12468  -0.19128  -0.62295
ATOM  H22     0.00326  -0.30603  -0.08835
ATOM  C23     0.15314  -0.31551  -0.45833
ATOM  H24     0.20497  -0.37791  -0.17856
ATOM  N25     0.06443  -0.24374  -0.76581
ATOM  H26     0.24216  -0.34347  -0.49690
ATOM  H27     0.14739  -0.24613  -0.80092
ATOM  H28     0.00559  -0.13329  -0.83827
ENERGY -36.97 kcal/mol with atom-centered charges.
COMMENT d = 1.444 g/cc.  Lowest E and highest density structure.
COMMENT Volume additivity calcns suggest d = 1.436 g/cc.
COMMENT Conformation # 3 for N-S bond; no intramolecular H-bond.
COMMENT Probably not the best structure based on only one
COMMENT N-H...O of 2.363 Angs.

TITL Ammon VI 2
CELL    7.5510   23.0988    6.7945   90.0000   82.4743   90.0000
SPACEGROUP P21/c
ATOM  H1       0.18648   0.01820  -0.26368
ATOM  C2       0.21815   0.01031  -0.11494
ATOM  C3       0.28329   0.05539  -0.00794
ATOM  C4       0.19733  -0.04446  -0.02866
ATOM  C5       0.24241  -0.05382   0.16181
ATOM  C6       0.33009   0.04653   0.18162
ATOM  H7       0.14706  -0.07983  -0.11033
ATOM  S8       0.31246   0.12595  -0.11884
ATOM  C9       0.30909  -0.00848   0.26643
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ATOM  H10     0.22657  -0.09652   0.22805
ATOM  H11     0.38341   0.08225   0.25904
ATOM  O12     0.43530   0.15856  -0.00766
ATOM  O13     0.36180   0.11800  -0.33402
ATOM  N14     0.10360   0.14995  -0.07336
ATOM  H15     0.34547  -0.01592   0.41348
ATOM  C16     0.07030   0.20595  -0.07291
ATOM  N17    -0.11204   0.21873  -0.04391
ATOM  C18     0.18512   0.25547  -0.09686
ATOM  C19     0.11228   0.31004  -0.09140
ATOM  C20    -0.18567   0.27280  -0.03640
ATOM  H21    -0.19168   0.18330  -0.03724
ATOM  H22     0.32832   0.24852  -0.11691
ATOM  C23    -0.07385   0.32019  -0.06019
ATOM  H24     0.20121   0.34705  -0.10985
ATOM  N25    -0.37025   0.27527  -0.01434
ATOM  H26    -0.12881   0.36361  -0.05340
ATOM  H27    -0.42137   0.31534   0.01529
ATOM  H28    -0.43586   0.24480   0.07443
ENERGY -36.63 kcal/mol with atom-centered charges.
COMMENT d = 1.409 g/cc.  Second lowest E.
COMMENT Volume additivity calcns suggest d = 1.436 g/cc.
COMMENT Conformation # 3 for N-S bond; no intramolecular H-bond.
COMMENT Structure probably better than # 1 based on two
COMMENT intermolecular N-H...O of 2.317 and 2.379 Angs.

TITL Ammon VI 3
CELL    7.7390    6.6830   22.8172   90.0000   82.8960   90.0000
SPACEGROUP P21/c
ATOM  H1     -0.19415  -0.25650  -0.48096
ATOM  C2     -0.22452  -0.10153  -0.48929
ATOM  C3     -0.30645   0.01627  -0.44354
ATOM  C4     -0.18530  -0.01754  -0.54530
ATOM  C5     -0.22886   0.18150  -0.55523
ATOM  C6     -0.35183   0.21460  -0.45292
ATOM  H7     -0.12188  -0.10754  -0.58122
ATOM  S8     -0.35924  -0.09139  -0.37138
ATOM  C9     -0.31235   0.29709  -0.50918
ATOM  H10    -0.19865   0.24597  -0.59889
ATOM  H11    -0.41828   0.30068  -0.41665
ATOM  O12    -0.49251   0.03762  -0.33836
ATOM  O13    -0.40033  -0.30411  -0.37913
ATOM  N14    -0.16653  -0.07070  -0.34685
ATOM  H15    -0.34742   0.45092  -0.51706
ATOM  C16    -0.15525  -0.07327  -0.28971
ATOM  N17     0.01623  -0.06625  -0.27662
ATOM  C18    -0.28471  -0.08228  -0.23921
ATOM  C19    -0.23467  -0.08470  -0.18349
ATOM  C20     0.06721  -0.06669  -0.22144
ATOM  H21     0.10661  -0.07013  -0.31272
ATOM  H22    -0.42060  -0.08494  -0.24632
ATOM  C23    -0.05854  -0.07598  -0.17310
ATOM  H24    -0.33443  -0.09161  -0.14577
ATOM  N25     0.24486  -0.06725  -0.21886
ATOM  H26    -0.02166  -0.07504  -0.12880
ATOM  H27     0.27888  -0.04270  -0.17800
ATOM  H28     0.31835   0.01417  -0.25005
ENERGY -36.46 kcal/mol with atom-centered charges.
COMMENT d = 1.414 g/cc.  Third lowest E.
COMMENT Volume additivity calcns suggest d = 1.436 g/cc.
COMMENT Conformation # 3 for N-S bond; no intramolecular H-bond.
COMMENT Structure probably better than # 1 based on two
COMMENT intermolecular N-H...O of 2.330 and 2.345 Angs.



TITL Dzyabchenko VI 1
SPACEGROUP Pbca
CELL 10.862 8.379 23.845 90.00 90.00 90.00
ATOM S1   0.41730 -0.07120  0.13130
ATOM O2   0.29420 -0.09369  0.15241
ATOM O3   0.49956 -0.20807  0.13421
ATOM N'4  0.41156 -0.01016  0.06606
ATOM C11  0.30945  0.05178  0.04181
ATOM N12  0.32787  0.10570 -0.01143
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ATOM C13  0.23505  0.16614 -0.04402
ATOM C14  0.11937  0.17567 -0.02417
ATOM C15  0.09672  0.12576  0.03057
ATOM C16  0.18955  0.06620  0.06325
ATOM H17  0.41261  0.09909 -0.02767
ATOM N18  0.25956  0.21805 -0.09689
ATOM H19  0.34533  0.21209 -0.11198
ATOM H20  0.19180  0.26217 -0.12068
ATOM H26  0.04762  0.22152 -0.05107
ATOM H27  0.00519  0.13340  0.04805
ATOM H28  0.16830  0.03079  0.10571
ATOM C5   0.48691  0.08877  0.16840
ATOM C6   0.58569  0.05629  0.20303
ATOM C7   0.64582  0.17877  0.23061
ATOM C8   0.60790  0.33573  0.22412
ATOM C9   0.50797  0.36552  0.18992
ATOM C10  0.44733  0.24402  0.16240
ATOM H21  0.61605 -0.06544  0.20855
ATOM H22  0.72311  0.15161  0.25746
ATOM H23  0.65494  0.43223  0.24515
ATOM H24  0.47647  0.48682  0.18455
ATOM H25  0.36888  0.27044  0.13617
ENERGY -36.06 kcal/mol
COMMENT Density 1.526 g/cm3
COMMENT Confidence level 5 (1-10), by energy


TITL Dzyabchenko VI 2
SPACEGROUP Pbca
CELL 9.317 9.850 24.697 90.00 90.00 90.00
ATOM S1   0.04150 0.38020 0.11230
ATOM O2  -0.03512 0.42299 0.06457
ATOM O3   0.05432 0.23457 0.12101
ATOM N4   0.20227 0.44693 0.11218
ATOM C11  0.31775 0.38886 0.08825
ATOM N12  0.43824 0.46713 0.08962
ATOM C13  0.56782 0.42431 0.06973
ATOM C14  0.58140 0.30058 0.04725
ATOM C15  0.46023 0.21831 0.04369
ATOM C16  0.33058 0.26134 0.06329
ATOM H17  0.43220 0.55926 0.10647
ATOM N18  0.68415 0.50744 0.07233
ATOM H19  0.67511 0.59984 0.08876
ATOM H20  0.77874 0.47619 0.05781
ATOM H26  0.68532 0.26862 0.03266
ATOM H27  0.46696 0.11898 0.02535
ATOM H28  0.23893 0.19504 0.05907
ATOM C5  -0.04320 0.45166 0.17010
ATOM C6  -0.08740 0.36611 0.21114
ATOM C7  -0.14753 0.41860 0.25786
ATOM C8  -0.16475 0.55754 0.26422
ATOM C9  -0.12164 0.64124 0.22245
ATOM C10 -0.06199 0.58966 0.17569
ATOM H21 -0.07489 0.25768 0.20668
ATOM H22 -0.18133 0.35048 0.28966
ATOM H23 -0.21056 0.59945 0.30075
ATOM H24 -0.13489 0.74970 0.22645
ATOM H25 -0.03001 0.65732 0.14346
ENERGY -35.21 kcal/mol
COMMENT Density 1.461 g/cm3
COMMENT Confidence level 3 (1-10), by energy


TITL Dzyabchenko VI 3
SPACEGROUP Pbca
CELL 9.351 10.345 22.923 90.00 90.00 90.00
ATOM S1   0.05100 0.51770 0.41570
ATOM O2   0.03820 0.40339 0.45125
ATOM O3  -0.07136 0.60463 0.41478
ATOM N4   0.19369 0.59838 0.43455
ATOM C11  0.32841 0.55170 0.42939
ATOM N12  0.43202 0.63883 0.44349
ATOM C13  0.57470 0.60883 0.44357
ATOM C14  0.61933 0.48946 0.42909
ATOM C15  0.51749 0.39806 0.41289
ATOM C16  0.37498 0.42819 0.41249
ATOM H17  0.40246 0.72819 0.45496
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ATOM N18  0.67287 0.70034 0.45809
ATOM H19  0.64089 0.78953 0.46871
ATOM H20  0.77703 0.67843 0.45815
ATOM H26  0.73229 0.46789 0.43040
ATOM H27  0.54971 0.30171 0.40038
ATOM H28  0.29973 0.35493 0.39891
ATOM C5   0.08405 0.46739 0.34260
ATOM C6   0.15854 0.54908 0.30590
ATOM C7   0.19203 0.51061 0.24976
ATOM C8   0.15122 0.38990 0.22937
ATOM C9   0.07521 0.31034 0.26646
ATOM C10  0.04107 0.34813 0.32243
ATOM H21  0.19073 0.64346 0.32117
ATOM H22  0.25059 0.57542 0.22159
ATOM H23  0.17792 0.35869 0.18575
ATOM H24  0.04166 0.21624 0.25133
ATOM H25 -0.01931 0.28437 0.35044
ENERGY -34.58 kcal/mol
COMMENT Density 1.494 g/cm3
COMMENT Confidence level 1 (1-10), by energy
COMMENT
COMMENT The molecular structures VI 1-3 are all trans isomers
COMMENT with regard to the S-N=C-N fragment (treated here with
COMMENT fixed geometry). As concerns to the cis isomer, its packings
COMMENT within all space groups were found of much smaller energy,
COMMENT the difference could be hardly covered by its larger
COMMENT intramolecular energy

TITL ERK VI 1
CELL   12.6340   7.6702  24.8320  90.0000  81.0350  90.0000
SPACEGROUP C2/c
ATOM S1      0.08497    0.20491    0.61526
ATOM O2      0.15830    0.33979    0.59424
ATOM O3     -0.01867    0.27721    0.61505
ATOM N4      0.08498    0.16547    0.67898
ATOM N5      0.15159    0.10590    0.75809
ATOM C6      0.08774    0.01828    0.57490
ATOM C7      0.03853   -0.13687    0.59667
ATOM C8      0.04033   -0.28734    0.56410
ATOM C9      0.09175   -0.28389    0.50967
ATOM C10     0.14114   -0.12980    0.48775
ATOM C11     0.13864    0.02109    0.52017
ATOM C12     0.17023    0.12154    0.70291
ATOM C13     0.27542    0.09460    0.67480
ATOM C14     0.35852    0.05374    0.70431
ATOM C15     0.33549    0.03880    0.76129
ATOM C16     0.22987    0.06546    0.78705
ATOM H17     0.00111   -0.14045    0.63622
ATOM H18     0.00476   -0.39957    0.57997
ATOM H19     0.17928   -0.12786    0.44831
ATOM H20     0.17381    0.13299    0.50379
ATOM H21     0.29193    0.10497    0.63341
ATOM N22     0.20240    0.05363    0.84073
ATOM H23     0.39399    0.00939    0.78373
ATOM H24     0.43468    0.03473    0.68451
ATOM H25     0.08063    0.12571    0.77763
ATOM H26     0.13637    0.10637    0.85761
ATOM H27     0.24932   -0.00363    0.86250
ATOM H28     0.09366   -0.39355    0.48606
END

TITL ERK VI 2
CELL   16.5053  10.8960  14.1392  90.0000  62.5408  90.0000
SPACEGROUP A2/n
ATOM S1   0.09795    0.98999   -0.74826
ATOM O2   0.02368    1.01717   -0.77026
ATOM O3   0.05956    1.03096   -0.64028
ATOM N4   0.11815    0.84500   -0.76560
ATOM N5   0.07590    0.78200   -0.58817
ATOM C6   0.18781    1.08274   -0.83527
ATOM C7   0.26771    1.02983   -0.91621
ATOM C8   0.33849    1.10475   -0.98890
ATOM C9   0.33004    1.23321   -0.98141
ATOM C10  0.25080    1.28689   -0.90073
ATOM C11  0.18062    1.21168   -0.82740
ATOM C12  0.10951    0.75796   -0.69378
ATOM C13  0.13760    0.63752   -0.73073
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ATOM C14  0.13168    0.54504   -0.65830
ATOM C15  0.09822    0.57484   -0.54993
ATOM C16  0.06947    0.69563   -0.51711
ATOM H17  0.27488    0.93664   -0.92238
ATOM H18  0.39641    1.06568   -1.04697
ATOM H19  0.24377    1.38020   -0.89555
ATOM H20  0.12336    1.25082   -0.76897
ATOM H21  0.16238    0.61730   -0.80962
ATOM N22  0.03346    0.72887   -0.41552
ATOM H23  0.09331    0.50994   -0.49553
ATOM H24  0.15093    0.45714   -0.68406
ATOM H25  0.05528    0.86455   -0.56405
ATOM H26  0.00965    0.81104   -0.39492
ATOM H27  0.02869    0.66959   -0.36242
ATOM H28  0.38175    1.28711   -1.03472
END

TITL ERK VI 3
CELL  9.3689  16.9826   7.9324  90.0000  70.1234  90.0000
SPACEGROUP P21/c
ATOM S1     -0.76087   -0.61717   -0.91205
ATOM O2     -0.90174   -0.63147   -0.94533
ATOM O3     -0.65469   -0.56160   -1.03043
ATOM N4     -0.68499   -0.70227   -0.91673
ATOM H5     -0.88397   -0.53043   -0.20074
ATOM N6     -0.44367   -0.65168   -0.92435
ATOM C7     -0.80613   -0.58325   -0.69188
ATOM C8     -0.92754   -0.61697   -0.55852
ATOM C9     -0.95694   -0.59800   -0.38150
ATOM C10    -0.86373   -0.54418   -0.33254
ATOM C11    -0.74526   -0.50839   -0.46906
ATOM C12    -0.71526   -0.52792   -0.64616
ATOM C13    -0.54559   -0.71093   -0.90916
ATOM C14    -0.49416   -0.78740   -0.88419
ATOM C15    -0.35424   -0.79731   -0.87209
ATOM C16    -0.25666   -0.73380   -0.88545
ATOM C17    -0.30396   -0.66163   -0.91246
ATOM H18    -0.99446   -0.65767   -0.59109
ATOM H19    -1.04634   -0.62372   -0.28403
ATOM H20    -0.67825   -0.46783   -0.43604
ATOM H21    -0.62541   -0.50249   -0.74287
ATOM H22    -0.56372   -0.83496   -0.87360
ATOM N23    -0.21840   -0.59725   -0.92951
ATOM H24    -0.15151   -0.74197   -0.87607
ATOM H25    -0.31913   -0.85268   -0.85285
ATOM H26    -0.47475   -0.59973   -0.94657
ATOM H27    -0.11768   -0.60098   -0.92157
ATOM H28    -0.25674   -0.54666   -0.95076
END

TITL Hofmann VI 1
SPACEGROUP P-1
CELL       10.886   7.632   8.062   120.792  93.920  97.608
ATOM C1   -0.52408   0.00127   0.23107
ATOM C2   -0.39889  -0.01962   0.26256
ATOM C3   -0.54984   0.18375   0.24738
ATOM C4   -0.45171   0.34806   0.29638
ATOM C5   -0.32757   0.33096   0.33017
ATOM C6   -0.30117   0.14896   0.31410
ATOM N7   -0.31835  -0.33969   0.06327
ATOM C8   -0.20534  -0.31125   0.02679
ATOM C9   -0.17860  -0.45283  -0.15756
ATOM C10  -0.05765  -0.42986  -0.20066
ATOM C11   0.03525  -0.26495  -0.05885
ATOM C12   0.00547  -0.12503   0.12349
ATOM N13  -0.11267  -0.15021   0.16249
ATOM O14  -0.46070  -0.32619   0.25060
ATOM O15  -0.28464  -0.16639   0.38407
ATOM C16  -0.36721  -0.21724   0.24485    ! S16 ?
ATOM N17   0.09857   0.04515   0.26940
ATOM H18  -0.60166  -0.12358   0.19504
ATOM H19  -0.64613   0.19813   0.22288
ATOM H20  -0.47194   0.48940   0.30935
ATOM H21  -0.25164   0.45920   0.36956
ATOM H22  -0.20443   0.13836   0.34206
ATOM H23  -0.25156  -0.58019  -0.26625
ATOM H24  -0.03617  -0.53892  -0.34294
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ATOM H25   0.12935  -0.24473  -0.08994
ATOM H26  -0.13087  -0.03893   0.29801
ATOM H27   0.18990   0.06850   0.24276
ATOM H28   0.07624   0.15134   0.40453
ENERGY   -105.41
COMMENT d=1.352g/cc.

TITL Hofmann VI 2
SPACEGROUP P-1
CELL          5.385  11.543  10.840   69.779  65.184  73.649
ATOM C1   -0.21733  -0.08212  -0.32811
ATOM C2   -0.04300  -0.11918  -0.24887
ATOM C3   -0.18447  -0.14935  -0.42083
ATOM C4    0.02291  -0.25361  -0.43666
ATOM C5    0.19896  -0.29066  -0.36041
ATOM C6    0.16722  -0.22387  -0.26753
ATOM N7   -0.20375  -0.11813  -0.00049
ATOM C8   -0.08898  -0.21235   0.07668
ATOM C9   -0.25343  -0.26269   0.21583
ATOM C10  -0.13615  -0.36217   0.30276
ATOM C11   0.14457  -0.41050   0.24933
ATOM C12   0.30313  -0.35891   0.10954
ATOM N13   0.18515  -0.26217   0.02681
ATOM O14  -0.21347   0.05767  -0.16820
ATOM O15   0.16039  -0.03646  -0.16166
ATOM C16  -0.07400  -0.04837  -0.14594   ! S16 ?
ATOM N17   0.58906  -0.40759   0.05274
ATOM H18  -0.37755  -0.00063  -0.31852
ATOM H19  -0.31925  -0.12018  -0.48104
ATOM H20   0.04831  -0.30535  -0.50879
ATOM H21   0.36099  -0.37103  -0.37362
ATOM H22   0.30657  -0.25315  -0.20974
ATOM H23  -0.47101  -0.22425   0.25599
ATOM H24  -0.26198  -0.40156   0.41062
ATOM H25   0.23857  -0.48765   0.31517
ATOM H26   0.30982  -0.22949  -0.07727
ATOM H27   0.68435  -0.48228   0.11393
ATOM H28   0.70694  -0.37046  -0.05199
ENERGY   -104.64
COMMENT d=1.344g/cc.

TITL Hofmann VI 3
SPACEGROUP P21/c
CELL     10.743  15.792   7.107      90.000 111.861  90.000
ATOM C1   -0.35326  -0.13206  -0.28303
ATOM C2   -0.21509  -0.11842  -0.17238
ATOM C3   -0.41476  -0.10020  -0.47974
ATOM C4   -0.34006  -0.05397  -0.56835
ATOM C5   -0.20382  -0.03908  -0.46035
ATOM C6   -0.14171  -0.07076  -0.26365
ATOM N7   -0.06143  -0.22603   0.04181
ATOM C8    0.05761  -0.22683   0.03401
ATOM C9    0.12013  -0.30519   0.04105
ATOM C10   0.24903  -0.30848   0.03730
ATOM C11   0.31393  -0.23325   0.02595
ATOM C12   0.24850  -0.15595   0.01749
ATOM N13   0.12321  -0.15414   0.02145
ATOM O14  -0.22638  -0.17293   0.12060
ATOM O15  -0.07002  -0.09649   0.14784
ATOM C16  -0.14437  -0.15273   0.04244        ! S16 ?
ATOM N17   0.31248  -0.07862   0.00406
ATOM H18  -0.41334  -0.16698  -0.21611
ATOM H19  -0.52073  -0.11104  -0.56325
ATOM H20  -0.38802  -0.02920  -0.72057
ATOM H21  -0.14627  -0.00268  -0.52885
ATOM H22  -0.03609  -0.05822  -0.18103
ATOM H23   0.06866  -0.36309   0.04996
ATOM H24   0.29816  -0.36887   0.04293
ATOM H25   0.41369  -0.23468   0.02260
ATOM H26   0.07754  -0.09535   0.00915
ATOM H27   0.40849  -0.07831  -0.00018
ATOM H28   0.26327  -0.02096  -0.00505
ENERGY   -102.89
COMMENT d=1.361g/cc.

TITL Leusen VI 1
SPACEGROUP  P21/a
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CELL   15.941  8.976  7.801 90.000 86.034 90.000
ATOM  C1     0.20780   0.38006   0.10256
ATOM  H2     0.26250   0.44812   0.06908
ATOM  C3     0.21735   0.23305   0.15612
ATOM  H4     0.27985   0.18771   0.16556
ATOM  C5     0.14667   0.14460   0.19595
ATOM  H6     0.15473   0.02994   0.23451
ATOM  C7     0.06655   0.20500   0.18241
ATOM  S8    -0.02397   0.09665   0.22827
ATOM  C9     0.05665   0.35224   0.12983
ATOM H10    -0.00556   0.39789   0.11931
ATOM C11     0.12750   0.43959   0.08981
ATOM H12     0.12103   0.55396   0.04828
ATOM N13    -0.00697  -0.08225   0.28856
ATOM O14    -0.08010   0.10252   0.06799
ATOM O15    -0.08209   0.17733   0.37338
ATOM C16    -0.06389  -0.17733   0.31745
ATOM C17    -0.04384  -0.32175   0.35456
ATOM C18    -0.10571  -0.42675   0.38900
ATOM C19    -0.18978  -0.39278   0.38701
ATOM C20    -0.21486  -0.25202   0.34852
ATOM N21    -0.15314  -0.13562   0.31302
ATOM N22    -0.29814  -0.21383   0.34086
ATOM H23     0.02167  -0.35585   0.35728
ATOM H24    -0.08781  -0.54052   0.41836
ATOM H25    -0.23625  -0.47970   0.41586
ATOM H26    -0.17103  -0.02996   0.28368
ATOM H27    -0.34374  -0.28895   0.38178
ATOM H28    -0.31097  -0.10690   0.30554
ENERGY  -90.30 kcal/mol asymmetric unit
DENSITY 1.487 g/(cm^3)
COMMENT Lowest energy structure according to CVFF950 force field.
COMMENT 1 dimensional ribbon hydrogen bonding motif.
COMMENT Fair sampling and good energy separation, but molecular
COMMENT flexibility and potential for complex hydrogen bonding
COMMENT reduces confidence in prediction.

TITL Leusen VI 2
SPACEGROUP  P21/a
CELL   11.893 13.649  7.569 90.000 114.040 90.000
ATOM  C1     0.49941   0.39555   0.34674
ATOM  H2     0.50152   0.42934   0.21909
ATOM  C3     0.60887   0.37392   0.50511
ATOM  H4     0.69599   0.39051   0.49825
ATOM  C5     0.60562   0.33159   0.67067
ATOM  H6     0.69079   0.31481   0.79303
ATOM  C7     0.49186   0.31091   0.67534
ATOM  S8     0.48625   0.24847   0.87340
ATOM  C9     0.38175   0.33223   0.51723
ATOM H10     0.29372   0.31449   0.52023
ATOM C11     0.38614   0.37455   0.35281
ATOM H12     0.30206   0.39093   0.22816
ATOM N13     0.42970   0.13427   0.80155
ATOM O14     0.38363   0.29625   0.92990
ATOM O15     0.61409   0.24749   1.05850
ATOM C16     0.48999   0.06244   0.78340
ATOM C17     0.43176  -0.02430   0.70947
ATOM C18     0.49709  -0.10483   0.69447
ATOM C19     0.62273  -0.10223   0.75203
ATOM C20     0.68718  -0.01815   0.82473
ATOM N21     0.62427   0.06967   0.84246
ATOM N22     0.81273  -0.01215   0.88340
ATOM H23     0.33251  -0.03106   0.66193
ATOM H24     0.44772  -0.17277   0.63605
ATOM H25     0.67069  -0.16793   0.73931
ATOM H26     0.67338   0.13115   0.90493
ATOM H27     0.85984  -0.07310   0.87327
ATOM H28     0.85229   0.05510   0.92947
ENERGY  -90.04 kcal/mol asymmetric unit
DENSITY 1.476 g/(cm^3)
COMMENT Second lowest energy structure according to CVFF950 force field.
COMMENT 2 dimensional hydrogen bonding pattern.
COMMENT Fair sampling and good energy separation, but molecular
COMMENT flexibility and potential for complex hydrogen bonding
COMMENT reduces confidence in prediction.  Nevertheless, this structure
COMMENT seems plausible.
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TITL Leusen VI 3
SPACEGROUP  P21/c
CELL    8.086  8.674 16.118 90.000 98.043 90.000
ATOM  C1    -0.53958   1.00119   0.38208
ATOM  H2    -0.64399   1.01080   0.41717
ATOM  C3    -0.40519   1.10332   0.39706
ATOM  H4    -0.40454   1.19157   0.44458
ATOM  C5    -0.27235   1.09237   0.35072
ATOM  H6    -0.17010   1.17376   0.36133
ATOM  C7    -0.27352   0.97608   0.29066
ATOM  S8    -0.10469   0.95833   0.23430
ATOM  C9    -0.40604   0.87217   0.27609
ATOM H10    -0.40469   0.77964   0.23117
ATOM C11    -0.53988   0.88615   0.32147
ATOM H12    -0.64348   0.80651   0.31041
ATOM N13    -0.11947   1.09869   0.16011
ATOM O14    -0.10417   0.79830   0.18660
ATOM O15     0.06569   0.97634   0.29597
ATOM C16    -0.00827   1.12758   0.11520
ATOM C17    -0.03215   1.24052   0.05513
ATOM C18     0.08988   1.27408   0.00619
ATOM C19     0.23985   1.19660   0.01490
ATOM C20     0.27382   1.08379   0.07390
ATOM N21     0.15092   1.04174   0.12692
ATOM N22     0.42499   1.00800   0.08744
ATOM H23    -0.14815   1.30632   0.04542
ATOM H24     0.06800   1.36486  -0.04096
ATOM H25     0.33180   1.22695  -0.02554
ATOM H26     0.17782   0.96391   0.17440
ATOM H27     0.52006   1.04371   0.05606
ATOM H28     0.44193   0.93244   0.13663
ENERGY  -89.37 kcal/mol asymmetric unit
DENSITY 1.479 g/(cm^3)
COMMENT Third lowest energy structure according to CVFF950 force field.
COMMENT 0 dimensional dimer hydrogen bonding motif.
COMMENT This structure is considerably higher in energy than the first
COMMENT two and exhibits an unfavorable hydrogen bonding pattern.
COMMENT Unlikely to be stable.

TITL Mooy-VI-1
SPACEGROUP  P-1
CELL   10.663  8.738  9.473 92.346 55.726 60.248
ATOM  C1     0.70697   0.41783   0.22925
ATOM  H2     0.82895   0.27381   0.14573
ATOM  C3     0.54802   0.48137   0.24640
ATOM  H4     0.55464   0.38341   0.17439
ATOM  C5     0.37969   0.67891   0.36268
ATOM  H6     0.26412   0.72336   0.37508
ATOM  C7     0.37078   0.81330   0.46165
ATOM  S8     0.16591   1.05892   0.60496
ATOM  C9     0.53003   0.74876   0.44475
ATOM H10     0.52472   0.84448   0.51762
ATOM C11     0.69861   0.55174   0.32735
ATOM H12     0.81478   0.50638   0.31410
ATOM N13     0.21015   1.19682   0.49747
ATOM O14     0.11287   1.13031   0.80029
ATOM O15    -0.01865   1.09596   0.65459
ATOM C16     0.21549   1.21131   0.35418
ATOM C17     0.25156   1.33415   0.28346
ATOM C18     0.26541   1.35034   0.13017
ATOM C19     0.24245   1.24134   0.04837
ATOM C20     0.20450   1.12074   0.12513
ATOM N21     0.19047   1.11083   0.27503
ATOM N22     0.18004   1.01598   0.05048
ATOM H23     0.26582   1.41086   0.34687
ATOM H24     0.29087   1.44143   0.07874
ATOM H25     0.25140   1.25133  -0.06362
ATOM H26     0.16038   1.02884   0.32834
ATOM H27     0.19346   1.02049  -0.05917
ATOM H28     0.14914   0.93543   0.10546
ENERGY  -60.39 kcal/mol
COMMENT Density 1.461 g/cc
COMMENT Lowest-energy structure in Dreiding+Multipole force field
COMMENT Less confidence in both the sampling and the accuracy of the
COMMENT energy function for this flexible molecule
COMMENT Confidence (1-3) : 1
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TITL Mooy-VI-2
SPACEGROUP  P21/c
CELL   14.106  5.895 16.626 90.000 126.085 90.000
ATOM  C1     0.02414   0.63938   0.90397
ATOM  H2     0.09616   0.60011   0.97372
ATOM  C3    -0.06669   0.48163   0.84963
ATOM  H4    -0.06122   0.32784   0.88036
ATOM  C5    -0.16449   0.53444   0.75327
ATOM  H6    -0.22995   0.41820   0.71334
ATOM  C7    -0.17259   0.74647   0.71162
ATOM  S8    -0.29369   0.81794   0.59358
ATOM  C9    -0.08156   0.90377   0.76621
ATOM H10    -0.08610   1.05824   0.73642
ATOM C11     0.01624   0.85065   0.86212
ATOM H12     0.08173   0.96666   0.90116
ATOM N13    -0.26586   0.77778   0.50872
ATOM O14    -0.32830   1.07481   0.59262
ATOM O15    -0.40385   0.67091   0.56445
ATOM C16    -0.30180   0.60173   0.44601
ATOM C17    -0.26487   0.59595   0.38499
ATOM C18    -0.29679   0.41478   0.31960
ATOM C19    -0.36786   0.24144   0.31422
ATOM C20    -0.40342   0.25605   0.37675
ATOM N21    -0.36946   0.43242   0.44018
ATOM N22    -0.47323   0.09592   0.37308
ATOM H23    -0.21439   0.72390   0.38981
ATOM H24    -0.26936   0.40989   0.27504
ATOM H25    -0.39225   0.10803   0.26641
ATOM H26    -0.39515   0.43714   0.48330
ATOM H27    -0.49505  -0.03583   0.33066
ATOM H28    -0.50087   0.11001   0.41428
ENERGY  -60.00 kcal/mol
COMMENT Density 1.482 g/cc
COMMENT 2nd lowest-energy structure in Dreiding+Multipole force field

TITL Mooy-VI-3
SPACEGROUP  Pbca
CELL   23.316  8.798 10.753 90.000 90.000 90.000
ATOM  C1     0.26059   0.31598   0.47721
ATOM  H2     0.23050   0.24926   0.51929
ATOM  C3     0.30315   0.38649   0.54843
ATOM  H4     0.30387   0.37169   0.64249
ATOM  C5     0.34483   0.47671   0.49084
ATOM  H6     0.37576   0.52709   0.54394
ATOM  C7     0.34395   0.49711   0.36144
ATOM  S8     0.39686   0.60264   0.28804
ATOM  C9     0.30069   0.42821   0.29054
ATOM H10     0.29938   0.44267   0.19630
ATOM C11     0.25928   0.33738   0.34830
ATOM H12     0.22819   0.28651   0.29615
ATOM N13     0.43483   0.48567   0.19437
ATOM O14     0.44119   0.67085   0.38523
ATOM O15     0.37089   0.73535   0.20547
ATOM C16     0.42783   0.44922   0.07404
ATOM C17     0.38593   0.50898  -0.00413
ATOM C18     0.38146   0.45882  -0.12667
ATOM C19     0.41942   0.34898  -0.17106
ATOM C20     0.46101   0.29225  -0.08970
ATOM N21     0.46412   0.34493   0.02812
ATOM N22     0.49762   0.18408  -0.12746
ATOM H23     0.35936   0.58886   0.02861
ATOM H24     0.35079   0.50289  -0.18379
ATOM H25     0.41663   0.31150  -0.26055
ATOM H26     0.49384   0.30465   0.08264
ATOM H27     0.49130   0.13191  -0.20592
ATOM H28     0.52981   0.15509  -0.07532
ENERGY  -59.62 kcal/mol
COMMENT Density 1.501 g/cc
COMMENT 7th lowest-energy structure in Dreiding+Multipole force field
COMMENT Chosen because it is the first trans S-N=C-N conformer

TITL Scheraga VI 1
SPACEGROUP P21/c
CELL  9.0080  12.8570  15.8170  90.0000 133.5100  90.0000
ATOM S1       .43688   .11149   .18197
ATOM C2       .56124   .05819   .32010
ATOM C3       .48019  -.03020   .32582
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ATOM C4       .57746  -.07255   .43356
ATOM C5       .75329  -.02640   .53433
ATOM C6       .83215   .06227   .52774
ATOM C7       .73600   .10512   .42013
ATOM H8       .34287  -.06437   .24720
ATOM H9       .51586  -.14102   .43894
ATOM H10      .82815  -.05943   .61796
ATOM H11      .96757   .09834   .60594
ATOM H12      .79404   .17438   .41366
ATOM O13      .43769   .03224   .11660
ATOM N14      .20896   .13220   .12745
ATOM O15      .53374   .20852   .20029
ATOM C16      .16492   .17756   .18157
ATOM C17     -.03339   .16435   .14028
ATOM C18     -.07833   .21087   .19713
ATOM C19      .06498   .27295   .29765
ATOM C20      .25227   .28621   .33532
ATOM N21      .29662   .23957   .27777
ATOM H22     -.14010   .11666   .06474
ATOM H23     -.22777   .20001   .16564
ATOM H24      .02823   .30843   .34267
ATOM N25      .40509   .34767   .42735
ATOM H26      .43018   .25539   .30144
ATOM H27      .37886   .38082   .47304
ATOM H28      .47033   .39593   .41171
ENERGY 35.12 kcal/mol
COMMENT Lowest energy structure.
COMMENT The packing seems reasonable.
COMMENT Confidence level (1-10): 3, by energy

TITL Scheraga VI 2
SPACEGROUP P21/c
CELL  7.6560  11.1400  17.7970  90.0000 118.8100  90.0000
S1      -.04130   .07237   .13176
C2       .17839   .16000   .18010
C3       .18545   .25889   .22885
C4       .35727   .32732   .26720
C5       .51960   .29723   .25636
C6       .51055   .19885   .20706
C7       .33916   .12956   .16855
H8       .05796   .28180   .23588
H9       .36424   .40415   .30507
H10      .65275   .35088   .28611
H11      .63595   .17617   .19824
H12      .32914   .05381   .12946
O13     -.07371   .02525   .20032
N14     -.20856   .16984   .07503
O15     -.02041  -.01354   .07668
C16     -.19263   .24828   .02436
C17     -.31853   .35168  -.00226
C18     -.30073   .43350  -.05436
C19     -.16014   .42127  -.08407
C20     -.04291   .32180  -.05936
N21     -.06164   .23964  -.00719
H22     -.42329   .36053   .02106
H23     -.39560   .51132  -.07368
H24     -.14597   .48743  -.12456
N25      .09358   .29294  -.08545
H26      .01597   .16267   .00606
H27      .11417   .35298  -.12204
H28      .08644   .20899  -.10597
ENERGY 34.26 kcal/mol
COMMENT Releative E=+0.86 kcal/mol.
COMMENT Confidence level (1-10): 2, by energy

TITL Scheraga VI 3
SPACEGROUP P21/c
CELL  7.9210  14.9370  11.1970  90.0000 101.2700  90.0000
ATOM S1       .35235   .23211   .31309
ATOM C2       .17781   .19023   .20434
ATOM C3       .01212   .19939   .22597
ATOM C4      -.12492   .16723   .14091
ATOM C5      -.09591   .12595   .03576
ATOM C6       .07008   .11654   .01543
ATOM C7       .20819   .14877   .10001
ATOM H8      -.00813   .23060   .30833
ATOM H9      -.25380   .17397   .15683
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ATOM H10     -.20281   .10082  -.03000
ATOM H11      .09240   .08398  -.06569
ATOM H12      .33764   .14118   .08615
ATOM O13      .32591   .32798   .32349
ATOM N14      .33039   .18033   .43525
ATOM O15      .50857   .20429   .27763
ATOM C16      .30337   .09467   .44303
ATOM C17      .23524   .06033   .54288
ATOM C18      .20603  -.02856   .55031
ATOM C19      .24012  -.09019   .46189
ATOM C20      .30711  -.05706   .36814
ATOM N21      .33671   .03228   .36118
ATOM H22      .20872   .10756   .60875
ATOM H23      .15392  -.05365   .62555
ATOM H24      .21459  -.16035   .46809
ATOM N25      .35542  -.10755   .27824
ATOM H26     .39681   .05537   .29629
ATOM H27     .33129  -.17306   .27924
ATOM H28     .47156  -.09396   .26131
ENERGY 33.85 kcal/mol
COMMENT Releative E=+1.27 kcal/mol
COMMENT Confidence level (1-10): 2, by energy.

TITL Schmidt VI 1
SPACEGROUP C2/c
CELL  22.8663  5.5332 16.7342 90.0000 91.3230 90.0000
ATOM   S1         0.42176  0.48110  0.67397
ATOM   O1         0.43457  0.71256  0.70977
ATOM   O2         0.45051  0.42631  0.59943
ATOM   N1         0.43788  0.25480  0.72989
ATOM   C1         0.34565  0.46630  0.65640
ATOM   C2         0.32314  0.27134  0.61436
ATOM   C3         0.26338  0.24704  0.60242
ATOM   C4         0.22518  0.41774  0.63217
ATOM   C5         0.24858  0.61294  0.67312
ATOM   C6         0.30811  0.63878  0.68507
ATOM   C7         0.42248  0.24326  0.80747
ATOM   C8         0.38894  0.40491  0.85209
ATOM   C9         0.38073  0.36612  0.93182
ATOM   C10        0.40455  0.16417  0.97007
ATOM   C11        0.43518  0.00591  0.92663
ATOM   N2         0.44369  0.04536  0.84693
ATOM   N3         0.45927 -0.19609  0.95536
ATOM   H2         0.35220  0.13828  0.59655
ATOM   H3         0.24551  0.10100  0.57129
ATOM   H4         0.18024  0.39962  0.62314
ATOM   H5         0.22202  0.74529  0.69739
ATOM   H6         0.32531  0.78879  0.71477
ATOM   H8         0.37134  0.56067  0.82639
ATOM   H9         0.35840  0.49985  0.96236
ATOM   H10        0.39860  0.15624  1.03144
ATOM   H72        0.46733 -0.07614  0.81626
ATOM   H73        0.48169 -0.30618  0.91892
ATOM   H74        0.45513 -0.23929  1.01359
ENERGY -117.12 kJ/mol
COMMENT  Not the best one in energy, but sensible hydrogen bond system.
COMMENT  Confidence level (1-10): 3, by energy and chemical intuition
COMMENT  (hydrogen bonds, molecular conformation)
COMMENT  No intramolecular H bond. Torsion angle Ph-S-N=C = -71 degree.

TITL Schmidt VI 2
SPACEGROUP P-1
CELL   6.8517  7.7755 11.1569 83.7270 73.5560 69.9060
ATOM   S1         0.24922  0.18263  0.17498
ATOM   O1         0.28600  0.04570  0.08647
ATOM   O2         0.06251  0.20775  0.28217
ATOM   N1         0.44417  0.14844  0.23660
ATOM   C1         0.22173  0.39305  0.09355
ATOM   C2         0.11942  0.55286  0.16087
ATOM   C3         0.10319  0.72082  0.10126
ATOM   C4         0.18855  0.73166 -0.02674
ATOM   C5         0.28768  0.57050 -0.09261
ATOM   C6         0.30397  0.40258 -0.03391
ATOM   C7         0.52323 -0.00911  0.29803
ATOM   C8         0.45945 -0.16566  0.32037
ATOM   C9         0.55394 -0.30854  0.39075
ATOM   C10        0.71730 -0.30328  0.43989
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ATOM   C11        0.78245 -0.15548  0.41520
ATOM   N2         0.68709 -0.01196  0.34536
ATOM   N3         0.93918 -0.13452  0.45432
ATOM   H2         0.06758  0.54153  0.25756
ATOM   H3         0.02777  0.84275  0.15029
ATOM   H4         0.17618  0.85796 -0.07160
ATOM   H5         0.35632  0.57022 -0.18854
ATOM   H6         0.37559  0.28222 -0.08479
ATOM   H8         0.33510 -0.17394  0.28770
ATOM   H9         0.49067 -0.41549  0.40987
ATOM   H10        0.77165 -0.41359  0.49738
ATOM   H72        0.73876  0.09752  0.32949
ATOM   H73        0.97908 -0.01933  0.43191
ATOM   H74        1.01821 -0.23381  0.50643
ENERGY  -121.90 kJ/mol
COMMENT  Best energy, but one hydrogen bond is quite long.
COMMENT  Confidence level (1-10): 3, by energy and chemical intuition
COMMENT  (hydrogen bonds, molecular conformation)
COMMENT  No intramolecular H bond. Torsion angle Ph-S-N=C = -174 degree.

TITL Schmidt VI 3
SPACEGROUP P21/c
CELL    4.9458   9.3060  23.1190  90.000  96.542  90.000
ATOM  S1         0.63531   0.30004   0.33481
ATOM  O1         0.34837   0.30877   0.34024
ATOM  O2         0.72015   0.19046   0.29575
ATOM  N1         0.76319   0.44490   0.31229
ATOM  C1         0.80527   0.26838   0.40475
ATOM  C2         0.99442   0.15879   0.41172
ATOM  C3         1.14150   0.13458   0.46536
ATOM  C4         1.10123   0.21940   0.51295
ATOM  C5         0.90871   0.32717   0.50529
ATOM  C6         0.76075   0.35171   0.45199
ATOM  C7         0.66761   0.57668   0.32431
ATOM  C8         0.45698   0.61464   0.35728
ATOM  C9         0.38170   0.75533   0.36181
ATOM  C10        0.51469   0.86388   0.33473
ATOM  C11        0.72170   0.82760   0.30462
ATOM  N2         0.79613   0.68670   0.29979
ATOM  N3         0.86878   0.92069   0.27765
ATOM  H2         1.03295   0.10183   0.37483
ATOM  H3         1.28587   0.05311   0.47147
ATOM  H4         1.21164   0.20113   0.55331
ATOM  H5         0.87171   0.39493   0.53928
ATOM  H6         0.61279   0.43155   0.44696
ATOM  H8         0.34835   0.53690   0.37725
ATOM  H9         0.21405   0.77525   0.38399
ATOM  H10        0.43454   0.96647   0.33807
ATOM  H72        0.95100   0.66316   0.27645
ATOM  H73        1.02147   0.88515   0.25587
ATOM  H74        0.82769   1.02687   0.27898
ENERGY -117.12 kJ/mol
COMMENT  Not the best one in energy, but acceptable hydrogen bond system.
COMMENT  Confidence level (1-10): 2, by energy and chemical intuition
COMMENT  (hydrogen bonds, molecular conformation)
COMMENT  No intramolecular H bond. Torsion angle Ph-S-N=C = -87 degree.

TITL  Van Eijck VI 1
SPACEGROUP P-1
CELL    9.84721  30.49148  21.45812     4.868    90.486    90.507
ATOM C1           0.494229 -1.195248  1.927653
ATOM H2           0.582429 -1.429804  2.268802
ATOM C3           0.487087 -0.895477  1.449120
ATOM H4           0.569955 -0.899759  1.422588
ATOM C5           0.387228 -1.193018  1.966852
ATOM H6           0.392914 -1.424521  2.336453
ATOM C7           0.372367 -0.592266  1.008111
ATOM H8           0.365469 -0.359059  0.636237
ATOM C9           0.272252 -0.892285  1.529094
ATOM H10          0.188813 -0.893611  1.563317
ATOM C11          0.264619 -0.591659  1.049370
ATOM S12          0.120087 -0.212865  0.497013
ATOM O13          0.098831 -0.254243  0.489491
ATOM O14          0.008834 -0.427730  0.835496
ATOM N15          0.170429  0.349597 -0.276537
ATOM C16          0.171425  0.533722 -0.481261
ATOM C17          0.226348  1.052398 -1.208309
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ATOM H18          0.261068  1.256529 -1.538129
ATOM C19          0.233276  1.282443 -1.477587
ATOM H20          0.273291  1.669411 -2.021010
ATOM C21          0.186369  1.006817 -1.032752
ATOM H22          0.191653  1.192314 -1.250248
ATOM C23          0.135129  0.528051 -0.360385
ATOM N24          0.090254  0.265039  0.060970
ATOM H25          0.052645 -0.094454  0.565673
ATOM H26          0.090284  0.439927 -0.144007
ATOM N27          0.128439  0.300119 -0.095679
ATOM H28          0.088153 -0.058680  0.409556
ENERGY   -540.459 kJ/mol
COMMENT The best S-N-C-N cis structure, both in energy and free energy.
COMMENT Second best structures are more than 2 kJ/mol higher.
COMMENT Nevertheless, for an ad-hoc force field it is just a long shot.

TITL  Van Eijck VI 2
SPACEGROUP P-1
CELL    9.33781  16.23431   8.37868    34.447    94.099    71.972
ATOM C1           0.789836  0.296724  1.282332
ATOM H2           0.885996  0.164935  1.566983
ATOM C3           0.675736  0.311469  1.130791
ATOM H4           0.684283  0.190777  1.298073
ATOM C5           0.779726  0.452197  1.066704
ATOM H6           0.868568  0.439271  1.186562
ATOM C7           0.550303  0.483211  0.761305
ATOM H8           0.461021  0.496346  0.641382
ATOM C9           0.654234  0.623789  0.697110
ATOM H10          0.644812  0.744810  0.528985
ATOM C11          0.539331  0.639454  0.544070
ATOM S12          0.379400  0.854106  0.079212
ATOM O13          0.210907  0.879192  0.011732
ATOM O14          0.347651  1.007336 -0.079712
ATOM N15          0.490805  0.802952  0.003851
ATOM C16          0.633718  0.791987  0.002817
ATOM C17          0.705992  0.740842 -0.071713
ATOM H18          0.637604  0.715523 -0.121982
ATOM C19          0.854355  0.726169 -0.081491
ATOM H20          0.905189  0.689363 -0.140097
ATOM C21          0.944314  0.761176 -0.014007
ATOM H22          1.062481  0.750384 -0.023431
ATOM C23          0.880039  0.808540  0.055607
ATOM N24          0.954744  0.845476  0.113185
ATOM H25          0.901013  0.884960  0.156467
ATOM H26          1.062900  0.842763  0.096643
ATOM N27          0.727737  0.824152  0.061724
ATOM H28          0.681191  0.862920  0.108941
ENERGY   -538.030 kJ/mol
COMMENT The second best S-N-C-N cis in free energy (and #3 in energy).

TITL  Van Eijck VI 3
SPACEGROUP P21/c
CELL   13.02141   7.68092  11.94011    90.000    62.973    90.000
ATOM C1            .059817   .054095   .139062
ATOM H2            .017984  -.070778   .150930
ATOM C3            .134520   .082917   .192034
ATOM H4            .149958  -.019989   .244298
ATOM C5            .039045   .185785   .071060
ATOM H6           -.019243   .163412   .030875
ATOM C7            .188001   .245087   .177726
ATOM H8            .244971   .269382   .219327
ATOM C9            .093374   .347074   .055990
ATOM H10           .077814   .450012   .004085
ATOM C11           .167221   .377309   .109813
ATOM S12           .230772   .584050   .094990
ATOM O13           .170281   .702623   .053179
ATOM O14           .216943   .625984   .218063
ATOM N15           .365232   .549180  -.000641
ATOM C16           .417666   .558411  -.122865
ATOM C17           .362387   .600635  -.201691
ATOM H18           .271027   .627024  -.159491
ATOM C19           .422758   .611952  -.327699
ATOM H20           .379747   .645319  -.383645
ATOM C21           .545773   .580528  -.387474
ATOM H22           .593866   .590703  -.488432
ATOM C23           .599048   .539090  -.318012
ATOM N24           .711332   .505521  -.371336
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ATOM H25           .749465   .461848  -.318540
ATOM H26           .759306   .509801  -.464940
ATOM N27           .535585   .528403  -.188620
ATOM H28           .575637   .496817  -.136805
ENERGY   -531.502 kJ/mol
COMMENT The best S-N-C-N trans structure in free energy without imaginary
COMMENT    frequencies (and second best in energy).
COMMENT Many cis structures are much better. But a trans-structure may have
COMMENT    been synthesised and remain quite stable.
COMMENT Whether the substance is cis or trans should have been known to the
COMMENT    chemist who made the compound, and might have been given.
COMMENT    Even with that knowledge the problem is still difficult enough.

TITL Verwer VI 1
SPACEGROUP P21/a
CELL 7.0103  24.5200   6.6567  90.0000  85.2087  90.0000
ATOM   C1  0.82984  0.53734 -0.77117
ATOM   C2  0.64883  0.56244 -0.76041
ATOM   C3  0.48218  0.53031 -0.74933
ATOM   C4  0.49601  0.47304 -0.75116
ATOM   C5  0.67746  0.44764 -0.76369
ATOM   C6  0.84440  0.48010 -0.77204
ATOM   S7  0.69436  0.37681 -0.76761
ATOM   N8  0.65293  0.35284 -0.53021
ATOM   C9  0.65282  0.30021 -0.50062
ATOM  C10  0.69191  0.25678 -0.63084
ATOM  C11  0.66749  0.20363 -0.55908
ATOM  C12  0.60281  0.19781 -0.35671
ATOM  C13  0.57480  0.24394 -0.24399
ATOM  N14  0.60083  0.29251 -0.31137
ATOM  O15  0.90176  0.35795 -0.85645
ATOM  O16  0.54101  0.35142 -0.90423
ATOM  N17  0.51529  0.24271 -0.05854
ATOM  H18  0.95098  0.56079 -0.77884
ATOM  H19  0.63777  0.60403 -0.76050
ATOM  H20  0.35096  0.54886 -0.73977
ATOM  H21  0.37363  0.45001 -0.74349
ATOM  H22  0.97704  0.46227 -0.77927
ATOM  H23  0.73745  0.26375 -0.77522
ATOM  H24  0.69485  0.17034 -0.65114
ATOM  H25  0.57558  0.16087 -0.29310
ATOM  H26  0.58059  0.32267 -0.22570
ATOM  H27  0.48539  0.20809  0.00361
ATOM  H28  0.50494  0.27677  0.01152
ENERGY -756.34 kcal/mol
COMMENT d= 1.4522 g/cc
COMMENT structure ranked nr. 3 by energy
COMMENT structures nr. 1 and 2 have a very unlikely SO2-Ph torsion angle
COMMENT and have therefore been skipped.

TITL Verwer VI 2
SPACEGROUP An (A1n1)
CELL 7.0544  24.5406   6.6024  90.0000  93.8334  90.0000
ATOM   C1 -0.07830  0.54222  0.18082
ATOM   C2  0.10596  0.56396  0.17637
ATOM   C3  0.26330  0.52890  0.17394
ATOM   C4  0.23703  0.47207  0.17505
ATOM   C5  0.05232  0.45001  0.17917
ATOM   C6 -0.10534  0.48539  0.18200
ATOM   S7  0.01921  0.37970  0.17921
ATOM   N8 -0.03360  0.35806 -0.06069
ATOM   C9 -0.04504  0.30579 -0.09691
ATOM  C10 -0.01250  0.26073  0.02730
ATOM  C11 -0.04254  0.20863 -0.05221
ATOM  C12 -0.10893  0.20545 -0.25508
ATOM  C13 -0.13312  0.25288 -0.36075
ATOM  N14 -0.10022  0.30046 -0.28706
ATOM  O15 -0.14870  0.36304  0.31636
ATOM  O16  0.20837  0.35034  0.26720
ATOM  N17 -0.19425  0.25344 -0.54586
ATOM  H18 -0.19291  0.56777  0.18266
ATOM  H19  0.12639  0.60520  0.17476
ATOM  H20  0.39702  0.54502  0.17166
ATOM  H21  0.35316  0.44699  0.17319
ATOM  H22 -0.24023  0.46997  0.18460
ATOM  H23  0.03341  0.26561  0.17282
ATOM  H24 -0.01788  0.17423  0.03473
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ATOM  H25 -0.14012  0.16947 -0.32455
ATOM  H26 -0.11622  0.33147 -0.36942
ATOM  H27 -0.22362  0.21910 -0.60995
ATOM  H28 -0.20330  0.28798 -0.61296
ENERGY -756.26 kcal/mol
COMMENT d= 1.451 g/cc
COMMENT Structure ranked nr. 4 by energy (1 and 2 were left out)
COMMENT Spacegroup is Cc, unique axis b, cell choice 2, giving An

TITL Verwer  VI 3
SPACEGROUP Pbca
CELL 24.3839   7.1344  13.2808  90.0000  90.0000  90.0000
ATOM   C1 -0.03229  0.72541  1.11970
ATOM   C2 -0.06365  0.89013  1.12858
ATOM   C3 -0.03744  1.06482  1.13693
ATOM   C4  0.02015  1.07534  1.13787
ATOM   C5  0.05190  0.91022  1.13098
ATOM   C6  0.02539  0.73518  1.12091
ATOM   S7  0.12321  0.92141  1.13397
ATOM   N8  0.14782  0.87222  1.01812
ATOM   C9  0.20044  0.88456  1.00175
ATOM  C10  0.24411  0.92484  1.06483
ATOM  C11  0.29718  0.92620  1.02584
ATOM  C12  0.30253  0.88931  0.92335
ATOM  C13  0.25615  0.84887  0.87037
ATOM  N14  0.20770  0.84665  0.90736
ATOM  O15  0.14711  0.77349  1.21222
ATOM  O16  0.14340  1.12475  1.16652
ATOM  N17  0.25681  0.80863  0.77728
ATOM  H18 -0.05151  0.59857  1.11283
ATOM  H19 -0.10555  0.88401  1.12868
ATOM  H20 -0.06058  1.18420  1.14200
ATOM  H21  0.03869  1.20376  1.14376
ATOM  H22  0.04795  0.61445  1.11488
ATOM  H23  0.23745  0.95214  1.13772
ATOM  H24  0.33070  0.95511  1.07032
ATOM  H25  0.33929  0.89301  0.88810
ATOM  H26  0.17732  0.81694  0.86704
ATOM  H27  0.29111  0.81434  0.74193
ATOM  H28  0.22255  0.77902  0.74625
ENERGY -756.08 kcal/mol
COMMENT d= 1.4334 g/cc
COMMENT structure ranked nr. 7 by energy
COMMENT structures ranked 5 and 6 (and 2,3) were discarded in view of
COMMENT the unlikely SO2-Ph torsion angle.

TITL Williams VI 1
SPACEGROUP P21/c
CELL 13.31   12.03    7.15   90.00  101.26   90.00
ATOM H3           0.42383   0.44048   0.35819
ATOM H5           0.57320   0.31948   0.33676
ATOM N3           0.53404   0.25890   0.34119
ATOM H6           0.56300   0.19161   0.33647
ATOM C4           0.43475   0.27082   0.35455
ATOM C3           0.38665   0.37047   0.36223
ATOM N1           0.38156   0.17475   0.36040
ATOM H2           0.24694   0.43897   0.38170
ATOM H4           0.41530   0.11034   0.35508
ATOM C2           0.28247   0.36806   0.37606
ATOM C5           0.28027   0.16832   0.37379
ATOM N2           0.23144   0.07474   0.37909
ATOM S1           0.28928  -0.04206   0.36989
ATOM C1           0.22981   0.27197   0.38184
ATOM H1           0.15740   0.27007   0.39145
ATOM C6           0.19146  -0.13981   0.38165
ATOM O1           0.32171  -0.05480   0.18957
ATOM O2           0.37046  -0.05629   0.53475
ATOM C7           0.20769  -0.25340   0.38385
ATOM C8           0.12657  -0.32425   0.39327
ATOM C11          0.09564  -0.09614   0.38871
ATOM C9           0.03095  -0.28154   0.40035
ATOM C10          0.01544  -0.16739   0.39807
ATOM H7           0.27583  -0.28259   0.37876
ATOM H8           0.13749  -0.40485   0.39488
ATOM H9          -0.02608  -0.33196   0.40700
ATOM H10         -0.05232  -0.13709   0.40309
ATOM H11          0.08527  -0.01545   0.38705
```

```
ENERGY -168.14
COMMENT slightly nonplanar

TITL Williams VI 2
SPACEGROUP P21/c
CELL    14.06   11.73    6.98   90.00   76.54   90.00
ATOM H3           0.06041   0.43823   0.11615
ATOM H5          -0.08072   0.30363   0.18747
ATOM N3          -0.03853   0.24500   0.16302
ATOM H6          -0.06342   0.17429   0.17411
ATOM C4           0.05913   0.26475   0.11133
ATOM C3           0.10117   0.36985   0.09215
ATOM N1           0.11721   0.17107   0.07725
ATOM H2           0.23568   0.45029   0.02265
ATOM H4           0.08742   0.10294   0.09105
ATOM C2           0.20448   0.37539   0.03699
ATOM C5           0.21789   0.17231   0.02337
ATOM N2           0.27151   0.08083  -0.00826
ATOM S1           0.22079  -0.04247   0.01500
ATOM C1           0.26203   0.28165   0.00319
ATOM H1           0.33386   0.28529  -0.03517
ATOM C6           0.32317  -0.13443  -0.04276
ATOM O1           0.17110  -0.06248   0.21474
ATOM O2           0.15949  -0.05862  -0.12644
ATOM C7           0.41894  -0.09565  -0.09283
ATOM C8           0.49496  -0.17376  -0.13602
ATOM C11          0.30234  -0.24978  -0.03526
ATOM C9           0.47493  -0.28871  -0.12894
ATOM C10          0.37855  -0.32678  -0.07852
ATOM H7           0.43213  -0.01396  -0.09730
ATOM H8           0.56302  -0.14691  -0.17163
ATOM H9           0.52891  -0.34351  -0.15959
ATOM H10          0.36432  -0.40825  -0.07349
ATOM H11          0.23410  -0.27602   0.00046
ENERGY -166.11
COMMENT planar

TITL Williams VI 3
SPACEGROUP Pbca
CELL     7.83   11.99   23.96     90.00     90.00     90.00
ATOM H3           0.35084   0.01483   0.05421
ATOM H5           0.23072  -0.05032   0.19611
ATOM N3           0.26944  -0.02790   0.25078
ATOM H6           0.24959  -0.03799   0.32193
ATOM C4           0.35465   0.01938   0.22465
ATOM C3           0.38859   0.03685   0.11855
ATOM N1           0.40833   0.05064   0.31263
ATOM H2           0.50444   0.10037   0.03028
ATOM H4           0.38410   0.03807   0.38159
ATOM C2           0.47916   0.08731   0.10598
ATOM C5           0.49671   0.09994   0.30448
ATOM N2           0.54641   0.12896   0.39060
ATOM S1           0.50538   0.10778   0.51517
ATOM C1           0.53238   0.11832   0.19406
ATOM H1           0.59536   0.15341   0.18554
ATOM C6           0.59791   0.16070   0.59842
ATOM O1           0.32332   0.10664   0.53531
ATOM O2           0.59098   0.05559   0.53821
ATOM C7           0.68092   0.20648   0.55374
ATOM C8           0.74991   0.24607   0.62519
ATOM C11          0.58290   0.15393   0.71312
ATOM C9           0.73559   0.23969   0.73945
ATOM C10          0.65202   0.19358   0.78348
ATOM H7           0.69018   0.21051   0.47260
ATOM H8           0.80892   0.27863   0.59413
ATOM H9           0.78456   0.26778   0.78954
ATOM H10          0.64184   0.18904   0.86446
ATOM H11          0.52371   0.12127   0.74360
ENERGY -162.27
COMMENT planar

         II. Powder-assisted submission
         ==============================

TITL Dzyabchenko IV
SPACEGROUP P21/C
CELL 9.342 10.594 7.714 90. 95.00 90.
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```
ATOM O1   0.30596 0.42314 -0.16281
ATOM O2   0.30134 0.75411  0.19920
ATOM N1   0.30376 0.58389  0.02637
ATOM H1   0.30242 0.64273 -0.07513
ATOM C3   0.30788 0.36661  0.14060
ATOM C5   0.30530 0.55148  0.34281
ATOM C8   0.30583 0.45750 -0.01327
ATOM C9   0.30328 0.64031  0.18668
ATOM C1   0.06138 0.43997  0.24412
ATOM C4   0.38242 0.43130  0.29888
ATOM C2   0.15027 0.33434  0.17704
ATOM C6   0.14769 0.51890  0.37891
ATOM H11  0.36472 0.28236  0.10770
ATOM H12  0.36031 0.59857  0.45357
ATOM H2   0.01522 0.49798  0.13848
ATOM H10 -0.02925 0.39967  0.30226
ATOM H5   0.38415 0.36776  0.40852
ATOM H6   0.49359 0.45027  0.28002
ATOM H4   0.09556 0.29471  0.06044
ATOM H7   0.09122 0.60566  0.40056
ATOM H3   0.15763 0.25850  0.27096
ATOM H8   0.15468 0.46974  0.50201
COMMENT The structure solution was obtained starting from one of
COMMENT the energy minima (of the energy rank 31)found in space
COMMENT group P21/c in the 'ab initio' search, whose cell dimensions
COMMENT (a=3D9.16, b=3D10.57, c=3D7.72, beta=3D96.0)
COMMENT were close to those determined from the PD
COMMENT pattern. Structure optimisation with cell parameters based
COMMENT on experimental resulted in a model whose simulated PD
COMMENT pattern showed a similarity with experimental one. This
COMMENT model was improved by a procedure in which the
COMMENT potential energy was combined with an X-ray PD pattern
COMMENT  disagreement criterion. Note, the use of just an X-ray
COMMENT fitting, while giving quite a marginal gain in the PD
COMMENT quality fit, at the same time resulted in a markedly loss
COMMENT of the potential energy (of 0.2 kcal mol) indicating the
COMMENT loss of quality with respect to intermolecular contacts


TITL Hofmann IV second turn
SPACEGROUP P21/c
CELL 10.596 9.438 7.699  95.174 90.000 90.000
ATOM C1  -0.31383  0.12874 -0.20607
ATOM C2  -0.32857  0.02867 -0.35353
ATOM C3  -0.18650  0.00316 -0.42533
ATOM N4  -0.09826 -0.09008 -0.35711
ATOM C5  -0.13296 -0.16393 -0.22219
ATOM C6  -0.27288 -0.14539 -0.14200
ATOM C7  -0.25650 -0.05050  0.01171
ATOM C8  -0.38625 -0.09484 -0.28094
ATOM O9  -0.15069  0.06660 -0.54550
ATOM O10 -0.05046 -0.24558 -0.16538
ATOM H11 -0.42090  0.15134 -0.16442
ATOM H12 -0.26943  0.21792 -0.25600
ATOM H13 -0.40381  0.06383 -0.46248
ATOM H14 -0.00140 -0.10485 -0.40888
ATOM H15 -0.30720 -0.23896 -0.09431
ATOM H16 -0.35795 -0.04545  0.07468
ATOM H17 -0.17265 -0.08475  0.11178
ATOM H18 -0.48912 -0.07794 -0.22412
ATOM H19 -0.40620 -0.16564 -0.38773
ATOM C20 -0.21681  0.08330 -0.04677
ATOM H21 -0.10406  0.08403 -0.07835
ATOM H22 -0.22504  0.15063  0.06278
ENERGY -79.6860

TITL Mooy IV  powder
SPACEGROUP  P21/c
CELL    9.229 10.406  7.963 90.000 83.870 90.000
ATOM  C1    -0.06033   0.45132   0.73833
ATOM  C2    -0.15164   0.52637   0.88062
ATOM  C3    -0.30683   0.55827   0.83536
ATOM  C4    -0.38478   0.43183   0.79787
ATOM  C5    -0.30326   0.37229   0.63719
ATOM  C6    -0.14458   0.33759   0.66868
ATOM  C7    -0.30257   0.64324   0.68588
ATOM  N8    -0.30331   0.59394   0.52859
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ATOM  C9    -0.30630   0.46613   0.49822
ATOM O10    -0.29571   0.76249   0.70317
ATOM O11    -0.31031   0.42869   0.34956
ATOM H12    -0.02776   0.51826   0.63600
ATOM H13     0.03870   0.41488   0.78484
ATOM H14    -0.16135   0.46885   0.99589
ATOM H15    -0.09520   0.61537   0.90567
ATOM H16    -0.36787   0.60560   0.94238
ATOM H17    -0.38339   0.36547   0.90350
ATOM H18    -0.49846   0.45043   0.77956
ATOM H19    -0.36027   0.28524   0.60621
ATOM H20    -0.14837   0.25896   0.75924
ATOM H21    -0.08487   0.30348   0.55143
ATOM H22    -0.30201   0.65224   0.43261
ENERGY  -9.53 kcal/mol
COMMENT This structure was already submitted in the first
COMMENT round. It is the 2nd lowest-energy structure
COMMENT in the DREIDING+Multipole model
COMMENT Energy-minimized structure; not Rietveld refined

TITLE Price IV powder
CELL    9.372639    6.580034   13.997299   90.0 82.694186 90.0
SPACEGROUP P21/c
ATOM  N1      0.832327      0.584942      0.034838
ATOM  C1      0.644465      0.694938      0.191694
ATOM  C2      0.807846      1.047893      0.101658
ATOM  C3      0.651678      1.006502      0.086581
ATOM  C4      0.845389      0.948516      0.194058
ATOM  C5      0.614639      0.778684      0.094406
ATOM  C6      0.804377      0.721876      0.199678
ATOM  C7      0.701993      0.664399      0.013187
ATOM  C8      0.894323      0.606813      0.119895
ATOM  O1      0.665890      0.643642     -0.067342
ATOM  O2      1.014569      0.539232      0.126117
ATOM  H1      0.892840      0.511191     -0.019651
ATOM  H2      0.826091      1.211503      0.104448
ATOM  H3      0.880069      0.991529      0.039907
ATOM  H4      0.786580      1.024492      0.256573
ATOM  H5      0.579467      1.086501      0.141662
ATOM  H6      0.959934      0.964615      0.199700
ATOM  H7      0.629942      1.063403      0.016617
ATOM  H8      0.832496      0.658412      0.266839
ATOM  H9      0.502354      0.757271      0.083666
ATOM  H10     0.580184      0.776896      0.249953
ATOM  H11     0.614247      0.534743      0.198546
ENERGY 129.31 kJ/mol
COMMENT This structure, found in the original search, is
COMMENT among the group of lowest energy packings. As it
COMMENT gives a reasonable reproduction of the main features
COMMENT of the powder pattern, we would have included this
COMMENT in our guesses (replacing Price IV 3) had we had
COMMENT the powder data to guide our selection of possible
COMMENT structures.

TITL Schmidt IV Final calculated structure (Lattic par. set to exp. values)
SPACEGROUP P21/c
CELL   9.3300  10.6000   7.6700  90.000  94.670  90.000
ATOM        C1   0.29867   0.37156   0.12711
ATOM        C2   0.29838   0.46517  -0.02353
ATOM        N3   0.30301   0.59415   0.01458
ATOM        C4   0.30865   0.64125   0.18525
ATOM        C5   0.30898   0.54829   0.33665
ATOM        C6   0.15557   0.52252   0.38108
ATOM        C7   0.06717   0.45282   0.23715
ATOM        C8   0.14499   0.34096   0.16582
ATOM        C9   0.38092   0.42568   0.28934
ATOM       O10   0.29349   0.43055  -0.17843
ATOM       O11   0.31252   0.75705   0.20870
ATOM       H12   0.34831   0.28982   0.08732
ATOM       H13   0.36583   0.59029   0.44358
ATOM       H14   0.10553   0.60748   0.40636
ATOM       H15   0.16044   0.46927   0.49530
ATOM       H16   0.03816   0.51508   0.13558
ATOM       H17  -0.02769   0.42158   0.28519
ATOM       H18   0.14869   0.26781   0.25645
ATOM       H19   0.08810   0.30880   0.05223
ATOM       H20   0.37924   0.36203   0.39235
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ATOM       H21   0.48770   0.44168   0.26627
ATOM       H22   0.30298   0.65602  -0.08557
ENERGY -93.55 kJ/mol
COMMENT With the calculated packing, the powder diagram could be indexed.
COMMENT Using the reflections 100, 200, 020, 110 and 111 the cell parameters
COMMENT of the calculated packing were corrected:
COMMENT Old values:        8.9439  10.5165  7.6854  90.  95.375  90., V=719.7
COMMENT Corrected values:  9.33    10.60    7.67    90.  94.67   90., V=756.0
COMMENT Subsequently, the energy was minimized again, keeping the lattice
COMMENT parameters fixed.
COMMENT The structure was not fitted to the peak intensities.
END


TITL Schmidt IV Calculated minimum close to the experimental structure
SPACEGROUP P21/c
CELL   8.9439  10.5165   7.6854  90.000  95.375  90.000
ATOM        C1   0.29990   0.36944   0.12932
ATOM        C2   0.29799   0.46363  -0.02138
ATOM        N3   0.30101   0.59371   0.01626
ATOM        C4   0.30650   0.64142   0.18652
ATOM        C5   0.30845   0.54789   0.33798
ATOM        C6   0.14873   0.52033   0.38049
ATOM        C7   0.05720   0.44898   0.23595
ATOM        C8   0.13995   0.33700   0.16612
ATOM        C9   0.38525   0.42503   0.29210
ATOM       O10   0.29312   0.42852  -0.17594
ATOM       O11   0.30891   0.75820   0.20957
ATOM       H12   0.35284   0.28754   0.09051
ATOM       H13   0.36737   0.59094   0.44529
ATOM       H14   0.09529   0.60545   0.40479
ATOM       H15   0.15478   0.46683   0.49475
ATOM       H16   0.02584   0.51132   0.13398
ATOM       H17  -0.04130   0.41654   0.28282
ATOM       H18   0.14503   0.26341   0.25689
ATOM       H19   0.08084   0.30387   0.05214
ATOM       H20   0.38460   0.36097   0.39512
ATOM       H21   0.49647   0.44227   0.27036
ATOM       H22   0.29992   0.65596  -0.08392
ENERGY -95.32 kJ/mol
COMMENT This minimum has energy rank 9, Volume rank 5 (V=719.70 A3).
COMMENT This is the calculated packing, without fitting to powder data.
COMMENT The simulated powder diagram is similar to the exp. diagram.
COMMENT Using this calculated packing, the powder diagram could be indexed.
END


TITL  Van Eijck IV 4
SPACEGROUP P21/c
CELL   12.67161  10.50719   7.78715    90.000    45.453    90.000
ATOM C1            0.377679   0.925321   0.322606
ATOM H2            0.375340   0.859162   0.218136
ATOM H3            0.493447   0.941714   0.222352
ATOM C4            0.296765   0.868583   0.569123
ATOM H5            0.353317   0.781123   0.540413
ATOM C6            0.303533   1.050484   0.357101
ATOM H7            0.366462   1.093291   0.181143
ATOM C8            0.136392   0.836355   0.702883
ATOM H9            0.074558   0.810550   0.888689
ATOM H10           0.136229   0.752301   0.621567
ATOM C11           0.147423   1.021234   0.470393
ATOM H12           0.156063   0.969404   0.339651
ATOM H13           0.090437   1.110346   0.507139
ATOM C14           0.053575   0.943059   0.703174
ATOM H15           0.005894   1.007686   0.851384
ATOM H16          -0.039088   0.901058   0.739708
ATOM C17           0.303168   0.961368   0.712635
ATOM O18           0.306758   0.929745   0.856154
ATOM C19           0.302538   1.143218   0.509489
ATOM O20           0.300256   1.256716   0.495447
ATOM N21           0.302941   1.089530   0.671709
ATOM H22           0.303260   1.149767   0.771288
ENERGY   -208.868 kJ/mol
COMMENT The fifth in energy (sixth in ab-initio); bad in free energy.
COMMENT But a very good powder diffraction pattern, especially after
COMMENT     adjusting the cell parameters to: 12.58  10.63  7.65  47.8
COMMENT This is almost certainly the correct structure.
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TITL  Van Eijck IV 5
SPACEGROUP C2/c
CELL   18.62745  10.22354   8.04470    90.000    74.163    90.000
ATOM C1            0.938038   0.327937   0.632350
ATOM H2            0.934885   0.396811   0.736756
ATOM H3            0.996880   0.313698   0.566478
ATOM C4            0.897102   0.383406   0.507591
ATOM H5            0.924427   0.474293   0.455335
ATOM C6            0.902571   0.197789   0.703959
ATOM H7            0.934255   0.156396   0.786795
ATOM C8            0.815764   0.413356   0.605314
ATOM H9            0.784837   0.439752   0.512975
ATOM H10           0.814353   0.498968   0.686527
ATOM C11           0.822962   0.224362   0.813953
ATOM H12           0.825704   0.279207   0.928322
ATOM H13           0.795630   0.131741   0.859666
ATOM C14           0.775208   0.301021   0.719430
ATOM H15           0.753902   0.233133   0.640300
ATOM H16           0.726764   0.340885   0.814237
ATOM C17           0.902152   0.287341   0.359533
ATOM O18           0.902788   0.319063   0.216007
ATOM C19           0.904970   0.101699   0.556775
ATOM O20           0.906336  -0.014841   0.572805
ATOM N21           0.904648   0.156060   0.399079
ATOM H22           0.906431   0.094081   0.301607
ENERGY   -207.915 kJ/mol
COMMENT The tenth in energy (twelfth in ab-initio); bad in free energy.
COMMENT But an acceptable powder diffraction pattern, especially after
COMMENT     adjusting the cell parameters to: 19.66  10.61  7.65  71.6
COMMENT A second possibility, but structure #4 is much more likely.
COMMENT Of course, the two structures #4 and #5 are fairly similar.


TITL Verwer IV 1 from powder diffraction data
SPACEGROUP P21/a
CELL 7.7013  10.6358   9.3457  90.0000  94.9502  90.0000
ATOM   C1  0.74489  0.45225  0.06665
ATOM   C2  0.88561  0.52683  0.15887
ATOM   C3  0.83528  0.55645  0.30919
ATOM   C4  0.79474  0.43168  0.38243
ATOM   C5  0.63077  0.37616  0.29930
ATOM   C6  0.66894  0.34198  0.14652
ATOM   C7  0.68093  0.63865  0.30272
ATOM   N8  0.52153  0.59382  0.29805
ATOM   C9  0.49201  0.47146  0.29807
ATOM  O10  0.69381  0.75426  0.29617
ATOM  O11  0.33820  0.44291  0.29507
ATOM  H12  0.64292  0.51722  0.03036
ATOM  H13  0.79641  0.41576 -0.02699
ATOM  H14  1.00358  0.47178  0.16933
ATOM  H15  0.91179  0.61384  0.10511
ATOM  H16  0.94194  0.60249  0.37137
ATOM  H17  0.90206  0.36680  0.38393
ATOM  H18  0.77267  0.44875  0.49190
ATOM  H19  0.59408  0.29232  0.35360
ATOM  H20  0.76096  0.26525  0.15253
ATOM  H21  0.55225  0.30831  0.08526
ATOM  H22  0.42438  0.64879  0.29488
ENERGY -133.08 kcal/mol
COMMENT d=3D 1.279 g/cc
COMMENT structure ranked nr. 209 by energy
COMMENT R_P=3D9.01%, R_WP=3D11.57%. No large deviations from powder data after
COMMENT refinement by DBWS.

TITL Dzyabchenko V
SPACEGROUP P212121
CELL 7.261 10.634 15.634 90. 90. 90.
ATOM S1   0.53554  0.04820 0.18969
ATOM BR1  0.59558 -0.14307 0.48163
ATOM O3   0.47944 -0.01128 0.11210
ATOM O4   0.70486  0.11693 0.18831
ATOM N5   0.54912 -0.06467 0.26488
ATOM C6   0.35192  0.14027 0.23614
ATOM C7   0.33060  0.08537 0.32494
ATOM C8   0.44105 -0.03419 0.32566
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ATOM C9   0.38615 -0.10983 0.40321
ATOM C10  0.23397 -0.02239 0.44013
ATOM C11  0.33166  0.09388 0.48016
ATOM C12  0.40163  0.16703 0.40103
ATOM C13  0.14430  0.03279 0.35962
ATOM C14  0.05162 -0.06513 0.29961
ATOM C15  0.00190  0.13506 0.37663
ATOM H18  0.22112  0.13435 0.20350
ATOM H19  0.37942  0.23973 0.24185
ATOM H20  0.32428 -0.19719 0.38282
ATOM H21  0.14298 -0.07011 0.48409
ATOM H22  0.23966  0.14964 0.51899
ATOM H23  0.44256  0.06751 0.52256
ATOM H24  0.34920  0.26203 0.39908
ATOM H25  0.54965  0.17700 0.40094
ATOM H26  0.14697 -0.14021 0.28537
ATOM H27  0.01058 -0.02061 0.24052
ATOM H28 -0.06876 -0.10435 0.33017
ATOM H29  0.05929  0.20602 0.41825
ATOM H30 -0.11824  0.09489 0.40684
ATOM H31 -0.03890  0.17864 0.31718
COMMENT The stucture solution was obtained starting from minimum 5
COMMENT of the 'ab inition' search, whose cell parameters (a=7.57,
COMMENT b=10.01, and c=15.06 A) were close to experimental. By
COMMENT fitting the structure to the experimental cell parameters
COMMENT with energy minimization, we came to a model whose
COMMENT simulated X-ray PD pattern was in reasonable agreement with
COMMENT the experimental XPDP. The final list of coordinates was
COMMENT then obtained by fitting simulated PD patterns to the
COMMENT observed one with variation of the six rigid body
COMMENT parameters

TITL Hofmann V second turn
SPACEGROUP P212121
CELL 15.778 7.284 10.629  90.000 90.000 90.000
ATOM C1   0.10282 -0.14398 -0.05630
ATOM C2   0.04989 -0.05183 -0.02070
ATOM C3  -0.02121 -0.01455 -0.14756
ATOM C4   0.14749 -0.00226 -0.23683
ATOM C5   0.18931 -0.09323 -0.26481
ATOM C6   0.04954 -0.14820 -0.19697
ATOM C7  -0.12242 -0.09156 -0.20647
ATOM C8  -0.19320 -0.07550 -0.34249
ATOM C9  -0.29152 -0.12237 -0.13051
ATOM C10  0.04582 -0.23709 -0.25548
ATOM S11  0.21961 -0.22693 -0.37476
ATOM N12  0.28098 -0.12024 -0.36004
ATOM O13  0.40320 -0.27493 -0.35945
ATOM O14  0.16307 -0.23513 -0.51435
ATOM BR15 0.35472  0.05931 -0.16520
ATOM H16  0.25272 -0.15584 -0.04270
ATOM H17  0.02543 -0.19116  0.00052
ATOM H18 -0.05925 -0.05006  0.05238
ATOM H19  0.16825 -0.01602  0.01900
ATOM H20 -0.10637  0.04352 -0.13701
ATOM H21  0.10630  0.03110 -0.32435
ATOM H22 -0.27572 -0.13007 -0.37657
ATOM H23 -0.28225 -0.01838 -0.34445
ATOM H24 -0.08352 -0.06718 -0.41382
ATOM H25 -0.35105 -0.18004 -0.17435
ATOM H26 -0.26252 -0.13906 -0.03157
ATOM H27 -0.39867 -0.07227 -0.12974
ATOM H28  0.08688 -0.28710 -0.18777
ATOM H29 -0.08791 -0.25242 -0.29962
ENERGY -54.9553

TITL Leusen V 70
SPACEGROUP  P212121
CELL    7.359 10.941 15.586 90.000 90.000 90.000
ATOM  C1     0.83818   0.40034   0.02737
ATOM  C2     0.88451   0.34970   0.11938
ATOM  C3     0.81219   0.45313   0.18099
ATOM  C4     0.94037   0.56129   0.16931
ATOM  C5     0.90024   0.62146   0.08434
ATOM  C6     0.75107   0.52997   0.04956
ATOM  C7     0.63341   0.49863   0.13584
ATOM  C8     0.53436   0.61055   0.17484
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ATOM  C9     0.47937   0.40465   0.12225
ATOM C10     0.81863   0.42373   0.27577
ATOM S11     1.03224   0.48995   0.30708
ATOM N12     1.05588   0.59077   0.22554
ATOM Br13    1.11162   0.63098   0.01083
ATOM O14     1.02331   0.55837   0.39648
ATOM O15     1.19106   0.39212   0.30594
ATOM H16     0.95916   0.40666  -0.01433
ATOM H17     0.73847   0.34120  -0.00580
ATOM H18     0.81287   0.26249   0.13122
ATOM H19     1.03152   0.33167   0.12746
ATOM H20     0.84506   0.71436   0.09240
ATOM H21     0.66969   0.56870  -0.00313
ATOM H22     0.62234   0.68772   0.19322
ATOM H23     0.43297   0.64808   0.12956
ATOM H24     0.45982   0.58571   0.23397
ATOM H25     0.52052   0.31722   0.09316
ATOM H26     0.41384   0.37998   0.18358
ATOM H27     0.37207   0.44157   0.07983
ATOM H28     0.70994   0.46894   0.31266
ATOM H29     0.81281   0.32562   0.29101

TITL Mooy V  powder
SPACEGROUP  P212121
CELL    7.136 10.803 15.381 90.000 90.000 90.000
ATOM  C1    -0.15069  -0.09325   0.02065
ATOM  C2    -0.09760  -0.15468   0.10813
ATOM  C3    -0.17425  -0.05961   0.17521
ATOM  C4    -0.05345   0.04761   0.16795
ATOM  C5    -0.08821   0.11505   0.08911
ATOM  C6    -0.24385   0.02947   0.05165
ATOM  C7    -0.35804  -0.00994   0.13353
ATOM  C8    -0.17063  -0.10043   0.27146
ATOM  S9     0.04100  -0.02665   0.30831
ATOM N10     0.05915   0.07470   0.22952
ATOM C11    -0.45558   0.09881   0.18308
ATOM C12    -0.51373  -0.10871   0.11720
ATOM BR13    0.13012   0.13449   0.01620
ATOM O14     0.02051   0.04286   0.39847
ATOM O15     0.21671  -0.11644   0.30570
ATOM H16    -0.24948  -0.15036  -0.01554
ATOM H17    -0.02769  -0.07705  -0.01988
ATOM H18    -0.16673  -0.24417   0.11492
ATOM H19     0.05379  -0.16745   0.11385
ATOM H20    -0.14431   0.20615   0.10401
ATOM H21    -0.32711   0.07502   0.00168
ATOM H22    -0.16342  -0.20058   0.27863
ATOM H23    -0.29004  -0.06397   0.30756
ATOM H24    -0.35623   0.16688   0.20741
ATOM H25    -0.55311   0.14581   0.13971
ATOM H26    -0.53349   0.06337   0.23871
ATOM H27    -0.57115  -0.13981   0.17903
ATOM H28    -0.46310  -0.18995   0.08276
ATOM H29    -0.62594  -0.06783   0.07870
ENERGY  39.52 kcal/mol
COMMENT 9th lowest-energy structure in the Dreiding+Multipole model.
COMMENT Energy-minimized structure; not Rietveld refined


TITL Schmidt V Final calculated structure (Lattic par. set to exp. values)
SPACEGROUP P212121
CELL   7.2600  10.6400  15.6400  90.000  90.000  90.000, V=1208.13
ATOM        C1   0.29265  -0.07425   0.40717   -0.000060
ATOM        C2   0.43319  -0.00916   0.34479   -0.003340
ATOM        C3   0.38508  -0.05210   0.25588    0.052480
ATOM        C4   0.21957  -0.14154   0.27295   -0.022750
ATOM        C5   0.29341  -0.25964   0.31811   -0.048140
ATOM        C6   0.34657  -0.21437   0.40787   -0.043180
ATOM        C7   0.11831  -0.07248   0.34882   -0.039210
ATOM        C8   0.30622  -0.00261   0.48929   -0.009910
ATOM        S9   0.50507   0.09504   0.48265    1.442090
ATOM       N10   0.54192   0.07159   0.37728   -0.391920
ATOM       C11  -0.04503  -0.14692   0.38496   -0.032100
ATOM       C12   0.04928   0.05936   0.32535   -0.032100
ATOM       O13   0.64737   0.04251   0.53480   -0.566900
ATOM       O14   0.45072   0.22139   0.50096   -0.566900
ATOM      Br15   0.59262  -0.12223   0.19075   -0.082370
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ATOM       H16   0.34222   0.02453   0.21972    0.048810
ATOM       H17   0.13916  -0.15832   0.21911    0.031840
ATOM       H18   0.40567  -0.29798   0.28609    0.027020
ATOM       H19   0.19183  -0.32846   0.32066    0.027020
ATOM       H20   0.27444  -0.26196   0.45532    0.027570
ATOM       H21   0.48659  -0.22569   0.41961    0.027570
ATOM       H22   0.18860   0.05131   0.49905    0.017240
ATOM       H23   0.31684  -0.06327   0.54120    0.017240
ATOM       H24  -0.00992  -0.23846   0.40162    0.020000
ATOM       H25  -0.09489  -0.10225   0.43939    0.020000
ATOM       H26  -0.14989  -0.15071   0.33972    0.020000
ATOM       H27  -0.03913   0.05359   0.27318    0.020000
ATOM       H28  -0.02274   0.09819   0.37639    0.020000
ATOM       H29   0.15580   0.12067   0.30993    0.020000
ENERGY -90.05 kJ/mol
COMMENT  The structure of V could not be determined without indexing the
COMMENT  powder diagram, because the search was incomplete.
COMMENT  The corresponding packing would have
COMMENT  a=6.8356, b=10.3457, c=15.7930, energy=-95.44 (energy rank 10),
COMMENT  with a powder diagram reasonably similar to the experimental
COMMENT  powder diagram; but this packing was not found in the crystal
COMMENT  structure prediction step (Calculation time too short?).
COMMENT  The structure given here is not part of the Blind test, since
COMMENT  it was found only in a energy minimization with
COMMENT  lattice parameters fixed to the experimental values, after
COMMENT  indexing the powder diagram.
END

TITL  Van Eijck V 4
SPACEGROUP P212121
CELL   11.48923   6.99936  13.84368    90.000    90.000    90.000
ATOM C1            .913701   .547074   .621632
ATOM C2            .998033   .714077   .637238
ATOM H3            .955139   .849955   .650833
ATOM H4           1.052533   .734178   .573747
ATOM H5           1.055004   .684819   .698393
ATOM C6            .994383   .376828   .603024
ATOM H7           1.050881   .351522   .664760
ATOM H8           1.049760   .403899   .540590
ATOM H9            .947752   .245011   .588278
ATOM C10           .818093   .518639   .700878
ATOM H11           .854264   .495668   .772707
ATOM C12           .745939   .346575   .662341
ATOM H13           .660613   .335362   .695670
ATOM H14           .790742   .211274   .674135
ATOM C15           .736981   .394892   .554928
ATOM H16           .768818   .277709   .510503
ATOM H17           .646924   .423770   .534316
ATOM C18           .816152   .574842   .542835
ATOM C19           .745563   .738519   .585628
ATOM C20           .745675   .706346   .692507
ATOM BR21          .587359   .708953   .747903
ATOM H22           .791856   .822885   .727721
ATOM C23           .846845   .633664   .442252
ATOM H24           .937827   .604390   .426248
ATOM H25           .792361   .561765   .389550
ATOM N26           .729961   .891881   .536453
ATOM S27           .818905   .883880   .441834
ATOM O28           .755110   .935978   .356859
ATOM O29           .923113   .987888   .463792
ENERGY   -314.629 kJ/mol
COMMENT The powder spectrum has a certain resemblance to the observed one.


TITL  Van Eijck V 5
SPACEGROUP P212121
CELL    7.45973  13.16070  11.36013    90.000    90.000    90.000
ATOM C1            .034493   .882238   .084995
ATOM C2            .177583   .850445  -.004605
ATOM H3            .299154   .820951   .035699
ATOM H4            .216782   .915175  -.058565
ATOM H5            .125143   .791976  -.063304
ATOM C6           -.126849   .915601   .010584
ATOM H7           -.097489   .916067  -.083097
ATOM H8           -.168962   .992488   .032960
ATOM H9           -.241327   .865668   .023424
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ATOM C10          -.007562   .804752   .185954
ATOM H11          -.053094   .731459   .152935
ATOM C12          -.150865   .861778   .260655
ATOM H13          -.165709   .830995   .348872
ATOM H14          -.282131   .859953   .218571
ATOM C15          -.074452   .969428   .263085
ATOM H16          -.172672  1.024088   .230844
ATOM H17          -.036826   .991534   .352182
ATOM C18           .092024   .963488   .179647
ATOM C19           .233799   .906671   .250212
ATOM C20           .173160   .798460   .254749
ATOM BR21          .168857   .744669   .417161
ATOM H22           .267710   .750892   .206644
ATOM C23           .177594  1.060931   .142530
ATOM H24           .153542  1.076051   .049740
ATOM H25           .129479  1.124423   .194392
ATOM N26           .387680   .947626   .268487
ATOM S27           .409516  1.040242   .170186
ATOM O28           .485225  1.128174   .225328
ATOM O29           .495441  1.000971   .067127
ENERGY   -313.093 kJ/mol
COMMENT The powder spectrum has a certain resemblance to the observed one.
COMMENT It also looks remarkably like the one for structure #4.
COMMENT In a certain force field the structures even become equivalent.

TITL Verwer V 1 from powder diffraction data
SPACEGROUP P212121
CELL 10.6350  15.6238   7.2584  90.0000  90.0000  90.0000
ATOM  C88  0.39856  0.03225  0.84531
ATOM  C89  0.34489  0.12219  0.89038
ATOM  C90  0.44881  0.18330  0.81442
ATOM  C91  0.55722  0.17238  0.93390
ATOM  C92  0.61869  0.09160  0.90581
ATOM  C93  0.52754  0.05649  0.75535
ATOM  C94  0.49686  0.13731  0.63581
ATOM  C95  0.41811  0.28046  0.81555
ATOM  S96  0.49355  0.30943  1.02245
ATOM  N97  0.59253  0.23163  1.04102
ATOM  C98  0.61217  0.18028  0.53603
ATOM  C99  0.39796  0.12383  0.47816
ATOM BR10  0.63892  0.02176  1.12295
ATOM O101  0.55915  0.39831  1.00108
ATOM O102  0.39408  0.30058  1.18010
ATOM H103  0.33804 -0.00266  0.75037
ATOM H104  0.40823 -0.00689  0.96853
ATOM H105  0.25646  0.13302  0.81855
ATOM H106  0.32897  0.13037  1.03804
ATOM H107  0.71221  0.10186  0.85002
ATOM H108  0.56986  0.00430  0.67789
ATOM H109  0.31913  0.29595  0.82684
ATOM H110  0.46277  0.31629  0.70538
ATOM H111  0.68177  0.20685  0.62950
ATOM H112  0.65957  0.13326  0.45010
ATOM H113  0.58205  0.23307  0.44835
ATOM H114  0.37094  0.18518  0.41968
ATOM H115  0.31165  0.09305  0.52141
ATOM H116  0.43764  0.08411  0.36957
ENERGY -114.266 kcal/mol
COMMENT d=3D 1.610 g/cc
COMMENT structure ranked nr. 5 by energy
COMMENT R_P=3D23.91%; R_WP=3D29.88%; Refined using DBWS and partial energy
COMMENT minimization. Although the rms fit is rather bad, the overall fit
COMMENT looks sufficiently convincing. Some atomic coordinates may be
COMMENT off by a few 0.1A, since no attempt has been made to refine atomic
COMMENT positions.


TITL Dzyabchenko VI
SPACEGROUP=P21/C
CELL 8.240 8.947 15.056 90. 91.21 90.
ATOM S1   .18190  .38660 .34030
ATOM O2   .12440  .47516 .26614
ATOM O3   .13631  .43654 .42832
ATOM N4   .11947  .21529 .32745
ATOM C11  .15646  .10232 .38422
ATOM N12  .07881 -.02835 .36455
ATOM C13  .10509 -.15749 .41156
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ATOM C14  .21053 -.16033 .48097
ATOM C15  .28969 -.02844 .50498
ATOM C16  .26279  .10082 .45835
ATOM N18  .02357 -.28432 .38850
ATOM C5   .39450  .38029 .33404
ATOM C6   .48545  .48346 .38176
ATOM C7   .65314  .47898 .38052
ATOM C8   .73259  .37143 .33133
ATOM C9   .63952  .27054 .28316
ATOM C10  .47230  .27456 .28386
ATOM H17 -.03074 -.01742 .33678
ATOM H19  .02211 -.30908 .32372
ATOM H20  .04287 -.37367 .42630
ATOM H21  .42516  .56801 .42021
ATOM H22  .72269  .56019 .41832
ATOM H23  .86350  .36639 .33056
ATOM H24  .69898  .18643 .24398
ATOM H25  .40231  .19493 .24510
ATOM H26  .23080 -.26424 .51598
ATOM H27  .37377 -.02635 .56097
ATOM H28  .32510  .20105 .47993
COMMENT The structure was derived by starting from one marginal
COMMENT (45th lowest-energy, 4 kcal/mol above the global one)
COMMENT energy minimum in space group P21/c whose cell parameters,
COMMENT a=3D 8.65, b=3D9.16, c=3D14.66, beta=3D94.4 deg, were close to
COMMENT these determined from the Xray PD pattern. The energy
COMMENT minimization based on experimental cell dimensions resulted
COMMENT in a stucture whose simulated pattern showed a rough
COMMENT agreement with experimental one. This agreement was then
COMMENT improved by minimization of a penalty function combining
COMMENT both disagreement factor for PD patterns and the
COMMENT potential-energy function. At the same time our attempts to
COMMENT refine the structure by using the X-ray criterion only were
COMMENT unsuccessful since they resulted in inappropriate
COMMENT interatomic distances.


TITL Leusen VI PowderSolve
SPACEGROUP  P21/a  (P 1 21/a 1)
CELL   15.068  8.952  8.242 90.000 88.778 90.000
ATOM  C1     0.28182   1.27081  -0.12549
ATOM  C2     0.32541   1.37477  -0.22577
ATOM  C3     0.37832   1.48576  -0.15799
ATOM  C4     0.38878   1.49234   0.00994
ATOM  C5     0.34530   1.38743   0.10836
ATOM  C6     0.29147   1.27688   0.04232
ATOM  S7     0.34311   1.37673   0.30760
ATOM  N8     0.33074   1.22233   0.36359
ATOM  C9     0.37971   1.09957   0.34701
ATOM C10     0.45805   1.09778   0.24801
ATOM C11     0.50771   0.96869   0.23367
ATOM C12     0.48307   0.83529   0.31314
ATOM C13     0.40623   0.83647   0.40952
ATOM N14     0.35859   0.96537   0.42423
ATOM O15     0.26290   1.46001   0.35479
ATOM O16     0.43079   1.43558   0.36233
ATOM N17     0.37355   0.71527   0.49150
ATOM H18     0.24001   1.18459  -0.17829
ATOM H19     0.31774   1.36956  -0.35713
ATOM H20     0.41173   1.56773  -0.23624
ATOM H21     0.42928   1.57871   0.06530
ATOM H22     0.25748   1.19754   0.12256
ATOM H23     0.47645   1.20081   0.18597
ATOM H24     0.56816   0.96943   0.15809
ATOM H25     0.52162   0.73287   0.29937
ATOM H26     0.30372   0.97372   0.50312
ATOM H27     0.40713   0.61686   0.48830
ATOM H28     0.31563   0.72043   0.55708

TITL Schmidt VI Final calculated structure (Lattic par. set to exp. values)
SPACEGROUP P21/c
CELL    8.2414   8.9510  15.0597  90.000  91.171  90.000
ATOM  S1         0.40377   0.25018   0.13814
ATOM  O1         0.54620   0.30668   0.18397
ATOM  O2         0.42437   0.11600   0.08498
ATOM  N1         0.25750   0.20847   0.20195
ATOM  C1         0.32987   0.39300   0.06788
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ATOM  C2         0.23156   0.35410  -0.00380
ATOM  C3         0.16490   0.46334  -0.05826
ATOM  C4         0.19583   0.61326  -0.04204
ATOM  C5         0.29610   0.64977   0.02923
ATOM  C6         0.36338   0.54150   0.08368
ATOM  C7         0.19614   0.30708   0.26065
ATOM  C8         0.27750   0.40381   0.31996
ATOM  C9         0.19216   0.49030   0.37761
ATOM  C10        0.02327   0.48623   0.37780
ATOM  C11       -0.05445   0.39678   0.31910
ATOM  N2         0.03092   0.30954   0.26172
ATOM  N3        -0.21504   0.38447   0.31113
ATOM  H2         0.20223   0.24184  -0.01183
ATOM  H3         0.08989   0.43651  -0.11231
ATOM  H4         0.14581   0.69543  -0.08305
ATOM  H5         0.32232   0.76038   0.04504
ATOM  H6         0.44108   0.57015   0.13624
ATOM  H8         0.40356   0.40820   0.32340
ATOM  H9         0.25996   0.55280   0.42324
ATOM  H10       -0.03069   0.54980   0.42687
ATOM  H2        -0.03130   0.24276   0.21902
ATOM  H3        -0.26459   0.31475   0.26535
ATOM  H4        -0.28736   0.44487   0.35087
ENERGY -112.03 kJ/mol
COMMENT The minimum with energy rank 3 shows a simulated powder diagram
COMEMNT comparable to the experimental one. It was not submitted as
COMMENT predicted crystal structure, because other structures with
COMMENT similar energies seemed to be "intuitively more reliable".
COMMENT With the calculated packing, the powder diagram could be indexed.
COMMENT The lattice parameters were set to the experimental values.
COMMENT Subsequently, the energy was minimized keeping the lattice parameters
COMMENT fixed.
COMMENT The structure was not fitted to the peak intensities.
COMMENT The powder diagram is not reproduced as good as usual.
COMMENT Perhaps the structure is wrong.
END

TITL Schmidt VI Calculated minimum close to the experimental structure
SPACEGROUP P21/c
CELL   7.7745  9.4058 15.5886 90.0000 109.2720 90.0000
ATOM   S1         0.34296  0.23069  0.14821    1.495200
ATOM   O1         0.51730  0.23960  0.21911   -0.564330
ATOM   O2         0.31176  0.10678  0.08913   -0.564330
ATOM   N1         0.17230  0.23041  0.18410   -0.567920
ATOM   C1         0.31856  0.38372  0.08022   -0.035920
ATOM   C2         0.19072  0.38231 -0.00582   -0.071250
ATOM   C3         0.16133  0.50249 -0.05985   -0.063490
ATOM   C4         0.25969  0.62594 -0.02877   -0.062380
ATOM   C5         0.38853  0.62463  0.05695   -0.063490
ATOM   C6         0.41897  0.50512  0.11112   -0.071250
ATOM   C7         0.16124  0.31901  0.25058    0.094040
ATOM   C8         0.28812  0.41874  0.30193   -0.022670
ATOM   C9         0.25437  0.49368  0.36992   -0.055140
ATOM   C10        0.09278  0.47456  0.38869   -0.021700
ATOM   C11       -0.03083  0.38207  0.33760    0.101470
ATOM   N2         0.00331  0.30642  0.26987   -0.529770
ATOM   N3        -0.19172  0.35579  0.34720   -0.585230
ATOM   H2         0.11107  0.29159 -0.02585    0.060970
ATOM   H3         0.06508  0.50393 -0.12466    0.062220
ATOM   H4         0.23773  0.71630 -0.06943    0.062270
ATOM   H5         0.46509  0.71449  0.08410    0.062220
ATOM   H6         0.51865  0.50455  0.17495    0.060970
ATOM   H8         0.41219  0.43434  0.29153    0.066060
ATOM   H9         0.35836  0.55959  0.40879    0.062540
ATOM   H10        0.08316  0.53053  0.44446    0.066100
ATOM   H2        -0.09186  0.23700  0.23332    0.369420
ATOM   H3        -0.27749  0.28468  0.30613    0.357690
ATOM   H4        -0.22803  0.40695  0.39556    0.357690
ENERGY -118.80 kJ/mol
COMMENT This minimum has energy rank 3. It was not submitted as
COMMENT predicted crystal structure, because other structures with
COMMENT similar energies seemed to be "intuitively more reliable".
COMMENT This is the calculated packing, without fitting to powder data.
COMMENT The simulated powder diagram is similar to the exp. diagram.
COMMENT Using this calculated packing, the powder diagram could be indexed.
END
```

```
TITL  Van Eijck VI 4
SPACEGROUP C2/c
CELL   47.29542  10.62872  15.58563    90.000    15.895    90.000
ATOM C1           0.897459  0.499538 -0.543675
ATOM H2           0.925539  0.507329 -0.690651
ATOM C3           0.874576  0.607945 -0.429796
ATOM H4           0.884900  0.699506 -0.488415
ATOM C5           0.883760  0.380922 -0.466667
ATOM H6           0.900958  0.297491 -0.553665
ATOM C7           0.838026  0.597717 -0.239034
ATOM H8           0.819782  0.681084 -0.149395
ATOM C9           0.847688  0.370839 -0.276988
ATOM H10          0.836581  0.279707 -0.215347
ATOM C11          0.824804  0.479289 -0.162988
ATOM S12          0.777294  0.465856  0.081259
ATOM O13          0.832518  0.362828 -0.041117
ATOM O14          0.794435  0.584863  0.073185
ATOM N15          0.658503  0.434983  0.405429
ATOM C16          0.576946  0.500219  0.660537
ATOM C17          0.479445  0.446783  0.917249
ATOM H18          0.479517  0.357567  0.884090
ATOM C19          0.389090  0.505266  1.196092
ATOM H20          0.317676  0.462881  1.383945
ATOM C21          0.388679  0.624865  1.241921
ATOM H22          0.315852  0.670891  1.467346
ATOM C23          0.477538  0.677159  1.008688
ATOM N24          0.479186  0.786636  1.044972
ATOM H25          0.547141  0.824140  0.867159
ATOM H26          0.412123  0.832960  1.251814
ATOM N27          0.569524  0.615323  0.724464
ATOM H28          0.635508  0.654215  0.552335
ENERGY   -532.749 kJ/mol
COMMENT The powder spectrum has a certain resemblance to the observed one.
COMMENT There are not many structures with this property.


TITL  Van Eijck VI 5
SPACEGROUP P21/c
CELL   14.48583  10.56232  13.31071    90.000    32.350    90.000
ATOM C1          -0.690936  0.990273  1.085507
ATOM H2          -0.814841  0.985100  1.236324
ATOM C3          -0.610636  1.107521  0.998217
ATOM H4          -0.672410  1.192495  1.081516
ATOM C5          -0.610663  0.879889  0.977464
ATOM H6          -0.673212  0.789464  1.045108
ATOM C7          -0.450152  1.114676  0.803174
ATOM H8          -0.387264  1.204878  0.734401
ATOM C9          -0.449828  0.887092  0.782047
ATOM H10         -0.387604  0.802319  0.697875
ATOM C11         -0.369346  1.004520  0.694733
ATOM S12         -0.168418  1.017553  0.448894
ATOM O13         -0.077042  1.117382  0.416026
ATOM O14         -0.084454  0.896134  0.377440
ATOM N15         -0.237141  1.056334  0.402078
ATOM C16         -0.217392  0.996959  0.300032
ATOM C17         -0.293498  1.055469  0.281839
ATOM H18         -0.362014  1.143797  0.353302
ATOM C19         -0.278527  1.002254  0.176449
ATOM H20         -0.334402  1.047682  0.163103
ATOM C21         -0.185835  0.883921  0.080132
ATOM H22         -0.173040  0.842356 -0.005530
ATOM C23         -0.115800  0.826991  0.096083
ATOM N24         -0.031853  0.717737  0.011151
ATOM H25          0.019241  0.674847  0.025874
ATOM H26         -0.021087  0.675727 -0.066921
ATOM N27         -0.131795  0.883164  0.204067
ATOM H28         -0.078307  0.840759  0.214558
ENERGY   -529.008 kJ/mol
COMMENT The powder spectrum has a certain resemblance to the observed one.
COMMENT It also looks remarkably like the one for structure #4.
COMMENT Of course, these two structures are fairly similar.
COMMENT But this one has a higher energy and is less probable.
```

III. Post-predicted (high-rank and minimized experimental) structures

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TITL Dzyabchenko IV-31:  ab initio minimum closest to experimental
COMMENT  Energy=-2.835994E+01 Density=1.36816
CELL:    9.158  10.570   7.725       90.00     95.95     90.00
SPACEGROUP P21/c
at O1    .28226        .43881    -.17929
at O2    .30085        .76056     .20086
at N1    .29204        .59472     .01873
at H1    .28596        .65639    -.07992
at C3    .29975        .37400     .12186
at C5    .31014        .55372     .33420
at C8    .29052        .46920    -.02761
at C9    .30079        .64691     .18236
at C1    .05620        .44570     .24343
at C4    .38456        .43423     .27961
at C2    .14150        .34135     .16571
at C6    .15187        .52077     .37770
at H11c  .35463        .29028     .08132
at H12c  .37239        .59768     .44452
at H2    .00445        .50684     .14314
at H10c -.03307        .40415     .30481
at H5    .39142        .36762     .38616
at H6    .49650        .45328     .25535
at H4    .07932        .30502     .04990
at H7    .09679        .60731     .40706
at H3    .15309        .26283     .25556
at H8    .16495        .46818     .49818
end

TITLE Erk 1 Polymorph Predictor, #62 in P21/c, #116 of 10 space groups
CELL   7.8487  10.7661   9.4748  90.0000  96.1628  90.0000
SPACEGROUP P21/a
!SYMM -X+0.500,+Y+0.500,-Z
at C1       -0.51410   -0.52590   -0.20517
at C2       -0.37493   -0.62118   -0.20112
at C3       -0.20961   -0.56814   -0.11622
at C4       -0.17112   -0.44308   -0.18984
at C5       -0.32535   -0.36055   -0.19750
at H6       -0.58126   -0.35001   -0.20764
at H7       -0.41594   -0.70307   -0.14627
at C8       -0.33173   -0.65832   -0.35294
at H9       -0.23090   -0.55209   -0.00553
at H10      -0.10240   -0.63290   -0.11545
at C11      -0.11618   -0.47411   -0.33957
at H12      -0.06634   -0.39561   -0.12691
at N13      -0.48453   -0.40451   -0.20392
at O14      -0.66841   -0.55342   -0.21230
at O15      -0.31247   -0.24545   -0.20102
at C16      -0.25401   -0.54969   -0.43361
at H17      -0.35532   -0.48575   -0.47362
at H18      -0.19926   -0.58728   -0.52567
at H19      -0.44666   -0.69288   -0.41620
at H20      -0.23962   -0.73471   -0.34344
at H21       0.00272   -0.52788   -0.32640
at H22      -0.08938   -0.38795   -0.39420
END

TITLE Erk 1-S Systematic Search, #47 in P 21/c, #76 of 10 space groups
CELL  7.7469  10.9802   9.7430  90.0000  94.2288  90.0000
!SYMM -X+0.500,+Y+0.500,-Z
SPACEGROUP P21/a
at C1    -0.52430   -0.53578   -0.20159
at C2    -0.37100   -0.62252   -0.20187
at C3    -0.21536   -0.56809   -0.11836
at C4    -0.16811   -0.44736   -0.18349
at C5    -0.32021   -0.35959   -0.18305
at H6    -0.59163   -0.35088   -0.19081
at H7    -0.40856   -0.71020   -0.15410
at C8    -0.32433   -0.64781   -0.34911
at H9    -0.24334   -0.55528   -0.00948
at H10   -0.10421   -0.63169   -0.11668
at C11   -0.11741   -0.46916   -0.33035
at H12   -0.05577   -0.40564   -0.12214
at N13   -0.49133   -0.40820   -0.19146
at O14   -0.67588   -0.56656   -0.20889
at O15   -0.30797   -0.24907   -0.17539
at C16   -0.25745   -0.53525   -0.41935
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at H17   -0.36619   -0.47226   -0.44762
at H18   -0.20609   -0.56175   -0.51819
at H19   -0.43808   -0.68515   -0.41067
at H20   -0.22468   -0.72041   -0.34586
at H21    0.00386   -0.52310   -0.32516
at H22   -0.08627   -0.38138   -0.37878
END

TITLE Hofmann IV 358
CELL   9.220087  10.199856   7.632169  90.000000  94.629784  90.000000
SPACEGROUP       P21/c
ATOM  N1   -0.305001  -0.090668  -0.011251
ATOM  H2   -0.297769  -0.144709   0.077718
ATOM  C3   -0.299389  -0.145107  -0.176724
ATOM  O4   -0.284432  -0.263372  -0.190847
ATOM  C5   -0.308326  -0.053101  -0.330963
ATOM  H6   -0.357436  -0.103315  -0.433045
ATOM  C7   -0.392255   0.069425  -0.290326
ATOM  H8   -0.394305   0.132723  -0.390627
ATOM  H9   -0.496505   0.048545  -0.272668
ATOM  C10  -0.315692   0.133939  -0.128287
ATOM  H11  -0.365590   0.207567  -0.093684
ATOM  C12  -0.313222   0.042041   0.026086
ATOM  O13  -0.315995   0.077140   0.177680
ATOM  C14  -0.159909   0.173154  -0.163100
ATOM  H15  -0.172636   0.244888  -0.259117
ATOM  H16  -0.114805   0.212034  -0.052583
ATOM  C17  -0.072176   0.059721  -0.227503
ATOM  H18  -0.050174  -0.002984  -0.130478
ATOM  H19   0.017219   0.090500  -0.266434
ATOM  C20  -0.154071  -0.015935  -0.376192
ATOM  H21  -0.102972  -0.097171  -0.407761
ATOM  H22  -0.164455   0.033940  -0.482638
!ENERGY             -107.854
COMMENT predicted
COMMENT similarity    0.792
COMMENT rank            358
END

TITLE Hofmann IV minimized
CELL   9.200543  10.499852   7.731753  90.000000  84.182823  90.000000
SPACEGROUP       P21/c
ATOM  N1    0.193251   0.594278   0.519769
ATOM  H2    0.196477   0.647076   0.432249
ATOM  C3    0.195076   0.647369   0.683428
ATOM  O4    0.201473   0.762865   0.698028
ATOM  C5    0.192968   0.557671   0.835077
ATOM  H6    0.140209   0.603540   0.937555
ATOM  C7    0.117747   0.434105   0.796063
ATOM  H8    0.120398   0.372629   0.894552
ATOM  H9    0.011755   0.448388   0.781531
ATOM  C10   0.198995   0.375943   0.633568
ATOM  H11   0.154321   0.301720   0.600058
ATOM  C12   0.194631   0.465166   0.481953
ATOM  O13   0.194256   0.430983   0.332090
ATOM  C14   0.357974   0.346831   0.663530
ATOM  H15   0.350536   0.276568   0.757993
ATOM  H16   0.405886   0.311720   0.552932
ATOM  C17   0.437691   0.461802   0.725821
ATOM  H18   0.455079   0.523843   0.630043
ATOM  H19   0.529541   0.437074   0.761649
ATOM  C20   0.350277   0.530459   0.875378
ATOM  H21   0.395598   0.612126   0.905929
ATOM  H22   0.343606   0.481519   0.980268
END
!ENERGY             -106.041
!COMMENT minimized
!COMMENT similarity    0.170


TITLE Price IV optimised
SPACEGROUP P21/a
CELL    7.913986   10.590148    9.315490   90.000000   94.521726   90.000000
ATOM  N1      0.033750      0.908462      0.811589
ATOM  H1     -0.065633      0.847852      0.809607
ATOM  H2      0.448412      0.897006      0.866436
ATOM  H3A     0.405098      1.132927      0.885023
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ATOM  H4      0.102847      1.212228      0.855755
ATOM  H3B     0.274693      1.049877      0.997160
ATOM  H6A     0.277689      1.227292      0.650226
ATOM  H6B     0.064792      1.196960      0.590982
ATOM  H7A     0.127824      0.973972      0.547638
ATOM  H7B     0.273701      1.065642      0.462359
ATOM  H8A     0.410178      0.881912      0.601657
ATOM  H8B     0.494478      1.029528      0.656934
ATOM  C1      0.193877      0.853086      0.810736
ATOM  C2      0.340586      0.944730      0.809869
ATOM  C3      0.298155      1.067655      0.884927
ATOM  C4      0.141999      1.125899      0.803723
ATOM  C5     -0.007414      1.036708      0.804519
ATOM  C6      0.177792      1.155704      0.647254
ATOM  C7      0.234693      1.038604      0.567876
ATOM  C8      0.380559      0.970748      0.653508
ATOM  O1      0.209235      0.738027      0.807864
ATOM  O2     -0.155725      1.070937      0.796589
COMMENT Experimental structure minimised with same ab initio
COMMENT molecular geometry, and same model potential (DMA + exp-6)
COMMENT as used in submissions.
COMMENT Calculated lattice energy -131.2 kJ/mol is too high relative
COMMENT to global minimum of -139.0 kJ/mol, but reproduction of
COMMENT structure is acceptable.
end

TITL Scheraga IV: Exp structure optimized with the force field (AMBER)
!used for crystal structure prediction of target IV
SPACEGROUP P21/a
CELL   7.908 10.462  8.921  90.00  95.76  90.00
ATOM N1      -.00295  -.08925   .30514
ATOM H1      -.09038  -.14055   .29405
ATOM C1      -.03647   .04040   .29275
ATOM O1      -.18314   .07660   .26697
ATOM C2       .11292   .12985   .30810
ATOM H2       .06912   .21690   .35657
ATOM C3       .26034   .07089   .40583
ATOM H3A      .36988   .13305   .41274
ATOM H3B      .22957   .05739   .52001
ATOM C4       .30610  -.05494   .33411
ATOM H4       .40643  -.10446   .40181
ATOM C5       .15692  -.14479   .32546
ATOM O2       .16892  -.26028   .33309
ATOM C6       .36079  -.03191   .17606
ATOM H6A      .47695   .02259   .19505
ATOM H6B      .38782  -.12443   .13036
ATOM C7       .22988   .04215   .07490
ATOM H7A      .12012  -.01750   .04536
ATOM H7B      .28196   .07041  -.02746
ATOM C8       .16727   .16066   .15133
ATOM H8A      .06205   .20656   .08587
ATOM H8B      .26428   .23345   .16689
END

TITL Scheraga IV crystal structure corresponding to minimum 5;
!it is also the experimental structure of target IV optimized
!with our molecular geometry and AMBER force field
CELL   7.798 10.589  9.094  90.00  95.25  90.00
SPACEGROUP P21/a
ATOM N1      -.00084  -.09077   .30759
ATOM H1      -.09930  -.15164   .29866
ATOM C1      -.04391   .03574   .29621
ATOM O1      -.19102   .06743   .27731
ATOM C2       .10574   .12782   .30717
ATOM H2       .05823   .21263   .35547
ATOM C3       .25787   .07197   .40396
ATOM H3A      .36422   .13770   .41284
ATOM H3B      .22330   .05503   .51457
ATOM C4       .31129  -.05108   .33270
ATOM H4       .41410  -.09740   .39982
ATOM C5       .16204  -.14353   .32131
ATOM O2       .17984  -.25538   .32214
ATOM C6       .37084  -.02472   .17843
ATOM H6A      .48576   .03249   .19371
ATOM H6B      .40669  -.11230   .12863
ATOM C7       .23371   .04426   .07653
ATOM H7A      .13121  -.02034   .04047
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ATOM H7B      .28891   .07441  -.02234
ATOM C8       .15939   .15893   .15204
ATOM H8A      .05054   .19689   .08423
ATOM H8B      .25522   .23272   .16477
END

TITLE  Schweizer/Dunitz E=-113.33,  d=1.235
SPACEGROUP P21/c
CELL    9.4238  11.3517  7.7409  90.00  95.882  90.00
ATOM   H1      -0.1636    0.1978    0.1118
ATOM   C2      -0.2066    0.1290    0.1457
ATOM   C3      -0.2030   -0.0354    0.3533
ATOM   C4      -0.4414    0.0471    0.2286
ATOM   C5      -0.3592   -0.0123    0.3842
ATOM   C6      -0.3642    0.1537    0.1662
ATOM   C7      -0.1312    0.0795    0.3135
ATOM   C8      -0.1975   -0.1210    0.2060
ATOM   H9      -0.4535   -0.0122    0.1350
ATOM   H10     -0.3576    0.0349    0.4868
ATOM   H11     -0.3619    0.2204    0.2577
ATOM   H12     -0.1388    0.1380    0.4088
ATOM   C13     -0.1948    0.0440   -0.0012
ATOM   H14     -0.1537   -0.0751    0.4595
ATOM   H15     -0.5333    0.0690    0.2585
ATOM   H16     -0.4025   -0.0880    0.4155
ATOM   H17     -0.4082    0.1834    0.0526
ATOM   H18     -0.0265    0.0678    0.3050
ATOM   O19     -0.1901    0.0730   -0.1514
ATOM   N20     -0.1914   -0.0747    0.0415
ATOM   O21     -0.2013   -0.2276    0.2247
ATOM   H22     -0.1902   -0.1251   -0.0436
!ENERGY  -113.33 Kcal/mol
COMMENT Coordinates from compound IV refined
COMMENT  in PROMET/MINOPEC to test force field
COMENT  with correct structure
END

TITLE  Schweizer/Dunitz IV 9   868.41  -108.10,  d=  1.172
SPACEGROUP P21/c
CELL     9.73150  11.40970   7.85850  90.00000  95.58700  90.00000
ATOM  H1      0.3494    0.0776    0.4725
ATOM  C2      0.2984    0.0371    0.3588
ATOM  C3      0.2964   -0.1255    0.1495
ATOM  C4      0.0662   -0.0458    0.2323
ATOM  C5      0.1437   -0.1524    0.1711
ATOM  C6      0.1458    0.0146    0.3862
ATOM  C7      0.3691   -0.0774    0.3164
ATOM  C8      0.3065   -0.0377    0.0062
ATOM  H9      0.0467    0.0165    0.1282
ATOM  H10      0.1420   -0.2230    0.2640
ATOM  H11      0.1443   -0.0407    0.4988
ATOM  H12      0.3623   -0.1404    0.4188
ATOM  C13      0.3085    0.1252    0.2159
ATOM  H14      0.3459   -0.2044    0.1096
ATOM  H15     -0.0346   -0.0729    0.2661
ATOM  H16      0.0929   -0.1852    0.0515
ATOM  H17      0.0964    0.0965    0.4144
ATOM  H18      0.4782   -0.0632    0.3046
ATOM  O19      0.3095    0.2286    0.2372
ATOM  N20      0.3150    0.0788    0.0545
ATOM  O21      0.3060   -0.0647   -0.1404
ATOM  H22      0.3200    0.1369   -0.0402
!ENERGY  -108.10 Kcal/mol
COMMENT lowest energy structure found in
COMMENT P21/c run. This structure has been
COMMENT rejected because it did not form a
COMMENT dimeric H-bond pattern.
END

TITL Williams IV observed relaxed with W99 force field
SPACEGROUP P21/a
CELL   7.7927   10.6101    9.1641     90.00     95.32     90.00
ATOM N1           0.02680  -0.08579   0.80917
ATOM H1          -0.06307  -0.13932   0.80584
ATOM C1           0.18871  -0.13891   0.80623
ATOM O1           0.20235  -0.25322   0.79892
ATOM C2           0.33976  -0.05070   0.80831
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ATOM H2           0.43895  -0.09587   0.85951
ATOM C3           0.30168   0.07134   0.88486
ATOM H3A          0.39879   0.13121   0.88223
ATOM H3B          0.28694   0.05694   0.98970
ATOM C4           0.14131   0.12988   0.80445
ATOM H4           0.10633   0.20796   0.85290
ATOM C5          -0.00973   0.04211   0.80887
ATOM O2          -0.15809   0.07648   0.81016
ATOM C6           0.17189   0.15937   0.64497
ATOM H6A          0.26192   0.22549   0.65219
ATOM H6B          0.06295   0.19466   0.59775
ATOM C7           0.23313   0.04577   0.56387
ATOM H7A          0.13748  -0.01538   0.54635
ATOM H7B          0.27068   0.07156   0.46799
ATOM C8           0.38057  -0.02314   0.65044
ATOM H8A          0.41037  -0.10365   0.60435
ATOM H8B          0.48855   0.02654   0.65725
!ENERGY -89.23
END

TITL Williams IV 4
!Rank 4 prediction for I
SPACEGROUP P21/c
CELL  9.2240   10.6794    7.7948     90.00     84.90     90.00
ATOM H5           0.48879   0.05580   0.21685
ATOM H6           0.38557   0.13045   0.10069
ATOM C4           0.38601   0.07188   0.19833
ATOM H3           0.35992  -0.09317   0.05821
ATOM H7           0.35394   0.20570   0.39522
ATOM O2           0.30811  -0.25116   0.29157
ATOM C3           0.30884  -0.04984   0.15715
ATOM C8           0.31039  -0.14011   0.30722
ATOM H13          0.31214  -0.13992   0.55747
ATOM N1           0.31269  -0.08648   0.46833
ATOM C7           0.30690   0.03939   0.50964
ATOM O1           0.30183   0.07226   0.65627
ATOM C5           0.30528   0.12940   0.35929
ATOM H2           0.15548   0.02790   0.01130
ATOM H10          0.15143   0.22756   0.23659
ATOM C2           0.15090  -0.02274   0.11762
ATOM C6           0.14720   0.16149   0.32551
ATOM H1           0.10185  -0.10181   0.09307
ATOM H9           0.09586   0.19717   0.43045
ATOM C1           0.06400   0.04795   0.26411
ATOM H12          0.03953  -0.00942   0.36166
ATOM H11         -0.02970   0.07564   0.22551
!ENERGY -84.59
END

TITLE Dzyabchenko V rank 5 (ab initio)
SPACEGROUP P212121
CELL  7.569  10.006  15.060  90.00  90.00  90.00
ATOM S1      -.01637    .04344    .31332
ATOM BR1     -.01197   -.06874    .01105
ATOM O3      -.00202   -.04728    .38610
ATOM O4      -.15295    .14204    .31761
ATOM N5      -.04460   -.04899    .22104
ATOM C6       .19410    .11784    .28579
ATOM C7       .21946    .08196    .18897
ATOM C8       .08043   -.02041    .16766
ATOM C9       .12780   -.08614    .08070
ATOM C10      .30524   -.01359    .06102
ATOM C11      .26019    .13204    .03253
ATOM C12      .19766    .19740    .12016
ATOM C13      .38515    .00571    .15373
ATOM C14      .42522   -.12276    .20369
ATOM C15      .55258    .08952    .15590
ATOM H18      .30556    .08067    .32314
ATOM H19      .20045    .22519    .29254
ATOM H20      .15339   -.19100    .09184
ATOM H21      .38623   -.06605    .01336
ATOM H22      .37251    .18323    .00426
ATOM H23      .15978    .13555   -.01837
ATOM H24      .27496    .28445    .13714
ATOM H25      .06319    .23294    .11593
ATOM H26      .30730   -.17313    .22699
ATOM H27      .51001   -.10393    .26062
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ATOM H28      .49544   -.19132    .15963
ATOM H29      .54007    .18487    .12400
ATOM H30      .65882    .03390    .12333
ATOM H31      .59387    .10584    .22468
COMMENT ENERGY -1.240747E+02 Density=1.70168
END

TITL Erk 2 Polymorph Predictor, not hit by during the prediction
CELL   7.1990  10.6022  15.9858  90.0000  90.0000  90.0000
!LATT -1
!SYMM -X+0.500,-Y,+Z+0.500
!SYMM -X,+Y+0.500,-Z+0.500
!SYMM +X+0.500,-Y+0.500,-Z
SPACEGROUP P212121
ATOM S1     0.57051    1.06033    0.21816
ATOM BR2    0.48888    1.08602    0.52333
ATOM O3     0.63622    1.15597    0.16350
ATOM O4     0.40602    0.99906    0.18941
ATOM N5     0.54748    1.12077    0.31185
ATOM C6     0.75594    0.95166    0.23893
ATOM C7     0.77579    0.96273    0.33509
ATOM C8     0.65815    1.06651    0.36279
ATOM C9     0.69882    1.10132    0.44811
ATOM C10    0.86566    1.00832    0.46233
ATOM C11    0.78868    0.87161    0.47447
ATOM C12    0.71507    0.84246    0.38517
ATOM C13    0.96470    1.00331    0.37490
ATOM C14    1.05246    1.13138    0.34473
ATOM C15    1.12825    0.90669    0.36670
ATOM H16    0.71554    0.85741    0.21863
ATOM H17    0.88155    0.98064    0.20600
ATOM H18    0.74575    1.19906    0.45039
ATOM H19    0.95722    1.03825    0.51338
ATOM H20    0.89830    0.80658    0.49383
ATOM H21    0.67984    0.86653    0.52200
ATOM H22    0.77666    0.75612    0.35990
ATOM H23    0.56410    0.83102    0.38468
ATOM H24    0.95337    1.20847    0.33897
ATOM H25    1.11668    1.12105    0.28324
ATOM H26    1.15973    1.16148    0.38878
ATOM H27    1.18428    0.90581    0.30332
ATOM H28    1.08875    0.81011    0.37995
ATOM H29    1.23977    0.93168    0.40981
END

TITL Erk 2 Systematic Search, #6 in P 212121, #8 of 2 space groups
CELL   7.1111  10.9543  15.9166  90.0000  90.0000  90.0000
!LATT -1
!SYMM -X+0.500,-Y,+Z+0.500
!SYMM -X,+Y+0.500,-Z+0.500
!SYMM +X+0.500,-Y+0.500,-Z
SPACEGROUP P212121
ATOM S1     0.58294    1.06606    0.21577
ATOM BR2    0.50081    1.08729    0.52655
ATOM O3     0.63477    1.16391    0.16126
ATOM O4     0.41788    0.99811    0.19453
ATOM N5     0.55603    1.12562    0.31249
ATOM C6     0.77918    0.96611    0.23734
ATOM C7     0.79383    0.96786    0.33222
ATOM C8     0.66852    1.06981    0.36157
ATOM C9     0.71529    1.09766    0.45201
ATOM C10    0.87914    1.00573    0.46563
ATOM C11    0.79156    0.87571    0.47099
ATOM C12    0.72919    0.85032    0.37953
ATOM C13    0.97746    1.00393    0.37986
ATOM C14    1.06220    1.12817    0.35162
ATOM C15    1.13319    0.90914    0.37149
ATOM H16    0.75180    0.87534    0.21197
ATOM H17    0.90475    1.00345    0.20771
ATOM H18    0.76649    1.19134    0.45705
ATOM H19    0.96960    1.02889    0.51892
ATOM H20    0.89431    0.80891    0.49332
ATOM H21    0.67386    0.87014    0.51512
ATOM H22    0.79524    0.76806    0.35412
ATOM H23    0.57636    0.83769    0.37492
ATOM H24    0.96197    1.20181    0.34112
ATOM H25    1.13907    1.11901    0.29255
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ATOM H26    1.16232    1.16005    0.39881
ATOM H27    1.18530    0.90630    0.30697
ATOM H28    1.09800    0.81550    0.38717
ATOM H29    1.25108    0.93429    0.41196
END

TITL Gavezzotti compound 2
SPACEGROUP P212121
CELL    7.0548   10.3517   15.5275   90.0000   90.0000   90.0000
ATOM   C1    -0.2031    0.0658   -0.1796
ATOM   C2    -0.1864    0.1017   -0.2730
ATOM   S3     0.0265    0.0194   -0.3065
ATOM   O4     0.1854    0.1050   -0.3073
ATOM   O5    -0.0055   -0.0572   -0.3817
ATOM   N6     0.0478   -0.0811   -0.2223
ATOM   C7    -0.0742   -0.0481   -0.1659
ATOM   C8    -0.1265   -0.1092   -0.0816
ATOM  BR9     0.0782   -0.0911   -0.0019
ATOM   C10   -0.2926   -0.0226   -0.0538
ATOM   C11   -0.2056    0.1069   -0.0256
ATOM   C12   -0.1399    0.1658   -0.1103
ATOM   C13   -0.3903    0.0109   -0.1404
ATOM   C14   -0.5472    0.1124   -0.1353
ATOM   C15   -0.4665   -0.1060   -0.1892
ATOM   H16   -0.3059    0.0625   -0.3080
ATOM   H17   -0.1653    0.2048   -0.2784
ATOM   H18   -0.1768   -0.2065   -0.0925
ATOM   H19   -0.3856   -0.0658   -0.0067
ATOM   H20   -0.3147    0.1670    0.0022
ATOM   H21   -0.0836    0.0883    0.0146
ATOM   H22   -0.2153    0.2553   -0.1209
ATOM   H23    0.0127    0.1722   -0.1102
ATOM   H24   -0.6681    0.0725   -0.1019
ATOM   H25   -0.4958    0.1959   -0.1010
ATOM   H26   -0.5884    0.1403   -0.1998
ATOM   H27   -0.5878   -0.1449   -0.1556
ATOM   H28   -0.3574   -0.1790   -0.1933
ATOM   H29   -0.5082   -0.0771   -0.2533
COMMENT Structure closest to experimental,
COMMENT ranked 14th in my energy ordering
COMMENT energy -105 kJ/mol
END

TITL Gavezzotti compound 2 optimized experimental
SPACEGROUP P212121
CELL    6.9746   10.6970   15.2287   90.0000   90.0000   90.0000
ATOM    C1    -.1820     .0663    -.1912
ATOM    C2    -.1693     .0999    -.2870
ATOM    S3     .0512     .0236    -.3217
ATOM    O4     .2084     .1075    -.3185
ATOM    O5     .0274    -.0483    -.3985
ATOM    N6     .0724    -.0762    -.2363
ATOM    C7    -.0510    -.0447    -.1790
ATOM    C8    -.1052    -.1077    -.0951
ATOM   BR9     .1117    -.1372    -.0180
ATOM   C10    -.2610    -.0206    -.0598
ATOM   C11    -.1683     .1042    -.0345
ATOM   C12    -.1087     .1625    -.1228
ATOM   C13    -.3676     .0145    -.1479
ATOM   C14    -.4539    -.0955    -.1976
ATOM   C15    -.5274     .1137    -.1376
ATOM   H16    -.2890     .0588    -.3215
ATOM   H17    -.1532     .1998    -.2935
ATOM   H18    -.1700    -.1967    -.1106
ATOM   H19    -.3515    -.0610    -.0099
ATOM   H20    -.2749     .1631    -.0039
ATOM   H21    -.0415     .0862     .0041
ATOM   H22    -.1840     .2499    -.1317
ATOM   H23     .0458     .1672    -.1261
ATOM   H24    -.5732    -.1331    -.1609
ATOM   H25    -.3465    -.1672    -.2062
ATOM   H26    -.5034    -.0644    -.2613
ATOM   H27    -.6458     .0740    -.1015
ATOM   H28    -.4716     .1934    -.1025
ATOM   H29    -.5762     .1427    -.2018
COMMENT  Optimized experimental structure
COMMENT using UNI force field, Energy -108 kJ/mol
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END


TITL Scheraga minimized experimental structure target 2
SPACEGROUP  P212121
CELL   7.071 10.575 16.112  90.00  90.00  90.00
ATOM Br1      .60865   .63121   .01522
ATOM S2       .51310   .46918   .30060
ATOM O3       .66385   .38078   .30028
ATOM O4       .48625   .54215   .37279
ATOM N5       .54690   .56972   .22059
ATOM C6       .38648   .60599   .08403
ATOM H7       .33137   .68892   .09647
ATOM C8       .42894   .54085   .16413
ATOM C9       .29323   .43143   .17297
ATOM C10      .36672   .33281   .10954
ATOM H11      .50188   .31985   .11541
ATOM H12      .30262   .25228   .11615
ATOM C13      .31902   .39332   .02521
ATOM H14      .43228   .40434  -.00798
ATOM H15      .22977   .34171  -.00542
ATOM C16      .23186   .52147   .04771
ATOM H17      .15692   .56059   .00341
ATOM C18      .29515   .39700   .26363
ATOM H19      .29737   .30599   .27119
ATOM H20      .18597   .43161   .29216
ATOM C21      .11699   .48817   .12882
ATOM C22      .03299   .60117   .17450
ATOM H23     -.06220   .64003   .14054
ATOM H24      .13105   .66143   .18615
ATOM H25     -.02268   .57320   .22570
ATOM C26     -.04445   .39145   .11599
ATOM H27      .00827   .31075   .10169
ATOM H28     -.12577   .41985   .07211
ATOM H29     -.11613   .38380   .16636
END

TITL Schmidt V 46
!   Minimum rank 46, close to exp. structure
SPACEGROUP  P212121
CELL   6.8121 10.0585 16.7283 90.0000 90.0000 90.0000
ATOM   C1          0.23980  0.41510  0.18131
ATOM   C2          0.37380  0.53926  0.16446
ATOM   C3          0.31534  0.59234  0.08381
ATOM   C4          0.15133  0.49325  0.05852
ATOM   C5          0.24816  0.35819  0.04111
ATOM   C6          0.31184  0.30642  0.12335
ATOM   C7          0.04674  0.46459  0.14087
ATOM   C8          0.25766  0.38950  0.26916
ATOM   S9          0.45761  0.48667  0.30522
ATOM   N10         0.48509  0.57745  0.22109
ATOM   C11        -0.11400  0.35819  0.13530
ATOM   C12        -0.04351  0.58884  0.17931
ATOM   O13         0.62116  0.40106  0.32012
ATOM   O14         0.38910  0.56506  0.37086
ATOM   Br15        0.53431  0.61607  0.00859
ATOM   H16         0.25697  0.68727  0.09025
ATOM   H17         0.06054  0.52944  0.01352
ATOM   H18         0.36707  0.36744  0.00253
ATOM   H19         0.14790  0.29435  0.01420
ATOM   H20         0.24662  0.21573  0.13698
ATOM   H21         0.46324  0.29447  0.12692
ATOM   H22         0.12844  0.41492  0.29854
ATOM   H23         0.28226  0.28920  0.28048
ATOM   H24        -0.06489  0.27072  0.10887
ATOM   H25        -0.16433  0.33521  0.19235
ATOM   H26        -0.23096  0.39441  0.10179
ATOM   H27        -0.14374  0.63158  0.14008
ATOM   H28        -0.11722  0.56325  0.23152
ATOM   H29         0.06106  0.66010  0.19401
END

TITLE Hoffman V minimized
CELL   7.200000  10.499906  15.499795  90.000000  90.000000  90.000000
SPACEGROUP     P212121
ATOM BR1    0.596576   0.641240   0.027984
ATOM  S2    0.536981   0.450441   0.318934
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ATOM  O3    0.688567   0.364832   0.312144
ATOM  O4    0.514432   0.516629   0.397292
ATOM  N5    0.558218   0.559458   0.239505
ATOM  C6    0.386304   0.604933   0.102420
ATOM  H7    0.329907   0.685973   0.119772
ATOM  C8    0.438362   0.533093   0.181982
ATOM  C9    0.310738   0.419463   0.189159
ATOM  C10   0.380956   0.327694   0.117951
ATOM  H11   0.514634   0.316996   0.120985
ATOM  H12   0.322138   0.244815   0.122674
ATOM  C13   0.323551   0.395161   0.033913
ATOM  H14   0.430997   0.411656  -0.002155
ATOM  H15   0.235273   0.344196   0.001694
ATOM  C16   0.234768   0.520036   0.064155
ATOM  H17   0.155369   0.561792   0.021248
ATOM  C18   0.322744   0.376661   0.281684
ATOM  H19   0.329503   0.284573   0.285721
ATOM  H20   0.216911   0.406532   0.314727
ATOM  C21   0.131256   0.476772   0.149010
ATOM  C22   0.048427   0.584380   0.202604
ATOM  H23  -0.049839   0.624506   0.170778
ATOM  H24   0.143161   0.645950   0.215347
ATOM  H25  -0.000101   0.550438   0.255565
ATOM  C26  -0.024213   0.377332   0.134726
ATOM  H27   0.029560   0.298657   0.115579
ATOM  H28  -0.109364   0.408142   0.091924
ATOM  H29  -0.089388   0.363550   0.187964
END
!ENERGY             -156.972
!COMMENT minimized
!COMMENT similarity    0.241

TITL Williams V observed relaxed with W99 force field
SPACEGROUP P212121
CELL 7.0099 10.6873 15.4042 90.00 90.00 90.00
ATOM Br    0.61847 0.64269  0.02254
ATOM S     0.54783 0.46093  0.31658
ATOM O1    0.70643 0.37883  0.31233
ATOM O2    0.51854 0.52736  0.39443
ATOM N     0.57047 0.56653  0.23575
ATOM C1    0.39980 0.60574  0.09549
ATOM H1    0.33853 0.68489  0.11145
ATOM C2    0.45126 0.53768  0.17686
ATOM C3    0.32334 0.42445  0.18390
ATOM C4    0.40199 0.33372  0.11404
ATOM H4A   0.54220 0.32498  0.11877
ATOM H4B   0.34273 0.24996  0.11914
ATOM C5    0.34540 0.39731  0.02816
ATOM H5A   0.45940 0.41456 -0.00784
ATOM H5B   0.25618 0.34420 -0.00536
ATOM C6    0.24884 0.51938  0.05626
ATOM H6    0.16753 0.55870  0.01135
ATOM C7    0.33211 0.38463  0.27756
ATOM H7A   0.34176 0.29346  0.28274
ATOM H7B   0.21969 0.41351  0.30963
ATOM C8    0.13944 0.47732  0.14094
ATOM C9    0.04829 0.58304  0.19277
ATOM H9A  -0.05529 0.62153  0.15820
ATOM H9B   0.14592 0.64704  0.20637
ATOM H9C  -0.00484 0.54920  0.24750
ATOM C10  -0.01637 0.37716  0.12594
ATOM H10A  0.04412 0.29776  0.10755
ATOM H10B -0.10522 0.40617  0.08021
ATOM H10C -0.08780 0.36348  0.18056
!ENERGY -130.31
END

!Rank 1 prediction for V if observed molecular structure is used
TITL Williams Va observed molecular structure
SPACEGROUP P212121
CELL 15.4023 7.0097 10.6875 90.00 90.00 90.00
ATOM Br    0.02253 -0.11853 0.35730
ATOM S     0.31660 -0.04789 0.53906
ATOM O1    0.31236 -0.20650 0.62116
ATOM O2    0.39446 -0.01860 0.47263
ATOM N     0.23576 -0.07054 0.43347
ATOM C1    0.09549  0.10015 0.39425
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ATOM H1    0.11145  0.16141 0.31511
ATOM C2    0.17686  0.04869 0.46232
ATOM C3    0.18391  0.17660 0.57554
ATOM C4    0.11404  0.09797 0.66627
ATOM H4A   0.11876 -0.04225 0.67501
ATOM H4B   0.11914  0.15723 0.75003
ATOM C5    0.02814  0.15454 0.60268
ATOM H5A  -0.00786  0.04055 0.58542
ATOM H5B  -0.00538  0.24378 0.65579
ATOM C6    0.05625  0.25111 0.48061
ATOM H6    0.01133  0.33243 0.44129
ATOM C7    0.27758  0.16783 0.61536
ATOM H7A   0.28275  0.15819 0.70653
ATOM H7B   0.30965  0.28026 0.58648
ATOM C8    0.14094  0.36051 0.52266
ATOM C9    0.19278  0.45167 0.41695
ATOM H9A   0.15821  0.55525 0.37846
ATOM H9B   0.20639  0.35403 0.35295
ATOM H9C   0.24751  0.50480 0.45079
ATOM C10   0.12594  0.51633 0.62282
ATOM H10A  0.10754  0.45584 0.70222
ATOM H10B  0.08021  0.60518 0.59381
ATOM H10C  0.18057  0.58776 0.63650
!ENERGY -130.44
END

TITLE Dzyabchenko VI ab initio Energy=-3.443532E+01 Density=1.40403
SPACEGROUP P21/c
CELL:      8.335     9.718    14.823     90.00    100.79     90.00
!SO2 a      .3347     .1807     .1132    315.24    -31.79    304.08  -1.00000
!Pyr1a      .3340     .1857     .1111    247.13     52.40    140.46  -1.00000
!Phe1a      .3328     .1806     .1135    184.94    -62.99    256.43  -1.00000
AT S1       .33470    .18070    .11320
AT O2       .45482    .08600    .16042
AT O3       .31135    .18250    .01341
AT N4       .37936    .33593    .15248
AT N12      .42030    .56703    .14556
AT N18      .46778    .80689    .15510
AT C11      .36437    .45025    .09930
AT C13      .40954    .69424    .10506
AT C14      .34247    .70919    .01574
AT C15      .28738    .59218   -.03493
AT C16      .29894    .46497    .00537
AT C5       .14369    .14074    .14364
AT C6       .06480    .02170    .10908
AT C7      -.08743   -.01022    .12762
AT C8      -.16306    .07628    .18125
AT C9      -.08129    .19384    .21615
AT C10      .07069    .22617    .19819
AT H17      .46962    .55975    .21228
AT H26      .33324    .81095   -.01406
AT H27      .23453    .60027   -.10704
AT H28      .25668    .37672   -.03671
AT H21      .12243   -.04674    .06737
AT H22     -.14782   -.10353    .09997
AT H23     -.28249    .05269    .19546
AT H24     -.13759    .26219    .25853
AT H25      .13253    .31834    .22684
AT H20      .45992    .89976    .12554
AT H19      .51846    .79686    .22147
END

TITL Erk 3A Polymorph Predictor, #24 in P21/c, #54 of 5 space groups
CELL   8.5531   9.2111  15.0606  90.0000  88.0772  90.0000
!LATT  1
!SYMM -X,+Y+0.500,-Z+0.500
SPACEGROUP P21/c
ATOM S1   0.79553    0.36941    0.14418
ATOM O2   0.87071    0.44496    0.07187
ATOM O3   0.84463    0.44981    0.21893
ATOM N4   0.86665    0.21094    0.16174
ATOM N5   0.92339   -0.02981    0.14310
ATOM C6   0.59267    0.38691    0.15151
ATOM C7   0.50047    0.28099    0.19603
ATOM C8   0.33669    0.29540    0.20192
ATOM C9   0.26471    0.41600    0.16321
ATOM C10  0.35556    0.52245    0.11896
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ATOM C11  0.51945    0.50804    0.11343
ATOM C12  0.85065    0.08980    0.11248
ATOM C13  0.76450    0.07851    0.03413
ATOM C14  0.75393   -0.05658   -0.00920
ATOM C15  0.82939   -0.17821    0.02643
ATOM C16  0.91376   -0.16031    0.10402
ATOM H17  0.55237    0.19331    0.22420
ATOM H18  0.26967    0.21829    0.23408
ATOM H19  0.30185    0.60969    0.09092
ATOM H20  0.58569    0.58578    0.08166
ATOM H21  0.71101    0.16724    0.00854
ATOM N22  0.98541   -0.26863    0.14433
ATOM H23  0.82456   -0.27755   -0.00325
ATOM H24  0.69312   -0.06590   -0.06623
ATOM H25  0.98558   -0.02291    0.19486
ATOM H26  1.04496   -0.24966    0.19650
ATOM H27  0.97077   -0.36702    0.12349
ATOM H28  0.14567    0.42615    0.16692
END

TITL Erk 3A Systematic Search, #250 in P 21/c, #530 of 5 space groups
CELL   8.7254   9.3808  16.6470  90.0000  89.6745  90.0000
!LATT  1
!SYMM -X,+Y+0.500,-Z+0.500
SPACEGROUP P21/c
ATOM S1   0.84916    0.36138    0.14461
ATOM O2   0.89586    0.41651    0.06812
ATOM O3   0.93558    0.42922    0.20648
ATOM N4   0.89645    0.19681    0.15613
ATOM N5   0.92153   -0.04260    0.13322
ATOM C6   0.65593    0.38589    0.16814
ATOM C7   0.60519    0.37794    0.24866
ATOM C8   0.44908    0.39689    0.26780
ATOM C9   0.34282    0.42431    0.20640
ATOM C10  0.39250    0.43275    0.12595
ATOM C11  0.54866    0.41342    0.10696
ATOM C12  0.86811    0.08517    0.10724
ATOM C13  0.78838    0.09170    0.03352
ATOM C14  0.76580   -0.03403   -0.01114
ATOM C15  0.82297   -0.16414    0.01825
ATOM C16  0.90163   -0.16470    0.09175
ATOM H17  0.68213    0.35859    0.29348
ATOM H18  0.41292    0.39094    0.32632
ATOM H19  0.31511    0.45320    0.08136
ATOM H20  0.58435    0.41957    0.04845
ATOM H21  0.74732    0.18631    0.01236
ATOM N22  0.95910   -0.28341    0.12376
ATOM H23  0.80774   -0.25652   -0.01317
ATOM H24  0.70836   -0.03089   -0.06456
ATOM H25  0.97614   -0.04633    0.18347
ATOM H26  1.01289   -0.27924    0.17441
ATOM H27  0.94742   -0.37389    0.09644
ATOM H28  0.22934    0.43840    0.22028
END

TITL Erk 3A Syst Search plus compl minim, #33 in P21/c, #77 of 5 spgrps
CELL   8.0792   9.6002  15.9067  90.0000 104.4225  90.0000
!LATT  1
!SYMM -X,+Y+0.500,-Z+0.500
SPACEGROUP P21/c
ATOM S1   0.84506    0.28607    0.12234
ATOM O2   0.83431    0.32619    0.03470
ATOM O3   0.99984    0.34777    0.17060
ATOM N4   0.88170    0.12424    0.14612
ATOM N5   0.89729   -0.11186    0.14000
ATOM C6   0.68556    0.35484    0.16667
ATOM C7   0.66185    0.30673    0.24659
ATOM C8   0.52209    0.35304    0.27726
ATOM C9   0.40629    0.44916    0.22810
ATOM C10  0.43296    0.50243    0.15022
ATOM C11  0.57442    0.45738    0.12088
ATOM C12  0.85528    0.00905    0.09582
ATOM C13  0.78880    0.00346    0.00473
ATOM C14  0.77148   -0.12656   -0.03797
ATOM C15  0.82002   -0.24882    0.01095
ATOM C16  0.88183   -0.23717    0.10132
ATOM H17  0.74600    0.23721    0.28224
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ATOM H18  0.50338    0.31626    0.33461
ATOM H19  0.34911    0.57298    0.11469
ATOM H20  0.59671    0.49856    0.06578
ATOM H21  0.75494    0.09220   -0.03035
ATOM N22  0.92857   -0.34445    0.15493
ATOM H23  0.81194   -0.34407   -0.01827
ATOM H24  0.72585   -0.13239   -0.10400
ATOM H25  0.93917   -0.10982    0.20204
ATOM H26  0.96423   -0.32770    0.21672
ATOM H27  0.92864   -0.43878    0.13329
ATOM H28  0.30241    0.48033    0.24895
END

TITL Hofmann VI minimized
CELL   8.300603   8.799930  15.003333  90.000000  90.455475  90.000000
SPACEGROUP       P21/c
ATOM  H1    0.988519   0.514665   0.682230
ATOM  C2    0.834300   0.388894   0.616399
ATOM  C3    0.908105   0.650026   0.594302
ATOM  C4    0.817118   0.656055   0.520922
ATOM  H5    0.808942   0.745359   0.488041
ATOM  C6    0.738549   0.532370   0.495722
ATOM  H7    0.675843   0.536726   0.444069
ATOM  C8    0.745103   0.394516   0.543005
ATOM  H9    0.688389   0.309683   0.523141
ATOM  C10   0.593883   0.106840   0.659937
ATOM  C11   0.515455  -0.004183   0.614071
ATOM  H12   0.571275  -0.073772   0.579439
ATOM  C13   0.359408  -0.009553   0.620521
ATOM  H14   0.304008  -0.085608   0.590124
ATOM  C15   0.275336   0.089625   0.668832
ATOM  H16   0.163724   0.082168   0.670653
ATOM  C17   0.349392   0.198717   0.714317
ATOM  H18   0.290492   0.266886   0.748362
ATOM  C19   0.508116   0.209655   0.710989
ATOM  H20   0.561526   0.285696   0.742505
ATOM  N21   0.858423   0.275049   0.675524
ATOM  N22   0.913074   0.517600   0.639103
ATOM  N23   0.991732   0.764076   0.624760
ATOM  H24   0.990204   0.849654   0.597050
ATOM  H25   1.048482   0.753855   0.672610
ATOM  O26   0.848557   0.019052   0.729795
ATOM  O27   0.850673   0.052558   0.569120
ATOM  S28   0.800213   0.110614   0.655882
END
!ENERGY             -170.248
!COMMENT minimized
!COMMENT similarity    0.174


!Molecule VI: Not found. This is the experimental structure after
!minimization:
TITL Mooy VI MinimizedExperimental
CELL    8.653  9.197 14.454 90.000 84.314 90.000
SPACEGROUP  P21/c
ATOM  H1     0.97022   0.51481   0.70531
ATOM  C2     0.84005   0.40249   0.62449
ATOM  C3     0.91129   0.65026   0.60545
ATOM  C4     0.83049   0.66306   0.52681
ATOM  H5     0.82819   0.75940   0.49207
ATOM  C6     0.75424   0.54068   0.49654
ATOM  H7     0.69507   0.54638   0.43888
ATOM  C8     0.76104   0.41040   0.54536
ATOM  H9     0.70941   0.32079   0.52452
ATOM C10     0.58045   0.09584   0.65576
ATOM C11     0.52163  -0.03169   0.61926
ATOM H12     0.59471  -0.11390   0.59576
ATOM C13     0.36181  -0.04709   0.61458
ATOM H14     0.31879  -0.13983   0.58813
ATOM C15     0.26080   0.06523   0.64561
ATOM H16     0.14475   0.05493   0.64061
ATOM C17     0.31904   0.19148   0.68338
ATOM H18     0.24506   0.27271   0.70687
ATOM C19     0.47867   0.20700   0.68850
ATOM H20     0.52022   0.29994   0.71559
ATOM N21     0.84612   0.28233   0.67710
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ATOM N22     0.91277   0.52199   0.65104
ATOM N23     0.98566   0.76684   0.63513
ATOM H24     0.98278   0.85777   0.60099
ATOM H25     1.04122   0.76249   0.69042
ATOM O26     0.82928   0.02587   0.74649
ATOM O27     0.87651   0.04859   0.57089
ATOM S28     0.77876   0.11300   0.66019
COMMENT Experimental structure of Molecule VI minimized in the
COMMENT Dreiding + Multipole COMMENT model. Energy difference with
COMMENT the global minimum: 4.0 kcal/mol Not sampled
END

TITL  Van Eijck VI Prediction closest to the experimental structure, rank 340
SPACEGROUP P21/c
CELL    8.40817   9.17889  14.24270    90.000    91.530    90.000
ATOM C1            .273855   .890929   .186617
ATOM H2            .146572   .884764   .193401
ATOM C3            .339240   .991366   .124965
ATOM H4            .261683  1.062920   .084629
ATOM C5            .372594   .798392   .239765
ATOM H6            .320679   .721299   .287343
ATOM C7            .504374   .998455   .116048
ATOM H8            .556615  1.075962   .068799
ATOM C9            .537596   .806199   .231098
ATOM H10           .615100   .735411   .271921
ATOM C11           .603723   .905582   .168792
ATOM S12           .811852   .915398   .157202
ATOM O13           .842752   .988910   .070579
ATOM O14           .868478   .994642   .238108
ATOM N15           .873467   .748897   .161103
ATOM C16           .838797   .637302   .108554
ATOM C17           .726626   .635362   .028552
ATOM H18           .665311   .733884   .007750
ATOM C19           .698511   .511099  -.020581
ATOM H20           .615638   .510732  -.079915
ATOM C21           .779818   .377558   .007448
ATOM H22           .756767   .278357  -.031399
ATOM C23           .884117   .377570   .080536
ATOM N24           .961023   .258485   .110226
ATOM H25          1.033596   .261180   .167152
ATOM H26           .939437   .160998   .078747
ATOM N27           .910773   .505371   .128547
ATOM H28           .989677   .505137   .183650
!ENERGY   -518.982 kJ/mol
END

TITL Scheraga minimized experimental structure  TARGET3
SPACEGROUP P21/c
CELL   9.170 10.428 13.001  90.00  92.22  90.00
ATOM H17      .92282   .36524   .73713
ATOM C17      .78108   .27304   .64872
ATOM C18      .88644   .48174   .62726
ATOM C19      .82033   .49226   .53467
ATOM H19      .83147   .56575   .49520
ATOM C20      .73845   .39601   .49993
ATOM H20      .69313   .40336   .43488
ATOM C21      .71652   .28302   .55629
ATOM H21      .65834   .21716   .52925
ATOM C14      .52025   .06633   .67863
ATOM C15      .44420  -.02061   .62018
ATOM H13      .49124  -.08691   .58709
ATOM C16      .30315  -.00769   .61236
ATOM H12      .24936  -.06700   .57333
ATOM C11      .23229   .08723   .65788
ATOM H11      .13145   .09329   .64916
ATOM C12      .30426   .17302   .71550
ATOM H16      .25440   .23843   .74763
ATOM C13      .44785   .16464   .72706
ATOM H15      .49965   .22423   .76718
ATOM N12      .77577   .17890   .71998
ATOM N13      .86431   .37331   .68057
ATOM N14      .97051   .56971   .66861
ATOM H18B     .98607   .63968   .63574
ATOM H18A    1.01046   .55788   .72882
ATOM O11      .72188  -.03054   .78429
ATOM O12      .75934  -.01250   .60093
ATOM S11      .70545   .04673   .69411
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END


TITL Schmidt VI minimized experimental
!, Calculated packing, which corresponds to the
!TITL experimental structure (calculated a posteriori, without
!TITL intramolecular potential for the rotation around the Ph-S bond)
SPACEGROUP P21/c
CELL    8.2576   8.9015  14.8969  90.000  95.031  90.000
ATOM  S1         0.79030   0.07938   0.65383
ATOM  O1         0.78573   0.01333   0.56532
ATOM  O2         0.88008  -0.00234   0.72675
ATOM  N1         0.86798   0.24423   0.66063
ATOM  C1         0.58815   0.09955   0.68083
ATOM  C2         0.55869   0.18411   0.75539
ATOM  C3         0.40109   0.20853   0.77660
ATOM  C4         0.27044   0.14836   0.72368
ATOM  C5         0.30253   0.06249   0.65014
ATOM  C6         0.45929   0.03733   0.62871
ATOM  C7         0.82195   0.35462   0.60124
ATOM  C8         0.70508   0.35188   0.52685
ATOM  C9         0.68227   0.47460   0.47187
ATOM  C10        0.77217   0.60535   0.48919
ATOM  C11        0.88061   0.60917   0.56203
ATOM  N2         0.90416   0.48607   0.61680
ATOM  N3         0.97195   0.72762   0.58719
ATOM  H2         0.65747   0.23543   0.79115
ATOM  H3         0.37619   0.27251   0.83216
ATOM  H4         0.15192   0.16658   0.73967
ATOM  H5         0.20929   0.01576   0.60761
ATOM  H6         0.48217  -0.02976   0.57407
ATOM  H8         0.63757   0.25564   0.51028
ATOM  H9         0.60076   0.46216   0.41507
ATOM  H10        0.75258   0.68988   0.44128
ATOM  H72        0.98750   0.49240   0.67049
ATOM  H73        1.05083   0.72189   0.64288
ATOM  H74        0.96242   0.82321   0.55060
END

        IV. Comparison of predicted coordinates with experimental
        ==========================================================
NOTES:
    Left part of each table presents experimental structure as reference.
    Right part (target) presents a predicted-structure coordinate list
    changed with CRYCOM (Dzyabchenko, Acta Cryst. 1994, B50, 414) from
    original (from above sections I-III) to make a numerical correspondence
    with reference. 'Matrix code' and 'Origin shift' define the
    transformation of unit-cell axes required to get such a correspondence.
    The sequence of atoms is also changed while their original labels are
    saved.
       The last column presents the relative deviations in the lattice
    dimensions and the absolute ones in atomic coordinats. The latter are
    given in angstroms, they are calculated from the three components of
    the deviation vector in unit space by converting it into the Cartesian
    space with a transformation matrix based on the mean cell dimensions of
    reference and target. 'r.m.s.d.' is the root-mean-square deviation found
    by averaging the atomic deviations over the molecule.

TITL Leusen IV 3

                     REFERENCE                    TARGET

Matrix code (Det)  655565556   1.               655565556   1.
Origin shift    .0000   .0000   .0000         .0000   .0000   .0000

New cell dimensions, A,deg:                                      dp/p(%)
a                     9.3380                     9.1820          -1.6706
b                    10.6060                    10.5090           -.9146
c                     7.7050                     8.0240           4.1402
alpha                  90.00                      90.00              .00
beta                   95.03                      96.99             2.06
gamma                  90.00                      90.00              .00

Atom      x       y       z           Atom      x       y      z      Dev,A
O1      .3001  -.2552   .2029          O11     .2999  -.2626   .1972    .090
O2      .3080   .0733  -.1643          O10     .3035   .0622  -.1575    .137
N1      .3086  -.0883   .0240          N8      .2987  -.0958   .0255    .122
```

C1	.3064	-.1409	.1882	C7	.3017	-.1467	.1791	.101
C2	.3081	-.0521	.3403	C1	.3055	-.0563	.3358	.060
C3	.3822	.0702	.3002	C6	.3829	.0734	.3000	.035
C4	.3026	.1278	.1382	C5	.2978	.1293	.1330	.059
C5	.3073	.0395	-.0140	C9	.3001	.0286	-.0116	.135
C6	.1461	.1566	.1703	C4	.1398	.1648	.1697	.105
C7	.0675	.0428	.2339	C3	.0556	.0544	.2427	.183
C8	.1532	-.0252	.3828	C2	.1500	-.0220	.3813	.046
H1	.3056	-.1406	-.0638	H22	.2980	-.1567	-.0742	.198
H2	.3598	-.0975	.4424	H12	.3684	-.1044	.4438	.107
H3A	.3794	.1311	.3990	H20	.3814	.1406	.4055	.113
H3B	.4866	.0561	.2842	H21	.4996	.0573	.2851	.121
H4	.3467	.2013	.1040	H19	.3546	.2160	.0978	.181
H6A	.1532	.2262	.2650	H18	.1480	.2450	.2598	.207
H6B	.0992	.1914	.0600	H17	.0746	.2026	.0552	.256
H7A	.0506	-.0186	.1380	H15	.0139	-.0119	.1410	.350
H7B	-.0230	.0673	.2710	H16	-.0437	.0918	.2912	.368
H8A	.1085	-.1060	.4140	H13	.0905	-.1091	.4110	.169
H8B	.1595	.0233	.4879	H14	.1635	.0339	.4995	.146
						r.m.s.d.(A)=		.172

TITL Mooy-I-2

	REFERENCE			TARGET			
Matrix code (Det)	655565556	1.		655565556	1.		
Origin shift	.0000	.0000	.0000	.0000	.0000	.0000	

New cell dimensions, A,deg:			dp/p(%)
a	9.3380	9.2290	-1.1673
b	10.6060	10.4060	-1.8857
c	7.7050	7.9630	3.3485
alpha	90.00	90.00	.00
beta	95.03	96.13	1.15
gamma	90.00	90.00	.00

Atom	x	y	z	Atom	x	y	z	Dev,A
O1	.3001	-.2552	.2029	O10	.2957	-.2625	.2032	.087
O2	.3080	.0733	-.1643	O11	.3103	.0713	-.1504	.111
N1	.3086	-.0883	.0240	N8	.3033	-.0939	.0286	.087
C1	.3064	-.1409	.1882	C7	.3026	-.1432	.1859	.046
C2	.3081	-.0521	.3403	C3	.3068	-.0583	.3354	.076
C3	.3822	.0702	.3002	C4	.3848	.0682	.2979	.038
C4	.3026	.1278	.1382	C5	.3033	.1277	.1372	.011
C5	.3073	.0395	-.0140	C9	.3063	.0339	-.0018	.114
C6	.1461	.1566	.1703	C6	.1446	.1624	.1687	.064
C7	.0675	.0428	.2339	C1	.0603	.0487	.2383	.100
C8	.1532	-.0252	.3828	C2	.1516	-.0264	.3806	.025
H1	.3056	-.1406	-.0638	H22	.3020	-.1522	-.0674	.129
H2	.3598	-.0975	.4424	H16	.3679	-.1056	.4424	.113
H3A	.3794	.1311	.3990	H17	.3834	.1345	.4035	.060
H3B	.4866	.0561	.2842	H18	.4985	.0496	.2796	.138
H4	.3467	.2013	.1040	H19	.3603	.2148	.1062	.189
H6A	.1532	.2262	.2650	H20	.1484	.2410	.2592	.167
H6B	.0992	.1914	.0600	H21	.0849	.1965	.0514	.153
H7A	.0506	-.0186	.1380	H12	.0278	-.0183	.1360	.211
H7B	-.0230	.0673	.2710	H13	-.0387	.0851	.2848	.267
H8A	.1085	-.1060	.4140	H15	.0952	-.1154	.4057	.166
H8B	.1595	.0233	.4879	H14	.1613	.0312	.4959	.104
						r.m.s.d.(A)=		.127

TITL Dzyabchenko IV (powder)

	REFERENCE			TARGET			
Matrix code (Det)	655565556	1.		655565556	1.		
Origin shift	.0000	.0000	.0000	.0000	.0000	.0000	

New cell dimensions, A,deg:			dp/p(%)
a	9.3380	9.3420	.0428
b	10.6060	10.5940	-.1131
c	7.7050	7.7140	.1168
alpha	90.00	90.00	.00
beta	95.03	95.00	-.03
gamma	90.00	90.00	.00

Atom	x	y	z	Atom	x	y	z	Dev,A

O1	.3001	-.2552	.2029	O2	.3013	-.2541	.1992	.034
O2	.3080	.0733	-.1643	O1	.3060	.0769	-.1628	.044
N1	.3086	-.0883	.0240	N1	.3038	-.0839	.0264	.069
C1	.3064	-.1409	.1882	C9	.3033	-.1403	.1867	.031
C2	.3081	-.0521	.3403	C5	.3053	-.0515	.3428	.034
C3	.3822	.0702	.3002	C4	.3824	.0687	.2989	.019
C4	.3026	.1278	.1382	C3	.3079	.1334	.1406	.078
C5	.3073	.0395	-.0140	C8	.3058	.0425	-.0133	.035
C6	.1461	.1566	.1703	C2	.1503	.1657	.1770	.114
C7	.0675	.0428	.2339	C1	.0614	.0600	.2441	.209
C8	.1532	-.0252	.3828	C6	.1477	-.0189	.3789	.088
H1	.3056	-.1406	-.0638	H1	.3024	-.1427	-.0751	.093
H2	.3598	-.0975	.4424	H12	.3603	-.0986	.4536	.087
H3A	.3794	.1311	.3990	H5	.3841	.1322	.4085	.083
H3B	.4866	.0561	.2842	H6	.4936	.0497	.2800	.101
H4	.3467	.2013	.1040	H11	.3647	.2176	.1077	.241
H6A	.1532	.2262	.2650	H3	.1576	.2415	.2710	.173
H6B	.0992	.1914	.0600	H4	.0956	.2053	.0604	.151
H7A	.0506	-.0186	.1380	H2	.0152	.0020	.1385	.396
H7B	-.0230	.0673	.2710	H10	-.0292	.1003	.3023	.432
H8A	.1085	-.1060	.4140	H7	.0912	-.1057	.4006	.184
H8B	.1595	.0233	.4879	H8	.1547	.0303	.5020	.142
						r.m.s.d.(A)=		.168

TITL Mooy IV powder

	REFERENCE			TARGET		
Matrix code (Det)	655565556	1.		655565556	1.	
Origin shift	.0000	.0000	.0000	.0000	.0000	.0000

New cell dimensions, A,deg:			dp/p(%)
a	9.3380	9.2290	-1.1673
b	10.6060	10.4060	-1.8857
c	7.7050	7.9630	3.3485
alpha	90.00	90.00	.00
beta	95.03	96.13	1.15
gamma	90.00	90.00	.00

Atom	x	y	z	Atom	x	y	z	Dev,A
O1	.3001	-.2552	.2029	O10	.2957	-.2625	.2032	.087
O2	.3080	.0733	-.1643	O11	.3103	.0713	-.1504	.111
N1	.3086	-.0883	.0240	N8	.3033	-.0939	.0286	.087
C1	.3064	-.1409	.1882	C7	.3026	-.1432	.1859	.046
C2	.3081	-.0521	.3403	C3	.3068	-.0583	.3354	.076
C3	.3822	.0702	.3002	C4	.3848	.0682	.2979	.038
C4	.3026	.1278	.1382	C5	.3033	.1277	.1372	.011
C5	.3073	.0395	-.0140	C9	.3063	.0339	-.0018	.114
C6	.1461	.1566	.1703	C6	.1446	.1624	.1687	.064
C7	.0675	.0428	.2339	C1	.0603	.0487	.2383	.100
C8	.1532	-.0252	.3828	C2	.1516	-.0264	.3806	.025
H1	.3056	-.1406	-.0638	H22	.3020	-.1522	-.0674	.129
H2	.3598	-.0975	.4424	H16	.3679	-.1056	.4424	.113
H3A	.3794	.1311	.3990	H17	.3834	.1345	.4035	.060
H3B	.4866	.0561	.2842	H18	.4985	.0496	.2796	.138
H4	.3467	.2013	.1040	H19	.3603	.2148	.1062	.189
H6A	.1532	.2262	.2650	H20	.1484	.2410	.2592	.167
H6B	.0992	.1914	.0600	H21	.0849	.1965	.0514	.153
H7A	.0506	-.0186	.1380	H12	.0278	-.0183	.1360	.211
H7B	-.0230	.0673	.2710	H13	-.0387	.0851	.2848	.267
H8A	.1085	-.1060	.4140	H15	.0952	-.1154	.4057	.166
H8B	.1595	.0233	.4879	H14	.1613	.0312	.4959	.104
						r.m.s.d.(A)=		.127

TITL Schmidt IV Final calculated structure (Lattic par. set to exp. values)

	REFERENCE			TARGET		
Matrix code (Det)	655565556	1.		655565556	1.	
Origin shift	.0000	.0000	.0000	.0000	.0000	.0000

New cell dimensions, A,deg:			dp/p(%)
a	9.3380	9.3300	-.0857
b	10.6060	10.6000	-.0566
c	7.7050	7.6700	-.4542
alpha	90.00	90.00	.00
beta	95.03	94.67	-.38
gamma	90.00	90.00	.00

Atom	x	y	z	Atom	x	y	z	Dev,A
O1	.3001	-.2552	.2029	O11	.3125	-.2571	.2087	.122
O2	.3080	.0733	-.1643	O10	.2935	.0694	-.1784	.171
N1	.3086	-.0883	.0240	N3	.3030	-.0941	.0146	.106
C1	.3064	-.1409	.1882	C4	.3086	-.1412	.1852	.032
C2	.3081	-.0521	.3403	C5	.3090	-.0483	.3367	.050
C3	.3822	.0702	.3002	C9	.3809	.0743	.2893	.094
C4	.3026	.1278	.1382	C1	.2987	.1284	.1271	.090
C5	.3073	.0395	-.0140	C2	.2984	.0348	-.0235	.117
C6	.1461	.1566	.1703	C8	.1450	.1590	.1658	.044
C7	.0675	.0428	.2339	C7	.0672	.0472	.2371	.053
C8	.1532	-.0252	.3828	C6	.1556	-.0225	.3811	.039
H1	.3056	-.1406	-.0638	H22	.3030	-.1560	-.0856	.234
H2	.3598	-.0975	.4424	H13	.3658	-.0903	.4436	.095
H3A	.3794	.1311	.3990	H20	.3792	.1380	.3923	.089
H3B	.4866	.0561	.2842	H21	.4877	.0583	.2663	.141
H4	.3467	.2013	.1040	H12	.3483	.2102	.0873	.161
H6A	.1532	.2262	.2650	H18	.1487	.2322	.2564	.098
H6B	.0992	.1914	.0600	H19	.0881	.1912	.0522	.115
H7A	.0506	-.0186	.1380	H16	.0382	-.0151	.1356	.122
H7B	-.0230	.0673	.2710	H17	-.0277	.0784	.2852	.169
H8A	.1085	-.1060	.4140	H14	.1055	-.1075	.4064	.065
H8B	.1595	.0233	.4879	H15	.1604	.0307	.4953	.097
						r.m.s.d.(A)=		.115

TITL Schmidt IV Calculated minimum close to the experimental structure

	REFERENCE			TARGET		
Matrix code (Det)	655565556	1.		655565556	1.	
Origin shift	.0000	.0000	.0000	.0000	.0000	.0000

New cell dimensions, A,deg:			dp/p(%)
a	9.3380	8.9439	-4.2204
b	10.6060	10.5165	-.8439
c	7.7050	7.6854	-.2544
alpha	90.00	90.00	.00
beta	95.03	95.37	.35
gamma	90.00	90.00	.00

Atom	x	y	z	Atom	x	y	z	Dev,A
O1	.3001	-.2552	.2029	O11	.3089	-.2582	.2096	.097
O2	.3080	.0733	-.1643	O10	.2931	.0715	-.1759	.157
N1	.3086	-.0883	.0240	N3	.3010	-.0937	.0163	.104
C1	.3064	-.1409	.1882	C4	.3065	-.1414	.1865	.014
C2	.3081	-.0521	.3403	C5	.3085	-.0479	.3380	.048
C3	.3822	.0702	.3002	C9	.3853	.0750	.2921	.087
C4	.3026	.1278	.1382	C1	.2999	.1306	.1293	.076
C5	.3073	.0395	-.0140	C2	.2980	.0364	-.0214	.103
C6	.1461	.1566	.1703	C8	.1400	.1630	.1661	.092
C7	.0675	.0428	.2339	C7	.0572	.0510	.2359	.130
C8	.1532	-.0252	.3828	C6	.1487	-.0203	.3805	.067
H1	.3056	-.1406	-.0638	H22	.2999	-.1560	-.0839	.227
H2	.3598	-.0975	.4424	H13	.3674	-.0909	.4453	.099
H3A	.3794	.1311	.3990	H20	.3846	.1390	.3951	.102
H3B	.4866	.0561	.2842	H21	.4965	.0577	.2704	.147
H4	.3467	.2013	.1040	H12	.3528	.2125	.0905	.170
H6A	.1532	.2262	.2650	H18	.1450	.2366	.2569	.144
H6B	.0992	.1914	.0600	H19	.0808	.1961	.0521	.180
H7A	.0506	-.0186	.1380	H16	.0258	-.0113	.1340	.238
H7B	-.0230	.0673	.2710	H17	-.0413	.0835	.2828	.261
H8A	.1085	-.1060	.4140	H14	.0953	-.1054	.4048	.134
H8B	.1595	.0233	.4879	H15	.1548	.0332	.4947	.126
						r.m.s.d.(A)=		.141

TITL Van Eijck IV 4

	REFERENCE			TARGET		
Matrix code (Det)	655565556	1.		655565556	1.	
Origin shift	.0000	.0000	.0000	.0000	.0000	.0000

New cell dimensions, A,deg:			dp/p(%)
a	9.3380	9.0977	-2.5734
b	10.6060	10.5072	-.9315
c	7.7050	7.7871	1.0655

alpha	90.00	90.00	.00
beta	95.03	96.96	2.03
gamma	90.00	90.00	.00

Atom	x	y	z	Atom	x	y	z	Dev,A
O1	.3001	-.2552	.2029	O20	.3003	-.2567	.2043	.019
O2	.3080	.0733	-.1643	O18	.3068	.0702	-.1629	.036
N1	.3086	-.0883	.0240	N21	.3029	-.0895	.0254	.056
C1	.3064	-.1409	.1882	C19	.3025	-.1432	.1880	.043
C2	.3081	-.0521	.3403	C6	.3035	-.0505	.3394	.045
C3	.3822	.0702	.3002	C1	.3777	.0747	.2997	.063
C4	.3026	.1278	.1382	C4	.2968	.1314	.1341	.071
C5	.3073	.0395	-.0140	C17	.3032	.0386	-.0158	.040
C6	.1461	.1566	.1703	C8	.1364	.1637	.1607	.133
C7	.0675	.0428	.2339	C14	.0536	.0569	.2432	.214
C8	.1532	-.0252	.3828	C11	.1474	-.0212	.3822	.068
H1	.3056	-.1406	-.0638	H22	.3033	-.1498	-.0746	.128
H2	.3598	-.0975	.4424	H7	.3665	-.0933	.4524	.104
H3A	.3794	.1311	.3990	H2	.3753	.1408	.4065	.126
H3B	.4866	.0561	.2842	H3	.4934	.0583	.2842	.067
H4	.3467	.2013	.1040	H5	.3533	.2189	.1063	.196
H6A	.1532	.2262	.2650	H10	.1362	.2477	.2422	.318
H6B	.0992	.1914	.0600	H9	.0746	.1894	.0367	.275
H7A	.0506	-.0186	.1380	H15	.0059	-.0077	.1427	.433
H7B	-.0230	.0673	.2710	H16	-.0391	.0989	.2994	.434
H8A	.1085	-.1060	.4140	H13	.0904	-.1103	.4024	.186
H8B	.1595	.0233	.4879	H12	.1561	.0306	.5043	.155
						r.m.s.d.(A)=		.189

TITL Verwer IV 1 from powder diffraction data

	REFERENCE			TARGET		
Matrix code (Det)	655565556	1.		655565556	1.	
Origin shift	.0000	.0000	.0000	.0000	.0000	.0000

New cell dimensions, A,deg:			dp/p(%)
a	9.3380	9.3457	.0825
b	10.6060	10.6358	.2810
c	7.7050	7.7013	-.0480
alpha	90.00	90.00	.00
beta	95.03	94.95	-.09
gamma	90.00	90.00	.00

Atom	x	y	z	Atom	x	y	z	Dev,A
O1	.3001	-.2552	.2029	O10	.2962	-.2543	.1938	.077
O2	.3080	.0733	-.1643	O11	.2951	.0571	-.1618	.212
N1	.3086	-.0883	.0240	N8	.2980	-.0938	.0215	.115
C1	.3064	-.1409	.1882	C7	.3027	-.1387	.1809	.067
C2	.3081	-.0521	.3403	C3	.3092	-.0564	.3353	.062
C3	.3822	.0702	.3002	C4	.3824	.0683	.2947	.047
C4	.3026	.1278	.1382	C5	.2993	.1238	.1308	.075
C5	.3073	.0395	-.0140	C9	.2981	.0285	-.0080	.154
C6	.1461	.1566	.1703	C6	.1465	.1580	.1689	.019
C7	.0675	.0428	.2339	C1	.0667	.0477	.2449	.101
C8	.1532	-.0252	.3828	C2	.1589	-.0268	.3856	.058
H1	.3056	-.1406	-.0638	H22	.2949	-.1488	-.0756	.156
H2	.3598	-.0975	.4424	H16	.3714	-.1025	.4419	.121
H3A	.3794	.1311	.3990	H17	.3839	.1332	.4021	.052
H3B	.4866	.0561	.2842	H18	.4919	.0512	.2727	.117
H4	.3467	.2013	.1040	H19	.3536	.2077	.0941	.124
H6A	.1532	.2262	.2650	H20	.1525	.2348	.2610	.096
H6B	.0992	.1914	.0600	H21	.0853	.1917	.0523	.138
H7A	.0506	-.0186	.1380	H12	.0304	-.0172	.1429	.197
H7B	-.0230	.0673	.2710	H13	-.0270	.0842	.2964	.271
H8A	.1085	-.1060	.4140	H15	.1051	-.1138	.4118	.090
H8B	.1595	.0233	.4879	H14	.1693	.0282	.5036	.154
						r.m.s.d.(A)=		.128

TITL Dzyabchenko IV-31: ab initio minimum closest to experimental

	REFERENCE			TARGET		
Matrix code (Det)	655565556	1.		655565556	1.	
Origin shift	.0000	.0000	.0000	.0000	.0000	.0000

New cell dimensions, A,deg: dp/p(%)

a	9.3380	9.1580	-1.9276
b	10.6060	10.5700	-.3394
c	7.7050	7.7250	.2596
alpha	90.00	90.00	.00
beta	95.03	95.95	.96
gamma	90.00	90.00	.00

Atom	x	y	z	Atom	x	y	z	Dev,A
O1	.3001	-.2552	.2029	O2	.3009	-.2606	.2009	.059
O2	.3080	.0733	-.1643	O1	.2823	.0612	-.1793	.285
N1	.3086	-.0883	.0240	N1	.2920	-.0947	.0187	.169
C1	.3064	-.1409	.1882	C9	.3008	-.1469	.1824	.091
C2	.3081	-.0521	.3403	C5	.3101	-.0537	.3342	.055
C3	.3822	.0702	.3002	C4	.3846	.0658	.2796	.169
C4	.3026	.1278	.1382	C3	.2998	.1260	.1219	.128
C5	.3073	.0395	-.0140	C8	.2905	.0308	-.0276	.201
C6	.1461	.1566	.1703	C2	.1415	.1586	.1657	.057
C7	.0675	.0428	.2339	C1	.0562	.0543	.2434	.181
C8	.1532	-.0252	.3828	C6	.1519	-.0208	.3777	.062
H1	.3056	-.1406	-.0638	H1	.2860	-.1564	-.0799	.268
H2	.3598	-.0975	.4424	H12C	.3724	-.0977	.4445	.116
H3A	.3794	.1311	.3990	H5	.3914	.1324	.3862	.156
H3B	.4866	.0561	.2842	H6	.4965	.0467	.2553	.268
H4	.3467	.2013	.1040	H11C	.3546	.2097	.0813	.215
H6A	.1532	.2262	.2650	H3	.1531	.2372	.2556	.137
H6B	.0992	.1914	.0600	H4	.0793	.1950	.0499	.196
H7A	.0506	-.0186	.1380	H2	.0044	-.0068	.1431	.450
H7B	-.0230	.0673	.2710	H10C	-.0331	.0958	.3048	.416
H8A	.1085	-.1060	.4140	H7	.0968	-.1073	.4071	.117
H8B	.1595	.0233	.4879	H8	.1649	.0318	.4982	.127
						r.m.s.d.(A)=		.207

TITLE Erk IV Polymorph Predictor, #62 in P21/c, #116 of 10 space groups

	REFERENCE			TARGET		
Matrix code (Det)	655565556	1.		655565556	1.	
Origin shift	.0000	.0000	.0000	.0000	.0000	.0000

New cell dimensions, A,deg:			dp/p(%)
a	9.3380	9.4748	1.4650
b	10.6060	10.7661	1.5095
c	7.7050	7.8487	1.8650
alpha	90.00	90.00	.00
beta	95.03	96.16	1.19
gamma	90.00	90.00	.00

Atom	x	y	z	Atom	x	y	z	Dev,A
O1	.3001	-.2552	.2029	O15	.2990	-.2546	.1875	.119
O2	.3080	.0733	-.1643	O14	.2877	.0534	-.1684	.285
N1	.3086	-.0883	.0240	N13	.2961	-.0955	.0155	.150
C1	.3064	-.1409	.1882	C5	.3025	-.1394	.1746	.109
C2	.3081	-.0521	.3403	C4	.3102	-.0569	.3289	.106
C3	.3822	.0702	.3002	C3	.3838	.0681	.2904	.082
C4	.3026	.1278	.1382	C2	.2989	.1212	.1251	.126
C5	.3073	.0395	-.0140	C1	.2948	.0259	-.0141	.187
C6	.1461	.1566	.1703	C8	.1471	.1583	.1683	.026
C7	.0675	.0428	.2339	C16	.0664	.0497	.2460	.121
C8	.1532	-.0252	.3828	C11	.1604	-.0259	.3838	.068
H1	.3056	-.1406	-.0638	H6	.2924	-.1500	-.0813	.202
H2	.3598	-.0975	.4424	H12	.3731	-.1044	.4337	.165
H3A	.3794	.1311	.3990	H10	.3846	.1329	.3976	.054
H3B	.4866	.0561	.2842	H9	.4945	.0521	.2691	.151
H4	.3467	.2013	.1040	H7	.3537	.2031	.0841	.175
H6A	.1532	.2262	.2650	H20	.1566	.2347	.2604	.104
H6B	.0992	.1914	.0600	H19	.0838	.1929	.0533	.150
H7A	.0506	-.0186	.1380	H17	.0264	-.0143	.1447	.243
H7B	-.0230	.0673	.2710	H18	-.0257	.0873	.3007	.318
H8A	.1085	-.1060	.4140	H22	.1058	-.1120	.4106	.073
H8B	.1595	.0233	.4879	H21	.1736	.0279	.5027	.174
						r.m.s.d.(A)=		.161

TITLE Erk 1-S Systematic Search, #47 in P 21/c, #76 of 10 space groups

	REFERENCE			TARGET		
Matrix code (Det)	655565556	1.		655565556	1.	

Origin shift .0000 .0000 .0000 .0000 .0000 .0000

New cell dimensions, A,deg:			dp/p(%)
a	9.3380	9.7430	4.3371
b	10.6060	10.9802	3.5282
c	7.7050	7.7469	.5438
alpha	90.00	90.00	.00
beta	95.03	94.23	-.84
gamma	90.00	90.00	.00

Atom	x	y	z	Atom	x	y	z	Dev,A
O1	.3001	-.2552	.2029	O15	.3246	-.2509	.1920	.259
O2	.3080	.0733	-.1643	O14	.2911	.0666	-.1759	.192
N1	.3086	-.0883	.0240	N13	.3085	-.0918	.0087	.124
C1	.3064	-.1409	.1882	C5	.3169	-.1404	.1798	.124
C2	.3081	-.0521	.3403	C4	.3165	-.0526	.3319	.107
C3	.3822	.0702	.3002	C3	.3816	.0681	.2846	.122
C4	.3026	.1278	.1382	C2	.2981	.1225	.1290	.098
C5	.3073	.0395	-.0140	C1	.2984	.0358	-.0243	.119
C6	.1461	.1566	.1703	C8	.1509	.1478	.1757	.112
C7	.0675	.0428	.2339	C16	.0807	.0353	.2426	.160
C8	.1532	-.0252	.3828	C11	.1697	-.0308	.3826	.168
H1	.3056	-.1406	-.0638	H6	.3092	-.1491	-.0916	.239
H2	.3598	-.0975	.4424	H12	.3779	-.0944	.4442	.175
H3A	.3794	.1311	.3990	H10	.3833	.1317	.3958	.047
H3B	.4866	.0561	.2842	H9	.4905	.0553	.2567	.219
H4	.3467	.2013	.1040	H7	.3459	.2102	.0914	.136
H6A	.1532	.2262	.2650	H20	.1541	.2204	.2753	.101
H6B	.0992	.1914	.0600	H19	.0893	.1851	.0619	.118
H7A	.0506	-.0186	.1380	H17	.0524	-.0277	.1338	.106
H7B	-.0230	.0673	.2710	H18	-.0182	.0617	.2939	.189
H8A	.1085	-.1060	.4140	H22	.1212	-.1186	.4137	.183
H8B	.1595	.0233	.4879	H21	.1748	.0231	.5039	.184
						r.m.s.d.(A)=		.158

TITLE Hofmann IV 358

	REFERENCE			TARGET			
Matrix code (Det)	655565556	1.		655565556	1.		
Origin shift	.0000	.0000	.0000	.0000	.0000	.0000	

New cell dimensions, A,deg:			dp/p(%)
a	9.3380	9.2201	-1.2626
b	10.6060	10.1999	-3.8290
c	7.7050	7.6322	-.9448
alpha	90.00	90.00	.00
beta	95.03	94.63	-.42
gamma	90.00	90.00	.00

Atom	x	y	z	Atom	x	y	z	Dev,A
O1	.3001	-.2552	.2029	O4	.2844	-.2634	.1909	.186
O2	.3080	.0733	-.1643	O13	.3160	.0771	-.1777	.138
N1	.3086	-.0883	.0240	N1	.3050	-.0907	.0113	.104
C1	.3064	-.1409	.1882	C3	.2994	-.1451	.1767	.114
C2	.3081	-.0521	.3403	C5	.3083	-.0531	.3310	.073
C3	.3822	.0702	.3002	C7	.3923	.0694	.2903	.125
C4	.3026	.1278	.1382	C10	.3157	.1339	.1283	.162
C5	.3073	.0395	-.0140	C12	.3132	.0420	-.0261	.115
C6	.1461	.1566	.1703	C14	.1599	.1732	.1631	.224
C7	.0675	.0428	.2339	C17	.0722	.0597	.2275	.189
C8	.1532	-.0252	.3828	C20	.1541	-.0159	.3762	.109
H1	.3056	-.1406	-.0638	H2	.2978	-.1447	-.0777	.131
H2	.3598	-.0975	.4424	H6	.3574	-.1033	.4330	.095
H3A	.3794	.1311	.3990	H8	.3943	.1327	.3906	.158
H3B	.4866	.0561	.2842	H9	.4965	.0485	.2727	.154
H4	.3467	.2013	.1040	H11	.3656	.2076	.0937	.209
H6A	.1532	.2262	.2650	H15	.1726	.2449	.2591	.272
H6B	.0992	.1914	.0600	H16	.1148	.2120	.0526	.268
H7A	.0506	-.0186	.1380	H18	.0502	-.0030	.1305	.172
H7B	-.0230	.0673	.2710	H19	-.0172	.0905	.2664	.250
H8A	.1085	-.1060	.4140	H21	.1030	-.0972	.4078	.114
H8B	.1595	.0233	.4879	H22	.1645	.0339	.4826	.128
						r.m.s.d.(A)=		.168

TITLE Hoffmann IV minimized (ordered list)

	REFERENCE			TARGET			
Matrix code (Det)	655565556	1.		655565556	1.		
Origin shift	.0000	.0000	.0000	.0000	.0000	.0000	
New cell dimensions, A,deg:							dp/p(%)
a	9.3380			9.2005			-1.4725
b	10.6060			10.4999			-1.0004
c	7.7050			7.7318			.3478
alpha	90.00			90.00			.00
beta	95.03			95.82			.83
gamma	90.00			90.00			.00

Atom	x	y	z	Atom	x	y	z	Dev,A
O1	.3001	-.2552	.2029	O4	.2985	-.2629	.1980	.090
O2	.3080	.0733	-.1643	O13	.3057	.0690	-.1679	.056
N1	.3086	-.0883	.0240	N1	.3067	-.0943	.0198	.072
C1	.3064	-.1409	.1882	C3	.3049	-.1474	.1834	.078
C2	.3081	-.0521	.3403	C5	.3070	-.0577	.3351	.071
C3	.3822	.0702	.3002	C7	.3823	.0659	.2961	.056
C4	.3026	.1278	.1382	C10	.3010	.1241	.1336	.054
C5	.3073	.0395	-.0140	C12	.3054	.0348	-.0180	.060
C6	.1461	.1566	.1703	C14	.1420	.1532	.1635	.071
C7	.0675	.0428	.2339	C17	.0623	.0382	.2258	.089
C8	.1532	-.0252	.3828	C20	.1497	-.0305	.3754	.084
H1	.3056	-.1406	-.0638	H2	.3035	-.1471	-.0677	.077
H2	.3598	-.0975	.4424	H6	.3598	-.1035	.4376	.074
H3A	.3794	.1311	.3990	H8	.3796	.1274	.3946	.052
H3B	.4866	.0561	.2842	H9	.4882	.0516	.2815	.054
H4	.3467	.2013	.1040	H11	.3457	.1983	.1001	.044
H6A	.1532	.2262	.2650	H15	.1495	.2234	.2580	.068
H6B	.0992	.1914	.0600	H16	.0941	.1883	.0529	.076
H7A	.0506	-.0186	.1380	H18	.0449	-.0238	.1300	.095
H7B	-.0230	.0673	.2710	H19	-.0295	.0629	.2617	.101
H8A	.1085	-.1060	.4140	H21	.1044	-.1121	.4059	.095
H8B	.1595	.0233	.4879	H22	.1564	.0185	.4803	.081
						r.m.s.d.(A)=		.074

TITLE Price IV optimised

	REFERENCE			TARGET			
Matrix code (Det)	655565556	1.		655565556	1.		
Origin shift	.0000	.0000	.0000	.0000	.0000	.0000	
New cell dimensions, A,deg:							dp/p(%)
a	9.3380			9.3155			-.2410
b	10.6060			10.5901			-.1499
c	7.7050			7.9140			2.7125
alpha	90.00			90.00			.00
beta	95.03			94.52			-.54
gamma	90.00			90.00			.00

Atom	x	y	z	Atom	x	y	z	Dev,A
O1	.3001	-.2552	.2029	O1	.3079	-.2620	.2092	.111
O2	.3080	.0733	-.1643	O2	.2966	.0709	-.1557	.133
N1	.3086	-.0883	.0240	N1	.3116	-.0915	.0338	.086
C1	.3064	-.1409	.1882	C1	.3107	-.1469	.1939	.086
C2	.3081	-.0521	.3403	C2	.3099	-.0553	.3406	.037
C3	.3822	.0702	.3002	C3	.3849	.0676	.2982	.041
C4	.3026	.1278	.1382	C4	.3037	.1259	.1420	.037
C5	.3073	.0395	-.0140	C5	.3045	.0367	-.0074	.066
C6	.1461	.1566	.1703	C6	.1472	.1557	.1778	.059
C7	.0675	.0428	.2339	C7	.0679	.0386	.2347	.045
C8	.1532	-.0252	.3828	C8	.1535	-.0292	.3806	.047
H1	.3056	-.1406	-.0638	H1	.3096	-.1522	-.0656	.129
H2	.3598	-.0975	.4424	H2	.3664	-.1030	.4484	.095
H3A	.3794	.1311	.3990	H3A	.3850	.1329	.4051	.071
H3B	.4866	.0561	.2842	H3B	.4972	.0499	.2747	.144
H4	.3467	.2013	.1040	H4	.3557	.2122	.1028	.144
H6A	.1532	.2262	.2650	H6A	.1502	.2273	.2777	.106
H6B	.0992	.1914	.0600	H6B	.0910	.1970	.0648	.106
H7A	.0506	-.0186	.1380	H7A	.0476	-.0260	.1278	.114
H7B	-.0230	.0673	.2710	H7B	-.0376	.0656	.2737	.141
H8A	.1085	-.1060	.4140	H8A	.1017	-.1181	.4102	.145
H8B	.1595	.0233	.4879	H8B	.1569	.0295	.4945	.088

r.m.s.d.(A)= .099

TITL Scheraga IV : Exp structure optimized with the force field (AMBER)

	REFERENCE			TARGET		
Matrix code (Det)	655565556	1.		655565556	1.	
Origin shift	.0000	.0000	.0000	.0000	.0000	.0000

New cell dimensions, A,deg:			dp/p(%)
a	9.3380	8.9210	-4.4656
b	10.6060	10.4620	-1.3577
c	7.7050	7.9080	2.6347
alpha	90.00	90.00	.00
beta	95.03	95.76	.77
gamma	90.00	90.00	.00

Atom	x	y	z	Atom	x	y	z	Dev,A
O1	.3001	-.2552	.2029	O2	.3331	-.2603	.1689	.423
O2	.3080	.0733	-.1643	O1	.2670	.0766	-.1831	.391
N1	.3086	-.0883	.0240	N1	.3051	-.0892	-.0030	.210
C1	.3064	-.1409	.1882	C5	.3255	-.1448	.1569	.316
C2	.3081	-.0521	.3403	C4	.3341	-.0549	.3061	.375
C3	.3822	.0702	.3002	C3	.4058	.0709	.2603	.395
C4	.3026	.1278	.1382	C2	.3081	.1299	.1129	.209
C5	.3073	.0395	-.0140	C1	.2928	.0404	-.0365	.210
C6	.1461	.1566	.1703	C8	.1513	.1607	.1673	.070
C7	.0675	.0428	.2339	C7	.0749	.0421	.2299	.077
C8	.1532	-.0252	.3828	C6	.1761	-.0319	.3608	.291
H1	.3056	-.1406	-.0638	H1	.2941	-.1406	-.0904	.224
H2	.3598	-.0975	.4424	H4	.4018	-.1045	.4064	.502
H3A	.3794	.1311	.3990	H3A	.4127	.1330	.3699	.397
H3B	.4866	.0561	.2842	H3B	.5200	.0574	.2296	.547
H4	.3467	.2013	.1040	H2	.3566	.2169	.0691	.337
H6A	.1532	.2262	.2650	H8B	.1669	.2334	.2643	.147
H6B	.0992	.1914	.0600	H8A	.0859	.2066	.0620	.202
H7A	.0506	-.0186	.1380	H7A	.0454	-.0175	.1201	.144
H7B	-.0230	.0673	.2710	H7B	-.0275	.0704	.2820	.103
H8A	.1085	-.1060	.4140	H6B	.1304	-.1244	.3878	.356
H8B	.1595	.0233	.4879	H6A	.1951	.0226	.4769	.343

r.m.s.d.(A)= .314

TITL Scheraga IV crystal structure corresponding to minimum 5;

	REFERENCE			TARGET		
Matrix code (Det)	655565556	1.		655565556	1.	
Origin shift	.0000	.0000	.0000	.0000	.0000	.0000

New cell dimensions, A,deg:			dp/p(%)
a	9.3380	9.0940	-2.6130
b	10.6060	10.5890	-.1603
c	7.7050	7.7980	1.2070
alpha	90.00	90.00	.00
beta	95.03	95.25	.23
gamma	90.00	90.00	.00

Atom	x	y	z	Atom	x	y	z	Dev,A
O1	.3001	-.2552	.2029	O2	.3221	-.2554	.1798	.282
O2	.3080	.0733	-.1643	O1	.2773	.0674	-.1910	.341
N1	.3086	-.0883	.0240	N1	.3076	-.0908	-.0008	.194
C1	.3064	-.1409	.1882	C5	.3213	-.1435	.1620	.256
C2	.3081	-.0521	.3403	C4	.3327	-.0511	.3113	.333
C3	.3822	.0702	.3002	C3	.4040	.0720	.2579	.400
C4	.3026	.1278	.1382	C2	.3072	.1278	.1057	.259
C5	.3073	.0395	-.0140	C1	.2962	.0357	-.0439	.248
C6	.1461	.1566	.1703	C8	.1520	.1589	.1594	.108
C7	.0675	.0428	.2339	C7	.0765	.0443	.2337	.085
C8	.1532	-.0252	.3828	C6	.1784	-.0247	.3708	.258
H1	.3056	-.1406	-.0638	H1	.2987	-.1516	-.0993	.301
H2	.3598	-.0975	.4424	H4	.3998	-.0974	.4141	.446
H3A	.3794	.1311	.3990	H3A	.4128	.1377	.3642	.433
H3B	.4866	.0561	.2842	H3B	.5146	.0550	.2233	.558
H4	.3467	.2013	.1040	H2	.3555	.2126	.0582	.390
H6A	.1532	.2262	.2650	H8B	.1648	.2327	.2552	.153
H6B	.0992	.1914	.0600	H8A	.0842	.1969	.0505	.161
H7A	.0506	-.0186	.1380	H7A	.0405	-.0203	.1312	.105

H7B	-.0230	.0673	.2710	H7B	-.0223	.0744	.2889	.158
H8A	.1085	-.1060	.4140	H6B	.1286	-.1123	.4067	.210
H8B	.1595	.0233	.4879	H6A	.1937	.0325	.4858	.332
						r.m.s.d.(A)=		.299

TITLE Schweizer/Dunitz E=-113.33, d=1.235

	REFERENCE			TARGET			
Matrix code (Det)	655565556	1.		655565556	1.		
Origin shift	.0000	.0000	.0000	.0000	.0000	.0000	
New cell dimensions, A,deg:							dp/p(%)
a	9.3380			9.4238			.9188
b	10.6060			11.3517			7.0309
c	7.7050			7.7409			.4659
alpha	90.00			90.00			.00
beta	95.03			95.88			.89
gamma	90.00			90.00			.00

Atom	x	y	z	Atom	x	y	z	Dev,A
O1	.3001	-.2552	.2029	O21	.2987	-.2276	.2247	.348
O2	.3080	.0733	-.1643	O19	.3099	.0730	-.1514	.100
N1	.3086	-.0883	.0240	N20	.3086	-.0747	.0415	.201
C1	.3064	-.1409	.1882	C8	.3025	-.1210	.2060	.263
C2	.3081	-.0521	.3403	C3	.2970	-.0354	.3533	.238
C3	.3822	.0702	.3002	C7	.3688	.0795	.3135	.198
C4	.3026	.1278	.1382	C2	.2934	.1290	.1457	.109
C5	.3073	.0395	-.0140	C13	.3052	.0440	-.0012	.114
C6	.1461	.1566	.1703	C6	.1358	.1537	.1662	.104
C7	.0675	.0428	.2339	C4	.0586	.0471	.2286	.101
C8	.1532	-.0252	.3828	C5	.1408	-.0123	.3842	.184
H1	.3056	-.1406	-.0638	H22	.3098	-.1251	-.0436	.232
H2	.3598	-.0975	.4424	H14	.3463	-.0751	.4595	.312
H3A	.3794	.1311	.3990	H12	.3612	.1380	.4088	.208
H3B	.4866	.0561	.2842	H18	.4735	.0678	.3050	.247
H4	.3467	.2013	.1040	H1	.3364	.1978	.1118	.125
H6A	.1532	.2262	.2650	H11	.1381	.2204	.2577	.161
H6B	.0992	.1914	.0600	H17	.0918	.1834	.0526	.123
H7A	.0506	-.0186	.1380	H9	.0465	-.0122	.1350	.082
H7B	-.0230	.0673	.2710	H15	-.0333	.0690	.2585	.131
H8A	.1085	-.1060	.4140	H16	.0975	-.0880	.4155	.224
H8B	.1595	.0233	.4879	H10	.1424	.0349	.4868	.204
						r.m.s.d.(A)=		.196

TITLE Schweizer/Dunitz IV 9 868.41 -108.10, d= 1.172

	REFERENCE			TARGET			
Matrix code (Det)	655565556	1.		655565556	1.		
Origin shift	.0000	.0000	.0000	.0000	.0000	.0000	
New cell dimensions, A,deg:							dp/p(%)
a	9.3380			9.7315			4.2140
b	10.6060			11.4097			7.5778
c	7.7050			7.8585			1.9922
alpha	90.00			90.00			.00
beta	95.03			95.59			.59
gamma	90.00			90.00			.00

Atom	x	y	z	Atom	x	y	z	Dev,A
O1	.3001	-.2552	.2029	O19	.3095	-.2286	.2372	.401
O2	.3080	.0733	-.1643	O21	.3060	.0647	-.1404	.211
N1	.3086	-.0883	.0240	N20	.3150	-.0788	.0545	.261
C1	.3064	-.1409	.1882	C13	.3085	-.1252	.2159	.276
C2	.3081	-.0521	.3403	C2	.2984	-.0371	.3588	.243
C3	.3822	.0702	.3002	C7	.3691	.0774	.3164	.202
C4	.3026	.1278	.1382	C3	.2964	.1255	.1495	.113
C5	.3073	.0395	-.0140	C8	.3065	.0377	.0062	.159
C6	.1461	.1566	.1703	C5	.1437	.1524	.1711	.052
C7	.0675	.0428	.2339	C4	.0662	.0458	.2323	.037
C8	.1532	-.0252	.3828	C6	.1458	-.0146	.3862	.140
H1	.3056	-.1406	-.0638	H22	.3200	-.1369	-.0402	.223
H2	.3598	-.0975	.4424	H1	.3494	-.0776	.4725	.342
H3A	.3794	.1311	.3990	H12	.3623	.1404	.4188	.256
H3B	.4866	.0561	.2842	H18	.4782	.0632	.3046	.200
H4	.3467	.2013	.1040	H14	.3459	.2044	.1096	.056

H6A	.1532	.2262	.2650	H10	.1420	.2230	.2640	.112
H6B	.0992	.1914	.0600	H16	.0929	.1852	.0515	.109
H7A	.0506	-.0186	.1380	H9	.0467	-.0165	.1282	.085
H7B	-.0230	.0673	.2710	H15	-.0346	.0729	.2661	.129
H8A	.1085	-.1060	.4140	H17	.0964	-.0965	.4144	.156
H8B	.1595	.0233	.4879	H11	.1443	.0407	.4988	.259
						r.m.s.d.(A)=		.205

TITL PRICE V 1

	REFERENCE			TARGET			
Matrix code (Det)	655565556	1.		554565455	-1.		
Origin shift	.0000	.0000	.0000	.5000	-.5000	1.0000	
New cell dimensions, A,deg:							dp/p(%)
a	7.2640			7.1772			-1.1952
b	10.6390			10.4130			-2.1239
c	15.6330			16.2227			3.7722
alpha	90.00			90.00			.00
beta	90.00			90.00			.00
gamma	90.00			90.00			.00

Atom	x	y	z	Atom	x	y	z	Dev,A
BR1	.5913	.6333	.0158	BR1	.5732	.6334	.0207	.152
S2	.5322	.4505	.3059	S1	.5073	.4694	.3069	.269
O3	.6825	.3659	.2999	O1	.6600	.3816	.3030	.237
O4	.5099	.5173	.3830	O2	.4735	.5407	.3804	.363
N5	.5533	.5566	.2262	N1	.5241	.5724	.2273	.269
C6	.3829	.5989	.0899	C2	.3604	.6042	.0925	.176
C7	.4345	.5295	.1694	C1	.4103	.5395	.1727	.211
C8	.3080	.4175	.1775	C7	.2834	.4241	.1827	.208
C9	.3776	.3256	.1077	C6	.3556	.3242	.1194	.246
C10	.3207	.3906	.0238	C5	.2995	.3838	.0353	.250
C11	.2327	.5144	.0527	C3	.2084	.5123	.0598	.210
C12	.3199	.3770	.2696	C8	.2965	.3897	.2736	.225
C13	.1301	.4733	.1372	C4	.1028	.4768	.1412	.211
C14	.0480	.5805	.1894	C10	.0146	.5917	.1863	.273
C15	-.0240	.3749	.1239	C9	-.0516	.3766	.1292	.217
H16	.3270	.6792	.1064	H1	.3074	.6992	.1043	.256
H17	.5101	.3151	.1108	H5	.5045	.3098	.1253	.241
H18	.3193	.2439	.1131	H6	.2897	.2321	.1298	.364
H19	.4272	.4062	-.0121	H3	.4175	.3975	-.0049	.162
H20	.2332	.3397	-.0077	H4	.2010	.3238	.0027	.331
H21	.1540	.5548	.0098	H2	.1238	.5554	.0120	.221
H22	.3266	.2862	.2744	H8	.3116	.2884	.2861	.217
H23	.2150	.4071	.3021	H7	.1838	.4292	.3098	.347
H24	-.0494	.6195	.1575	H13	-.0843	.6397	.1461	.377
H25	.1419	.6415	.2015	H14	.1135	.6630	.2074	.320
H26	-.0001	.5480	.2422	H12	-.0618	.5593	.2400	.463
H27	.0293	.2969	.1056	H9	-.0067	.2906	.0977	.296
H28	-.1084	.4045	.0812	H11	-.1651	.4180	.0938	.477
H29	-.0886	.3623	.1768	H10	-.1080	.3480	.1885	.278
						r.m.s.d.(A)=		.283

TITL Van Eijck V 1

	REFERENCE			TARGET			
Matrix code (Det)	655565556	1.		655565556	1.		
Origin shift	.0000	.0000	.0000	.0000	.0000	.0000	
New cell dimensions, A,deg:							dp/p(%)
a	7.2640			7.1190			-1.9961
b	10.6390			9.9850			-6.1472
c	15.6330			15.8900			1.6440
alpha	90.00			90.00			.00
beta	90.00			90.00			.00
gamma	90.00			90.00			.00

Atom	x	y	z	Atom	x	y	z	Dev,A
BR1	.5913	.6333	.0158	BR21	.5229	.5871	-.0115	.809
S2	.5322	.4505	.3059	S27	.4360	.5001	.3045	.861
O3	.6825	.3659	.2999	O28	.5889	.4398	.3494	1.282
O4	.5099	.5173	.3830	O29	.3378	.6075	.3443	1.664
N5	.5533	.5566	.2262	N26	.5113	.5531	.2114	.383

C6	.3829	.5989	.0899	C20	.3253	.5766	.0758	.523
C7	.4345	.5295	.1694	C19	.3909	.5149	.1564	.404
C8	.3080	.4175	.1775	C18	.2485	.4066	.1786	.443
C9	.3776	.3256	.1077	C15	.2938	.2927	.1144	.700
C10	.3207	.3906	.0238	C12	.2115	.3440	.0319	.929
C11	.2327	.5144	.0527	C10	.1499	.4885	.0560	.655
C12	.3199	.3770	.2696	C23	.2726	.3768	.2700	.340
C13	.1301	.4733	.1372	C1	.0596	.4689	.1449	.523
C14	.0480	.5805	.1894	C2	-.0104	.5967	.1882	.452
C15	-.0240	.3749	.1239	C6	-.1084	.3733	.1478	.715
H16	.3270	.6792	.1064	H22	.2814	.6795	.0873	.445
H17	.5101	.3151	.1108	H17	.4445	.2769	.1085	.616
H18	.3193	.2439	.1131	H16	.2296	.1981	.1330	.859
H19	.4272	.4062	-.0121	H13	.3148	.3422	-.0184	1.048
H20	.2332	.3397	-.0077	H14	.0920	.2838	.0123	1.209
H21	.1540	.5548	.0098	H11	.0541	.5338	.0106	.750
H22	.3266	.2862	.2744	H25	.3290	.2774	.2800	.128
H23	.2150	.4071	.3021	H24	.1403	.3864	.3037	.579
H24	-.0494	.6195	.1575	H5	-.1141	.6458	.1483	.558
H25	.1419	.6415	.2015	H3	.1007	.6687	.2011	.408
H26	-.0001	.5480	.2422	H4	-.0771	.5741	.2484	.623
H27	.0293	.2969	.1056	H8	-.0673	.2693	.1496	1.022
H28	-.1084	.4045	.0812	H9	-.2083	.3975	.0982	.770
H29	-.0886	.3623	.1768	H7	-.1821	.3788	.2078	.848
						r.m.s.d.(A)=		.777

TITL Williams V 3

	REFERENCE			TARGET		
Matrix code (Det)	655565556	1.		545655556	1.	
Origin shift	.0000	.0000	.0000	1.0000	.0000	-.5000

New cell dimensions, A,deg:			dp/p(%)
a	7.2640	6.9300	-4.5980
b	10.6390	10.6600	.1974
c	15.6330	15.5800	-.3390
alpha	90.00	90.00	.00
beta	90.00	90.00	.00
gamma	90.00	90.00	.00

Atom	x	y	z	Atom	x	y	z	Dev,A
BR1	.5913	.6333	.0158	BR1	.6101	.6424	.0218	.190
S2	.5322	.4505	.3059	S1	.5479	.4648	.3160	.246
O3	.6825	.3659	.2999	O2	.7058	.3793	.3088	.259
O4	.5099	.5173	.3830	O1	.5145	.5301	.3944	.227
N5	.5533	.5566	.2262	N1	.5631	.5700	.2355	.215
C6	.3829	.5989	.0899	C5	.3922	.6062	.0960	.139
C7	.4345	.5295	.1694	C6	.4466	.5393	.1778	.188
C8	.3080	.4175	.1775	C1	.3173	.4252	.1858	.167
C9	.3776	.3256	.1077	C2	.3890	.3294	.1182	.187
C10	.3207	.3906	.0238	C3	.3307	.3913	.0317	.143
C11	.2327	.5144	.0527	C4	.2380	.5164	.0593	.112
C12	.3199	.3770	.2696	C8	.3287	.3891	.2800	.216
C13	.1301	.4733	.1372	C7	.1334	.4770	.1428	.098
C14	.0480	.5805	.1894	C9	.0416	.5870	.1921	.093
C15	-.0240	.3749	.1239	C10	-.0216	.3759	.1272	.056
H16	.3270	.6792	.1064	H5	.3366	.6882	.1101	.131
H17	.5101	.3151	.1108	H22	.5285	.3138	.1231	.233
H18	.3193	.2439	.1131	H21	.3224	.2489	.1269	.223
H19	.4272	.4062	-.0121	H32	.4408	.4034	-.0070	.129
H20	.2332	.3397	-.0077	H31	.2345	.3400	.0013	.141
H21	.1540	.5548	.0098	H4	.1579	.5560	.0150	.087
H22	.3266	.2862	.2744	H81	.3410	.2990	.2910	.309
H23	.2150	.4071	.3021	H82	.2224	.4243	.3140	.267
H24	-.0494	.6195	.1575	H93	-.0655	.6228	.1578	.120
H25	.1419	.6415	.2015	H91	.1402	.6526	.2024	.119
H26	-.0001	.5480	.2422	H92	-.0090	.5566	.2477	.141
H27	.0293	.2969	.1056	H101	.0361	.3047	.0955	.184
H28	-.1084	.4045	.0812	H102	-.1285	.4121	.0931	.248
H29	-.0886	.3623	.1768	H103	-.0720	.3459	.1830	.232
						r.m.s.d.(A)=		.187

TITL Dzyabchenko V (powder)

	REFERENCE	TARGET

Matrix code (Det) 655565556 1. 655545554 1.
Origin shift .0000 .0000 .0000 .0000 .5000 .5000

New cell dimensions, A,deg:			dp/p(%)
a	7.2640	7.2610	-.0413
b	10.6390	10.6340	-.0470
c	15.6330	15.6340	.0064
alpha	90.00	90.00	.00
beta	90.00	90.00	.00
gamma	90.00	90.00	.00

Atom	x	y	z	Atom	x	y	z	Dev,A
BR1	.5913	.6333	.0158	BR1	.5956	.6431	.0184	.116
S2	.5322	.4505	.3059	S1	.5355	.4518	.3103	.074
O3	.6825	.3659	.2999	O4	.7049	.3831	.3117	.306
O4	.5099	.5173	.3830	O3	.4794	.5113	.3879	.243
N5	.5533	.5566	.2262	N5	.5491	.5647	.2351	.167
C6	.3829	.5989	.0899	C9	.3862	.6098	.0968	.160
C7	.4345	.5295	.1694	C8	.4410	.5342	.1743	.104
C8	.3080	.4175	.1775	C7	.3306	.4146	.1751	.171
C9	.3776	.3256	.1077	C12	.4016	.3330	.0990	.235
C10	.3207	.3906	.0238	C11	.3317	.4061	.0198	.193
C11	.2327	.5144	.0527	C10	.2340	.5224	.0599	.141
C12	.3199	.3770	.2696	C6	.3519	.3597	.2639	.310
C13	.1301	.4733	.1372	C13	.1443	.4672	.1404	.132
C14	.0480	.5805	.1894	C14	.0516	.5651	.2004	.239
C15	-.0240	.3749	.1239	C15	.0019	.3649	.1234	.216
H16	.3270	.6792	.1064	H20	.3243	.6972	.1172	.256
H17	.5101	.3151	.1108	H25	.5497	.3230	.0991	.351
H18	.3193	.2439	.1131	H24	.3492	.2380	.1009	.296
H19	.4272	.4062	-.0121	H23	.4426	.4325	-.0226	.343
H20	.2332	.3397	-.0077	H22	.2397	.3504	-.0190	.215
H21	.1540	.5548	.0098	H21	.1430	.5701	.0159	.205
H22	.3266	.2862	.2744	H19	.3794	.2603	.2581	.536
H23	.2150	.4071	.3021	H18	.2211	.3656	.2965	.452
H24	-.0494	.6195	.1575	H28	-.0688	.6043	.1698	.288
H25	.1419	.6415	.2015	H26	.1470	.6402	.2146	.209
H26	-.0001	.5480	.2422	H27	.0106	.5206	.2595	.405
H27	.0293	.2969	.1056	H29	.0593	.2940	.0818	.433
H28	-.1084	.4045	.0812	H30	-.1182	.4051	.0932	.200
H29	-.0886	.3623	.1768	H31	-.0389	.3214	.1828	.573
						r.m.s.d.(A)=		.289

TITL Leusen V 70

REFERENCE TARGET

Matrix code (Det) 655565556 1. 655565556 1.
Origin shift .0000 .0000 .0000 -.5000 .0000 .0000

New cell dimensions, A,deg:			dp/p(%)
a	7.2640	7.3590	1.3078
b	10.6390	10.9410	2.8386
c	15.6330	15.5860	-.3006
alpha	90.00	90.00	.00
beta	90.00	90.00	.00
gamma	90.00	90.00	.00

Atom	x	y	z	Atom	x	y	z	Dev,A
BR1	.5913	.6333	.0158	BR13	.6116	.6310	.0108	.169
S2	.5322	.4505	.3059	S11	.5322	.4900	.3071	.426
O3	.6825	.3659	.2999	O15	.6911	.3921	.3059	.305
O4	.5099	.5173	.3830	O14	.5233	.5584	.3965	.500
N5	.5533	.5566	.2262	N12	.5559	.5908	.2255	.369
C6	.3829	.5989	.0899	C5	.4002	.6215	.0843	.288
C7	.4345	.5295	.1694	C4	.4404	.5613	.1693	.346
C8	.3080	.4175	.1775	C3	.3122	.4531	.1810	.389
C9	.3776	.3256	.1077	C2	.3845	.3497	.1194	.322
C10	.3207	.3906	.0238	C1	.3382	.4003	.0274	.175
C11	.2327	.5144	.0527	C6	.2511	.5300	.0496	.221
C12	.3199	.3770	.2696	C10	.3186	.4237	.2758	.513
C13	.1301	.4733	.1372	C7	.1334	.4986	.1358	.275
C14	.0480	.5805	.1894	C8	.0344	.6105	.1748	.408
C15	-.0240	.3749	.1239	C9	-.0206	.4047	.1222	.323
H16	.3270	.6792	.1064	H20	.3451	.7144	.0924	.457
H17	.5101	.3151	.1108	H19	.5315	.3317	.1275	.352
H18	.3193	.2439	.1131	H18	.3129	.2625	.1312	.350

H19	.4272	.4062	-.0121	H16	.4592	.4067	-.0143	.236
H20	.2332	.3397	-.0077	H17	.2385	.3412	-.0058	.051
H21	.1540	.5548	.0098	H21	.1697	.5687	-.0031	.276
H22	.3266	.2862	.2744	H29	.3128	.3256	.2910	.508
H23	.2150	.4071	.3021	H28	.2099	.4689	.3127	.688
H24	-.0494	.6195	.1575	H23	-.0670	.6481	.1296	.549
H25	.1419	.6415	.2015	H22	.1223	.6877	.1932	.535
H26	-.0001	.5480	.2422	H24	-.0402	.5857	.2340	.518
H27	.0293	.2969	.1056	H25	.0205	.3172	.0932	.300
H28	-.1084	.4045	.0812	H27	-.1279	.4416	.0798	.425
H29	-.0886	.3623	.1768	H26	-.0862	.3800	.1836	.219
						r.m.s.d.(A)=		.387

TITL Mooy V powder

	REFERENCE			TARGET		
Matrix code (Det)	655565556	1.		655565556	1.	
Origin shift	.0000	.0000	.0000	.5000	.5000	.0000

New cell dimensions, A,deg:			dp/p(%)
a	7.2640	7.1360	-1.7621
b	10.6390	10.8030	1.5415
c	15.6330	15.3810	-1.6120
alpha	90.00	90.00	.00
beta	90.00	90.00	.00
gamma	90.00	90.00	.00

Atom	x	y	z	Atom	x	y	z	Dev,A
BR1	.5913	.6333	.0158	BR13	.6301	.6345	.0162	.280
S2	.5322	.4505	.3059	S9	.5410	.4733	.3083	.256
O3	.6825	.3659	.2999	O15	.7167	.3836	.3057	.323
O4	.5099	.5173	.3830	O14	.5205	.5429	.3985	.372
N5	.5533	.5566	.2262	N10	.5591	.5747	.2295	.205
C6	.3829	.5989	.0899	C5	.4118	.6151	.0891	.271
C7	.4345	.5295	.1694	C4	.4466	.5476	.1680	.214
C8	.3080	.4175	.1775	C3	.3257	.4404	.1752	.279
C9	.3776	.3256	.1077	C2	.4024	.3453	.1081	.277
C10	.3207	.3906	.0238	C1	.3493	.4067	.0207	.273
C11	.2327	.5144	.0527	C6	.2562	.5295	.0517	.234
C12	.3199	.3770	.2696	C8	.3294	.3996	.2715	.253
C13	.1301	.4733	.1372	C7	.1420	.4901	.1335	.207
C14	.0480	.5805	.1894	C11	.0444	.5988	.1831	.221
C15	-.0240	.3749	.1239	C12	-.0137	.3913	.1172	.217
H16	.3270	.6792	.1064	H20	.3557	.7061	.1040	.357
H17	.5101	.3151	.1108	H19	.5538	.3325	.1139	.369
H18	.3193	.2439	.1131	H18	.3333	.2558	.1149	.165
H19	.4272	.4062	-.0121	H17	.4723	.4229	-.0199	.390
H20	.2332	.3397	-.0077	H16	.2505	.3496	-.0155	.204
H21	.1540	.5548	.0098	H21	.1729	.5750	.0017	.285
H22	.3266	.2862	.2744	H22	.3366	.2994	.2786	.172
H23	.2150	.4071	.3021	H23	.2100	.4360	.3076	.324
H24	-.0494	.6195	.1575	H25	-.0531	.6458	.1397	.395
H25	.1419	.6415	.2015	H24	.1438	.6669	.2074	.287
H26	-.0001	.5480	.2422	H26	-.0335	.5634	.2387	.296
H27	.0293	.2969	.1056	H28	.0369	.3101	.0828	.385
H28	-.1084	.4045	.0812	H29	-.1259	.4322	.0787	.325
H29	-.0886	.3623	.1768	H27	-.0712	.3602	.1790	.132
						r.m.s.d.(A)=		.284

TITL Verwer V 1 from powder diffraction data

	REFERENCE			TARGET		
Matrix code (Det)	655565556	1.		556655565	1.	
Origin shift	.0000	.0000	.0000	-.5000	.0000	.0000

New cell dimensions, A,deg:			dp/p(%)
a	7.2640	7.2584	-.0771
b	10.6390	10.6350	-.0376
c	15.6330	15.6238	-.0589
alpha	90.00	90.00	.00
beta	90.00	90.00	.00
gamma	90.00	90.00	.00

Atom	x	y	z	Atom	x	y	z	Dev,A

BR1	.5913	.6333	.0158	BR10	.6229	.6389	.0218	.255
S2	.5322	.4505	.3059	S96	.5224	.4936	.3094	.467
O3	.6825	.3659	.2999	O102	.6801	.3941	.3006	.300
O4	.5099	.5173	.3830	O101	.5011	.5591	.3983	.509
N5	.5533	.5566	.2262	N97	.5410	.5925	.2316	.402
C6	.3829	.5989	.0899	C92	.4058	.6187	.0916	.270
C7	.4345	.5295	.1694	C91	.4339	.5572	.1724	.299
C8	.3080	.4175	.1775	C90	.3144	.4488	.1833	.348
C9	.3776	.3256	.1077	C89	.3904	.3449	.1222	.319
C10	.3207	.3906	.0238	C88	.3453	.3986	.0322	.238
C11	.2327	.5144	.0527	C93	.2553	.5275	.0565	.224
C12	.3199	.3770	.2696	C95	.3156	.4181	.2805	.470
C13	.1301	.4733	.1372	C94	.1358	.4969	.1373	.254
C14	.0480	.5805	.1894	C98	.0360	.6122	.1803	.376
C15	-.0240	.3749	.1239	C99	-.0218	.3980	.1238	.246
H16	.3270	.6792	.1064	H107	.3500	.7122	.1019	.395
H17	.5101	.3151	.1108	H106	.5380	.3290	.1304	.396
H18	.3193	.2439	.1131	H105	.3185	.2565	.1330	.339
H19	.4272	.4062	-.0121	H104	.4685	.4082	-.0069	.312
H20	.2332	.3397	-.0077	H103	.2504	.3380	-.0027	.149
H21	.1540	.5548	.0098	H108	.1779	.5699	.0043	.251
H22	.3266	.2862	.2744	H109	.3268	.3191	.2959	.486
H23	.2150	.4071	.3021	H110	.2054	.4628	.3163	.636
H24	-.0494	.6195	.1575	H112	-.0499	.6596	.1333	.570
H25	.1419	.6415	.2015	H111	.1295	.6818	.2069	.446
H26	-.0001	.5480	.2422	H113	-.0516	.5821	.2331	.540
H27	.0293	.2969	.1056	H115	.0214	.3117	.0931	.258
H28	-.1084	.4045	.0812	H116	-.1304	.4376	.0841	.390
H29	-.0886	.3623	.1768	H114	-.0803	.3709	.1852	.171
						r.m.s.d.(A)=		.375

TITLE Dzyabchenko V rank 5 (ab initio)

	REFERENCE			TARGET		
Matrix code (Det)	655565556	1.		455545556	1.	
Origin shift	.0000	.0000	.0000	.5000	.5000	.0000

New cell dimensions, A,deg:			dp/p(%)
a	7.2640	7.5690	4.1988
b	10.6390	10.0060	-5.9498
c	15.6330	15.0600	-3.6653
alpha	90.00	90.00	.00
beta	90.00	90.00	.00
gamma	90.00	90.00	.00

Atom	x	y	z	Atom	x	y	z	Dev,A
BR1	.5913	.6333	.0158	BR1	.5120	.5687	.0111	.892
S2	.5322	.4505	.3059	S1	.5164	.4566	.3133	.175
O3	.6825	.3659	.2999	O4	.6529	.3580	.3176	.359
O4	.5099	.5173	.3830	O3	.5020	.5473	.3861	.319
N5	.5533	.5566	.2262	N5	.5446	.5490	.2210	.129
C6	.3829	.5989	.0899	C9	.3722	.5861	.0807	.209
C7	.4345	.5295	.1694	C8	.4196	.5204	.1677	.148
C8	.3080	.4175	.1775	C7	.2805	.4180	.1890	.269
C9	.3776	.3256	.1077	C12	.3023	.3026	.1202	.636
C10	.3207	.3906	.0238	C11	.2398	.3680	.0325	.658
C11	.2327	.5144	.0527	C10	.1948	.5136	.0610	.309
C12	.3199	.3770	.2696	C6	.3059	.3822	.2858	.275
C13	.1301	.4733	.1372	C13	.1149	.4943	.1537	.352
C14	.0480	.5805	.1894	C14	.0748	.6228	.2037	.527
C15	-.0240	.3749	.1239	C15	-.0526	.4105	.1559	.649
H16	.3270	.6792	.1064	H20	.3466	.6910	.0918	.293
H17	.5101	.3151	.1108	H25	.4368	.2671	.1159	.740
H18	.3193	.2439	.1131	H24	.2250	.2156	.1371	.843
H19	.4272	.4062	-.0121	H23	.3402	.3645	.0184	.782
H20	.2332	.3397	-.0077	H22	.1275	.3168	.0043	.839
H21	.1540	.5548	.0098	H21	.1138	.5660	.0134	.325
H22	.3266	.2862	.2744	H19	.2995	.2748	.2925	.363
H23	.2150	.4071	.3021	H18	.1944	.4193	.3231	.379
H24	-.0494	.6195	.1575	H28	.0046	.6913	.1596	.843
H25	.1419	.6415	.2015	H26	.1927	.6731	.2270	.634
H26	-.0001	.5480	.2422	H27	-.0100	.6039	.2606	.647
H27	.0293	.2969	.1056	H29	-.0401	.3151	.1240	.616
H28	-.1084	.4045	.0812	H30	-.1588	.4661	.1233	.981
H29	-.0886	.3623	.1768	H31	-.0939	.3942	.2247	.806

r.m.s.d.(A)= .581

TITL Erk 2 Polymorph Predictor, not hit by during the prediction

	REFERENCE			TARGET			
Matrix code (Det)	655565556	1.		455565554	1.		
Origin shift	.0000	.0000	.0000	1.0000	-.5000	.5000	
New cell dimensions, A,deg:							dp/p(%)
a	7.2640			7.1990			-.8948
b	10.6390			10.6022			-.3459
c	15.6330			15.9858			2.2568
alpha	90.00			90.00			.00
beta	90.00			90.00			.00
gamma	90.00			90.00			.00

Atom	x	y	z	Atom	x	y	z	Dev,A
BR1	.5913	.6333	.0158	BR2	.5111	.5860	-.0233	.985
S2	.5322	.4505	.3059	S1	.4295	.5603	.2818	1.434
O3	.6825	.3659	.2999	O4	.5940	.4991	.3106	1.562
O4	.5099	.5173	.3830	O3	.3638	.6560	.3365	1.956
N5	.5533	.5566	.2262	N5	.4525	.6208	.1881	1.165
C6	.3829	.5989	.0899	C9	.3012	.6013	.0519	.843
C7	.4345	.5295	.1694	C8	.3418	.5665	.1372	.929
C8	.3080	.4175	.1775	C7	.2242	.4627	.1649	.798
C9	.3776	.3256	.1077	C12	.2849	.3425	.1148	.703
C10	.3207	.3906	.0238	C11	.2113	.3716	.0255	.817
C11	.2327	.5144	.0527	C10	.1343	.5083	.0377	.753
C12	.3199	.3770	.2696	C6	.2441	.4517	.2611	.974
C13	.1301	.4733	.1372	C13	.0353	.5033	.1251	.780
C14	.0480	.5805	.1894	C14	-.0525	.6314	.1553	1.054
C15	-.0240	.3749	.1239	C15	-.1283	.4067	.1333	.839
H16	.3270	.6792	.1064	H18	.2542	.6991	.0496	1.062
H17	.5101	.3151	.1108	H23	.4359	.3310	.1153	.567
H18	.3193	.2439	.1131	H22	.2233	.2561	.1401	.825
H19	.4272	.4062	-.0121	H21	.3202	.3665	-.0220	.895
H20	.2332	.3397	-.0077	H20	.1017	.3066	.0062	1.037
H21	.1540	.5548	.0098	H19	.0428	.5382	-.0134	.901
H22	.3266	.2862	.2744	H16	.2845	.3574	.2814	.823
H23	.2150	.4071	.3021	H17	.1184	.4806	.2940	1.055
H24	-.0494	.6195	.1575	H26	-.1597	.6615	.1112	1.171
H25	.1419	.6415	.2015	H24	.0466	.7085	.1610	1.179
H26	-.0001	.5480	.2422	H25	-.1167	.6211	.2168	1.214
H27	.0293	.2969	.1056	H28	-.0888	.3101	.1201	.895
H28	-.1084	.4045	.0812	H29	-.2398	.4317	.0902	1.003
H29	-.0886	.3623	.1768	H27	-.1843	.4058	.1967	.889

r.m.s.d.(A)= 1.041

TITL Erk 2 Systematic Search, #6 in P 212121, #8 of 2 space groups

	REFERENCE			TARGET			
Matrix code (Det)	655565556	1.		655565556	1.		
Origin shift	.0000	.0000	.0000	.0000	.0000	.0000	
New cell dimensions, A,deg:							dp/p(%)
a	7.2640			7.1111			-2.1049
b	10.6390			10.9543			2.9636
c	15.6330			15.9166			1.8141
alpha	90.00			90.00			.00
beta	90.00			90.00			.00
gamma	90.00			90.00			.00

Atom	x	y	z	Atom	x	y	z	Dev,A
BR1	.5913	.6333	.0158	BR2	.4992	.5873	-.0265	1.064
S2	.5322	.4505	.3059	S1	.4171	.5661	.2842	1.536
O3	.6825	.3659	.2999	O4	.5821	.4981	.3055	1.602
O4	.5099	.5173	.3830	O3	.3652	.6639	.3387	2.018
N5	.5533	.5566	.2262	N5	.4440	.6256	.1875	1.243
C6	.3829	.5989	.0899	C9	.2847	.5977	.0480	.967
C7	.4345	.5295	.1694	C8	.3315	.5698	.1384	.988
C8	.3080	.4175	.1775	C7	.2062	.4679	.1678	.925
C9	.3776	.3256	.1077	C12	.2708	.3503	.1205	.837
C10	.3207	.3906	.0238	C11	.2084	.3757	.0290	.827

C11	.2327	.5144	.0527	C10	.1209	.5057	.0344	.859
C12	.3199	.3770	.2696	C6	.2208	.4661	.2627	1.202
C13	.1301	.4733	.1372	C13	.0225	.5039	.1201	.883
C14	.0480	.5805	.1894	C14	-.0622	.6282	.1484	1.145
C15	-.0240	.3749	.1239	C15	-.1332	.4091	.1285	.871
H16	.3270	.6792	.1064	H18	.2335	.6913	.0430	1.213
H17	.5101	.3151	.1108	H23	.4236	.3377	.1251	.705
H18	.3193	.2439	.1131	H22	.2048	.2681	.1459	1.007
H19	.4272	.4062	-.0121	H21	.3261	.3701	-.0151	.826
H20	.2332	.3397	-.0077	H20	.1057	.3089	.0067	1.001
H21	.1540	.5548	.0098	H19	.0304	.5289	-.0189	1.036
H22	.3266	.2862	.2744	H17	.0953	.5034	.2923	2.889
H23	.2150	.4071	.3021	H16	.2482	.3753	.2880	.473
H24	-.0494	.6195	.1575	H26	-.1623	.6600	.1012	1.280
H25	.1419	.6415	.2015	H24	.0380	.7018	.1589	1.197
H26	-.0001	.5480	.2422	H25	-.1391	.6190	.2075	1.373
H27	.0293	.2969	.1056	H27	-.1853	.4063	.1930	2.383
H28	-.1084	.4045	.0812	H28	-.0980	.3155	.1128	1.085
H29	-.0886	.3623	.1768	H29	-.2511	.4343	.0880	1.982
						r.m.s.d.(A)=		1.325

TITL Gavezzotti compound 2

	REFERENCE			TARGET		
Matrix code (Det)	655565556	1.		655545554	1.	
Origin shift	.0000	.0000	.0000	.5000	.5000	.0000

New cell dimensions, A,deg:			dp/p(%)
a	7.2640	7.0548	-2.8800
b	10.6390	10.3517	-2.7004
c	15.6330	15.5275	-.6749
alpha	90.00	90.00	.00
beta	90.00	90.00	.00
gamma	90.00	90.00	.00

Atom	x	y	z	Atom	x	y	z	Dev,A
BR1	.5913	.6333	.0158	BR9	.5782	.5911	.0019	.502
S2	.5322	.4505	.3059	S3	.5265	.4806	.3065	.319
O3	.6825	.3659	.2999	O4	.6854	.3950	.3073	.327
O4	.5099	.5173	.3830	O5	.4945	.5572	.3817	.434
N5	.5533	.5566	.2262	N6	.5478	.5811	.2223	.267
C6	.3829	.5989	.0899	C8	.3735	.6092	.0816	.181
C7	.4345	.5295	.1694	C7	.4258	.5481	.1659	.212
C8	.3080	.4175	.1775	C1	.2969	.4342	.1796	.195
C9	.3776	.3256	.1077	C12	.3601	.3342	.1103	.160
C10	.3207	.3906	.0238	C11	.2944	.3931	.0256	.192
C11	.2327	.5144	.0527	C10	.2074	.5226	.0538	.201
C12	.3199	.3770	.2696	C2	.3136	.3983	.2730	.234
C13	.1301	.4733	.1372	C13	.1097	.4891	.1404	.227
C14	.0480	.5805	.1894	C15	.0335	.6060	.1892	.287
C15	-.0240	.3749	.1239	C14	-.0472	.3876	.1353	.277
H16	.3270	.6792	.1064	H18	.3232	.7065	.0925	.360
H17	.5101	.3151	.1108	H23	.5127	.3278	.1102	.135
H18	.3193	.2439	.1131	H22	.2847	.2447	.1209	.276
H19	.4272	.4062	-.0121	H21	.4164	.4117	-.0146	.104
H20	.2332	.3397	-.0077	H20	.1853	.3330	-.0022	.360
H21	.1540	.5548	.0098	H19	.1144	.5658	.0067	.310
H22	.3266	.2862	.2744	H17	.3347	.2952	.2784	.127
H23	.2150	.4071	.3021	H16	.1941	.4375	.3080	.364
H24	-.0494	.6195	.1575	H27	-.0878	.6449	.1556	.384
H25	.1419	.6415	.2015	H28	.1426	.6790	.1933	.414
H26	-.0001	.5480	.2422	H29	-.0082	.5771	.2533	.356
H27	.0293	.2969	.1056	H25	.0042	.3041	.1010	.208
H28	-.1084	.4045	.0812	H24	-.1681	.4275	.1019	.587
H29	-.0886	.3623	.1768	H26	-.0884	.3597	.1998	.359
						r.m.s.d.(A)=		.309

TITL Gavezzotti compound 2 optimized experimental

	REFERENCE			TARGET		
Matrix code (Det)	655565556	1.		655545554	1.	
Origin shift	.0000	.0000	.0000	.5000	.5000	.0000

New cell dimensions, A,deg:			dp/p(%)
a	7.2640	6.9746	-3.9840
b	10.6390	10.6970	.5452
c	15.6330	15.2287	-2.5862
alpha	90.00	90.00	.00
beta	90.00	90.00	.00
gamma	90.00	90.00	.00

Atom	x	y	z	Atom	x	y	z	Dev,A
BR1	.5913	.6333	.0158	BR9	.6117	.6372	.0180	.155
S2	.5322	.4505	.3059	S3	.5512	.4764	.3217	.393
O3	.6825	.3659	.2999	O4	.7084	.3925	.3185	.444
O4	.5099	.5173	.3830	O5	.5274	.5483	.3985	.427
N5	.5533	.5566	.2262	N6	.5724	.5762	.2363	.294
C6	.3829	.5989	.0899	C8	.3948	.6077	.0951	.150
C7	.4345	.5295	.1694	C7	.4490	.5447	.1790	.243
C8	.3080	.4175	.1775	C1	.3180	.4337	.1912	.282
C9	.3776	.3256	.1077	C12	.3913	.3375	.1228	.283
C10	.3207	.3906	.0238	C11	.3317	.3958	.0345	.191
C11	.2327	.5144	.0527	C10	.2390	.5206	.0598	.136
C12	.3199	.3770	.2696	C2	.3307	.4001	.2870	.372
C13	.1301	.4733	.1372	C13	.1324	.4855	.1479	.211
C14	.0480	.5805	.1894	C14	.0461	.5955	.1976	.204
C15	-.0240	.3749	.1239	C15	-.0274	.3863	.1376	.245
H16	.3270	.6792	.1064	H18	.3300	.6967	.1106	.199
H17	.5101	.3151	.1108	H23	.5458	.3328	.1261	.395
H18	.3193	.2439	.1131	H22	.3160	.2501	.1317	.295
H19	.4272	.4062	-.0121	H21	.4585	.4138	-.0041	.267
H20	.2332	.3397	-.0077	H20	.2251	.3369	.0039	.190
H21	.1540	.5548	.0098	H19	.1485	.5610	.0099	.077
H22	.3266	.2862	.2744	H17	.3468	.3002	.2935	.360
H23	.2150	.4071	.3021	H16	.2110	.4412	.3215	.472
H24	-.0494	.6195	.1575	H24	-.0732	.6331	.1609	.229
H25	.1419	.6415	.2015	H25	.1535	.6672	.2062	.295
H26	-.0001	.5480	.2422	H26	-.0034	.5644	.2613	.344
H27	.0293	.2969	.1056	H28	.0284	.3066	.1025	.114
H28	-.1084	.4045	.0812	H27	-.1458	.4260	.1015	.471
H29	-.0886	.3623	.1768	H29	-.0762	.3573	.2018	.399
						r.m.s.d.(A)=		.301

TITLE Hofmann V minimized

	REFERENCE			TARGET		
Matrix code (Det)	655565556	1.		655565556	1.	
Origin shift	.0000	.0000	.0000	.0000	.0000	.0000

New cell dimensions, A,deg:			dp/p(%)
a	7.2640	7.2000	-.8811
b	10.6390	10.4999	-1.3074
c	15.6330	15.4998	-.8521
alpha	90.00	90.00	.00
beta	90.00	90.00	.00
gamma	90.00	90.00	.00

Atom	x	y	z	Atom	x	y	z	Dev,A
BR1	.5913	.6333	.0158	BR1	.5966	.6412	.0280	.211
S2	.5322	.4505	.3059	S2	.5370	.4504	.3189	.206
O3	.6825	.3659	.2999	O3	.6886	.3648	.3121	.196
O4	.5099	.5173	.3830	O4	.5144	.5166	.3973	.225
N5	.5533	.5566	.2262	N5	.5582	.5595	.2395	.212
C6	.3829	.5989	.0899	C6	.3863	.6049	.1024	.207
C7	.4345	.5295	.1694	C8	.4384	.5331	.1820	.201
C8	.3080	.4175	.1775	C9	.3107	.4195	.1892	.184
C9	.3776	.3256	.1077	C10	.3810	.3277	.1180	.163
C10	.3207	.3906	.0238	C13	.3236	.3952	.0339	.166
C11	.2327	.5144	.0527	C16	.2348	.5200	.0642	.189
C12	.3199	.3770	.2696	C18	.3227	.3767	.2817	.189
C13	.1301	.4733	.1372	C21	.1313	.4768	.1490	.188
C14	.0480	.5805	.1894	C22	.0484	.5844	.2026	.210
C15	-.0240	.3749	.1239	C26	-.0242	.3773	.1347	.170
H16	.3270	.6792	.1064	H7	.3299	.6860	.1198	.221
H17	.5101	.3151	.1108	H11	.5146	.3170	.1210	.163
H18	.3193	.2439	.1131	H12	.3221	.2448	.1227	.151
H19	.4272	.4062	-.0121	H14	.4310	.4117	-.0022	.167
H20	.2332	.3397	-.0077	H15	.2353	.3442	.0017	.154
H21	.1540	.5548	.0098	H17	.1554	.5618	.0212	.193

H22	.3266	.2862	.2744	H19	.3295	.2846	.2857	.178
H23	.2150	.4071	.3021	H20	.2169	.4065	.3147	.197
H24	-.0494	.6195	.1575	H23	-.0498	.6245	.1708	.213
H25	.1419	.6415	.2015	H24	.1432	.6460	.2153	.221
H26	-.0001	.5480	.2422	H25	-.0001	.5504	.2556	.210
H27	.0293	.2969	.1056	H27	.0296	.2987	.1156	.156
H28	-.1084	.4045	.0812	H28	-.1094	.4081	.0919	.171
H29	-.0886	.3623	.1768	H29	-.0894	.3636	.1880	.174
						r.m.s.d.(A)=		.190

TITL Scheraga minimized experimental structure target 2

	REFERENCE			TARGET		
Matrix code (Det)	655565556	1.		655565556	1.	
Origin shift	.0000	.0000	.0000	.0000	.0000	.0000

New cell dimensions, A,deg:			dp/p(%)
a	7.2640	7.0710	-2.6569
b	10.6390	10.5750	-.6016
c	15.6330	16.1120	3.0640
alpha	90.00	90.00	.00
beta	90.00	90.00	.00
gamma	90.00	90.00	.00

Atom	x	y	z	Atom	x	y	z	Dev,A
BR1	.5913	.6333	.0158	BR1	.6087	.6312	.0152	.127
S2	.5322	.4505	.3059	S2	.5131	.4692	.3006	.255
O3	.6825	.3659	.2999	O3	.6639	.3808	.3003	.207
O4	.5099	.5173	.3830	O4	.4863	.5422	.3728	.353
N5	.5533	.5566	.2262	N5	.5469	.5697	.2206	.171
C6	.3829	.5989	.0899	C6	.3865	.6060	.0840	.122
C7	.4345	.5295	.1694	C8	.4289	.5408	.1641	.152
C8	.3080	.4175	.1775	C9	.2932	.4314	.1730	.195
C9	.3776	.3256	.1077	C10	.3667	.3328	.1095	.113
C10	.3207	.3906	.0238	C13	.3190	.3933	.0252	.038
C11	.2327	.5144	.0527	C16	.2319	.5215	.0477	.109
C12	.3199	.3770	.2696	C18	.2952	.3970	.2636	.292
C13	.1301	.4733	.1372	C21	.1170	.4882	.1288	.227
C14	.0480	.5805	.1894	C22	.0330	.6012	.1745	.340
C15	-.0240	.3749	.1239	C26	-.0444	.3914	.1160	.261
H16	.3270	.6792	.1064	H7	.3314	.6889	.0965	.191
H17	.5101	.3151	.1108	H11	.5019	.3198	.1154	.107
H18	.3193	.2439	.1131	H12	.3026	.2523	.1161	.157
H19	.4272	.4062	-.0121	H14	.4323	.4043	-.0080	.077
H20	.2332	.3397	-.0077	H15	.2298	.3417	-.0054	.049
H21	.1540	.5548	.0098	H17	.1569	.5606	.0034	.120
H22	.3266	.2862	.2744	H19	.2974	.3060	.2712	.301
H23	.2150	.4071	.3021	H20	.1860	.4316	.2922	.368
H24	-.0494	.6195	.1575	H23	-.0622	.6400	.1405	.358
H25	.1419	.6415	.2015	H24	.1311	.6614	.1861	.332
H26	-.0001	.5480	.2422	H25	-.0227	.5732	.2257	.408
H27	.0293	.2969	.1056	H27	.0083	.3108	.1017	.219
H28	-.1084	.4045	.0812	H28	-.1258	.4198	.0721	.251
H29	-.0886	.3623	.1768	H29	-.1161	.3838	.1664	.344
						r.m.s.d.(A)=		.239

TITL Schmidt V 46

	REFERENCE			TARGET		
Matrix code (Det)	655565556	1.		655565556	1.	
Origin shift	.0000	.0000	.0000	.0000	.0000	.0000

New cell dimensions, A,deg:			dp/p(%)
a	7.2640	6.8121	-6.2211
b	10.6390	10.0585	-5.4563
c	15.6330	16.7283	7.0063
alpha	90.00	90.00	.00
beta	90.00	90.00	.00
gamma	90.00	90.00	.00

Atom	x	y	z	Atom	x	y	z	Dev,A
BR1	.5913	.6333	.0158	BR15	.5343	.6161	.0086	.454
S2	.5322	.4505	.3059	S9	.4576	.4867	.3052	.645
O3	.6825	.3659	.2999	O13	.6212	.4011	.3201	.653

O4	.5099	.5173	.3830	O14	.3891	.5651	.3709	1.003
N5	.5533	.5566	.2262	N10	.4851	.5774	.2211	.533
C6	.3829	.5989	.0899	C3	.3153	.5923	.0838	.490
C7	.4345	.5295	.1694	C2	.3738	.5393	.1645	.446
C8	.3080	.4175	.1775	C1	.2398	.4151	.1813	.485
C9	.3776	.3256	.1077	C6	.3118	.3064	.1234	.564
C10	.3207	.3906	.0238	C5	.2482	.3582	.0411	.672
C11	.2327	.5144	.0527	C4	.1513	.4933	.0585	.620
C12	.3199	.3770	.2696	C8	.2577	.3895	.2692	.457
C13	.1301	.4733	.1372	C7	.0467	.4646	.1409	.597
C14	.0480	.5805	.1894	C12	-.0435	.5888	.1793	.670
C15	-.0240	.3749	.1239	C11	-.1140	.3582	.1353	.682
H16	.3270	.6792	.1064	H16	.2570	.6873	.0903	.564
H17	.5101	.3151	.1108	H21	.4632	.2945	.1269	.472
H18	.3193	.2439	.1131	H20	.2466	.2157	.1370	.704
H19	.4272	.4062	-.0121	H18	.3671	.3674	.0025	.629
H20	.2332	.3397	-.0077	H19	.1479	.2943	.0142	.840
H21	.1540	.5548	.0098	H17	.0605	.5294	.0135	.711
H22	.3266	.2862	.2744	H23	.2823	.2892	.2805	.329
H23	.2150	.4071	.3021	H22	.1284	.4149	.2985	.617
H24	-.0494	.6195	.1575	H27	-.1437	.6316	.1401	.732
H25	.1419	.6415	.2015	H29	.0611	.6601	.1940	.613
H26	-.0001	.5480	.2422	H28	-.1172	.5633	.2315	.857
H27	.0293	.2969	.1056	H24	-.0649	.2707	.1089	.718
H28	-.1084	.4045	.0812	H26	-.2310	.3944	.1018	.931
H29	-.0886	.3623	.1768	H25	-.1643	.3352	.1924	.653
						r.m.s.d.(A)=		.649

TITL Williams V observed relaxed with W99 force field

	REFERENCE			TARGET		
Matrix code (Det)	655565556	1.		655565556	1.	
Origin shift	.0000	.0000	.0000	.0000	.0000	.0000

New cell dimensions, A,deg:			dp/p(%)
a	7.2640	7.0099	-3.4981
b	10.6390	10.6873	.4540
c	15.6330	15.4042	-1.4636
alpha	90.00	90.00	.00
beta	90.00	90.00	.00
gamma	90.00	90.00	.00

Atom	x	y	z	Atom	x	y	z	Dev,A
BR1	.5913	.6333	.0158	BR	.6185	.6427	.0225	.242
S2	.5322	.4505	.3059	S	.5478	.4609	.3166	.229
O3	.6825	.3659	.2999	O1	.7064	.3788	.3123	.292
O4	.5099	.5173	.3830	O2	.5185	.5274	.3944	.216
N5	.5533	.5566	.2262	N	.5705	.5665	.2358	.220
C6	.3829	.5989	.0899	C1	.3998	.6057	.0955	.166
C7	.4345	.5295	.1694	C2	.4513	.5377	.1769	.188
C8	.3080	.4175	.1775	C3	.3233	.4245	.1839	.165
C9	.3776	.3256	.1077	C4	.4020	.3337	.1140	.218
C10	.3207	.3906	.0238	C5	.3454	.3973	.0282	.202
C11	.2327	.5144	.0527	C6	.2488	.5194	.0563	.138
C12	.3199	.3770	.2696	C7	.3321	.3846	.2776	.172
C13	.1301	.4733	.1372	C8	.1394	.4773	.1409	.098
C14	.0480	.5805	.1894	C9	.0483	.5830	.1928	.059
C15	-.0240	.3749	.1239	C10	-.0164	.3772	.1259	.067
H16	.3270	.6792	.1064	H1	.3385	.6849	.1115	.129
H17	.5101	.3151	.1108	H4A	.5422	.3250	.1188	.281
H18	.3193	.2439	.1131	H4B	.3427	.2500	.1191	.202
H19	.4272	.4062	-.0121	H5A	.4594	.4146	-.0078	.255
H20	.2332	.3397	-.0077	H5B	.2562	.3442	-.0054	.175
H21	.1540	.5548	.0098	H6	.1675	.5587	.0114	.108
H22	.3266	.2862	.2744	H7A	.3418	.2935	.2827	.186
H23	.2150	.4071	.3021	H7B	.2197	.4135	.3096	.139
H24	-.0494	.6195	.1575	H9A	-.0553	.6215	.1582	.049
H25	.1419	.6415	.2015	H9B	.1459	.6470	.2064	.100
H26	-.0001	.5480	.2422	H9C	-.0048	.5492	.2475	.090
H27	.0293	.2969	.1056	H10A	.0441	.2978	.1076	.110
H28	-.1084	.4045	.0812	H10B	-.1052	.4062	.0802	.033
H29	-.0886	.3623	.1768	H10C	-.0878	.3635	.1806	.060
						r.m.s.d.(A)=		.173

TITL Williams Va observed molecular structure

	REFERENCE			TARGET			
Matrix code (Det)	655565556	1.		545554655	1.		
Origin shift	.0000	.0000	.0000	.5000	1.0000	.0000	
New cell dimensions, A,deg:							dp/p(%)
a	7.2640			7.0097			-3.5008
b	10.6390			10.6875			.4559
c	15.6330			15.4023			-1.4757
alpha	90.00			90.00			.00
beta	90.00			90.00			.00
gamma	90.00			90.00			.00

Atom	x	y	z	Atom	x	y	z	Dev,A
BR1	.5913	.6333	.0158	BR	.6185	.6427	.0225	.242
S2	.5322	.4505	.3059	S	.5479	.4609	.3166	.229
O3	.6825	.3659	.2999	O1	.7065	.3788	.3124	.293
O4	.5099	.5173	.3830	O2	.5186	.5274	.3945	.217
N5	.5533	.5566	.2262	N	.5705	.5665	.2358	.220
C6	.3829	.5989	.0899	C1	.3999	.6057	.0955	.166
C7	.4345	.5295	.1694	C2	.4513	.5377	.1769	.188
C8	.3080	.4175	.1775	C3	.3234	.4245	.1839	.166
C9	.3776	.3256	.1077	C4	.4020	.3337	.1140	.218
C10	.3207	.3906	.0238	C5	.3455	.3973	.0281	.202
C11	.2327	.5144	.0527	C6	.2489	.5194	.0562	.139
C12	.3199	.3770	.2696	C7	.3322	.3846	.2776	.172
C13	.1301	.4733	.1372	C8	.1395	.4773	.1409	.099
C14	.0480	.5805	.1894	C9	.0483	.5831	.1928	.059
C15	-.0240	.3749	.1239	C10	-.0163	.3772	.1259	.068
H16	.3270	.6792	.1064	H1	.3386	.6849	.1115	.129
H17	.5101	.3151	.1108	H4A	.5422	.3250	.1188	.281
H18	.3193	.2439	.1131	H4B	.3428	.2500	.1191	.203
H19	.4272	.4062	-.0121	H5A	.4595	.4146	-.0079	.256
H20	.2332	.3397	-.0077	H5B	.2562	.3442	-.0054	.175
H21	.1540	.5548	.0098	H6	.1676	.5587	.0113	.108
H22	.3266	.2862	.2744	H7A	.3418	.2935	.2828	.186
H23	.2150	.4071	.3021	H7B	.2197	.4135	.3097	.140
H24	-.0494	.6195	.1575	H9A	-.0552	.6215	.1582	.048
H25	.1419	.6415	.2015	H9B	.1460	.6471	.2064	.101
H26	-.0001	.5480	.2422	H9C	-.0048	.5492	.2475	.090
H27	.0293	.2969	.1056	H10A	.0442	.2978	.1075	.111
H28	-.1084	.4045	.0812	H10B	-.1052	.4062	.0802	.033
H29	-.0886	.3623	.1768	H10C	-.0878	.3635	.1806	.060
						r.m.s.d.(A)=		.174

TITL Dzyabchenko VI (powder)

	REFERENCE			TARGET			
Matrix code (Det)	655565556	1.		655565556	1.		
Origin shift	.0000	.0000	.0000	.0000	.0000	.0000	
New cell dimensions, A,deg:							dp/p(%)
a	8.2510			8.2400			-.1333
b	8.9640			8.9470			-.1896
c	15.0870			15.0560			-.2055
alpha	90.00			90.00			.00
beta	91.21			91.21			.00
gamma	90.00			90.00			.00

Atom	x	y	z	Atom	x	y	z	Dev,A
S1	.3065	.1271	.1571	S1	.3181	.1134	.1597	.160
O2	.3553	.0380	.2313	O2	.3756	.0248	.2339	.208
O3	.3571	.0691	.0714	O3	.3637	.0635	.0717	.074
N4	.3651	.2887	.1764	N4	.3805	.2847	.1725	.145
N5	.4200	.5264	.1396	N12	.4212	.5283	.1355	.066
N6	.4991	.7682	.1249	N18	.4764	.7843	.1115	.308
C7	.3407	.3998	.1170	C11	.3435	.3977	.1158	.036
C8	.4149	.6559	.0945	C13	.3949	.6575	.0884	.187
C9	.3232	.6610	.0209	C14	.2895	.6603	.0190	.279
C10	.2441	.5393	-.0042	C15	.2103	.5284	-.0050	.295
C11	.2508	.4045	.0434	C16	.2372	.3992	.0417	.124
C12	.0989	.1234	.1598	C5	.1055	.1197	.1660	.112
C13	.0199	.0139	.1141	C6	.0146	.0165	.1182	.081

C14	-.1371	.0087	.1195	C7	-.1531	.0210	.1195	.172
C15	-.2216	.1066	.1666	C8	-.2326	.1286	.1687	.219
C16	-.1470	.2142	.2119	C9	-.1395	.2295	.2168	.167
C17	.0127	.2249	.2096	C10	.0277	.2254	.2161	.157
H18	.4960	.5240	.1830	H17	.5307	.5174	.1632	.422
H19	.3149	.7483	-.0122	H26	.2692	.7642	-.0160	.406
H20	.1809	.5430	-.0560	H27	.1262	.5264	-.0610	.479
H21	.1937	.3210	.0236	H28	.1749	.2989	.0201	.256
H22	.0760	-.0548	.0803	H21	.0748	-.0680	.0798	.119
H23	-.1929	-.0663	.0892	H22	-.2227	-.0602	.0817	.274
H24	-.3339	.0993	.1677	H23	-.3635	.1336	.1694	.394
H25	-.2062	.2815	.2451	H24	-.1990	.3136	.2560	.336
H26	.0665	.2999	.2410	H25	.0977	.3051	.2549	.332
H27	.4975	.8519	.0970	H20	.4571	.8737	.0737	.517
H28	.5563	.7587	.1729	H19	.4779	.8091	.1763	.791
						r.m.s.d.(A)=		.303

TITL Leusen VI PowderSolve

	REFERENCE			TARGET		
Matrix code (Det)	655565556	1.		556545455	-1.	
Origin shift	.0000	.0000	.0000	.0000	1.5000	.5000

New cell dimensions, A,deg:			Dev
a	8.2510	8.2420	-.0090
b	8.9640	8.9520	-.0120
c	15.0870	15.0680	-.0190
alpha	90.00	90.00	.00
beta	91.21	91.22	.01
gamma	90.00	90.00	.00

Atom	x	y	z	Atom	x	y	z	Dev,A
S1	.3065	.1271	.1571	S7	.3076	.1233	.1569	.035
O2	.3553	.0380	.2313	O15	.3548	.0400	.2371	.089
O3	.3571	.0691	.0714	O16	.3623	.0644	.0692	.069
N4	.3651	.2887	.1764	N8	.3636	.2777	.1693	.146
N5	.4200	.5264	.1396	N14	.4242	.5346	.1414	.086
N6	.4991	.7682	.1249	N17	.4915	.7847	.1265	.163
C7	.3407	.3998	.1170	C9	.3470	.4004	.1203	.071
C8	.4149	.6559	.0945	C13	.4095	.6635	.0938	.082
C9	.3232	.6610	.0209	C12	.3131	.6647	.0169	.107
C10	.2441	.5393	-.0042	C11	.2337	.5313	-.0077	.123
C11	.2508	.4045	.0434	C10	.2480	.4022	.0419	.037
C12	.0989	.1234	.1598	C5	.1084	.1126	.1547	.147
C13	.0199	.0139	.1141	C4	.0099	.0077	.1112	.108
C14	-.1371	.0087	.1195	C3	-.1580	.0142	.1217	.183
C15	-.2216	.1066	.1666	C2	-.2258	.1252	.1746	.209
C16	-.1470	.2142	.2119	C1	-.1255	.2292	.2182	.240
C17	.0127	.2249	.2096	C6	.0423	.2231	.2085	.246
H18	.4960	.5240	.1830	H26	.5031	.5263	.1963	.208
H19	.3149	.7483	-.0122	H25	.2994	.7671	-.0216	.253
H20	.1809	.5430	-.0560	H24	.1581	.5306	-.0682	.283
H21	.1937	.3210	.0236	H23	.1860	.2992	.0236	.206
H22	.0760	-.0548	.0803	H21	.0653	-.0787	.0707	.272
H23	-.1929	-.0663	.0892	H20	-.2362	-.0677	.0883	.358
H24	-.3339	.0993	.1677	H19	-.3571	.1304	.1823	.406
H25	-.2062	.2815	.2451	H18	-.1783	.3154	.2600	.440
H26	.0665	.2999	.2410	H22	.1226	.3025	.2425	.463
H27	.4975	.8519	.0970	H27	.4883	.8831	.0929	.296
H28	.5563	.7587	.1729	H28	.5571	.7796	.1844	.255
						r.m.s.d.(A)=		.231

TITLE Dzyabchenko VI ab initio Energy=-3.443532E+01 Density=1.40403

	REFERENCE			TARGET		
Matrix code (Det)	655565556	1.		655565556	1.	
Origin shift	.0000	.0000	.0000	.0000	.0000	.0000

New cell dimensions, A,deg:			dp/p(%)
a	8.2510	8.3350	1.0180
b	8.9640	9.7180	8.4114
c	15.0870	14.8230	-1.7499
alpha	90.00	90.00	.00
beta	91.21	100.79	10.50

gamma		90.00			90.00		.00	
Atom	x	y	z	Atom	x	y	z	Dev,A
S1	.3065	.1271	.1571	S1	.3347	.1807	.1132	.877
O2	.3553	.0380	.2313	O2	.4548	.0860	.1604	1.479
O3	.3571	.0691	.0714	O3	.3113	.1825	.0134	1.396
N4	.3651	.2887	.1764	N4	.3794	.3359	.1525	.588
N5	.4200	.5264	.1396	N12	.4203	.5670	.1456	.390
N6	.4991	.7682	.1249	N18	.4678	.8069	.1551	.653
C7	.3407	.3998	.1170	C11	.3644	.4502	.0993	.584
C8	.4149	.6559	.0945	C13	.4095	.6942	.1051	.396
C9	.3232	.6610	.0209	C14	.3425	.7092	.0157	.487
C10	.2441	.5393	-.0042	C15	.2874	.5922	-.0349	.786
C11	.2508	.4045	.0434	C16	.2989	.4650	.0054	.922
C12	.0989	.1234	.1598	C5	.1437	.1407	.1436	.491
C13	.0199	.0139	.1141	C6	.0648	.0217	.1091	.394
C14	-.1371	.0087	.1195	C7	-.0874	-.0102	.1276	.453
C15	-.2216	.1066	.1666	C8	-.1631	.0763	.1813	.585
C16	-.1470	.2142	.2119	C9	-.0813	.1938	.2161	.574
C17	.0127	.2249	.2096	C10	.0707	.2262	.1982	.527
H18	.4960	.5240	.1830	H17	.4696	.5598	.2123	.609
H19	.3149	.7483	-.0122	H26	.3332	.8109	-.0141	.606
H20	.1809	.5430	-.0560	H27	.2345	.6003	-.1070	1.067
H21	.1937	.3210	.0236	H28	.2567	.3767	-.0367	1.207
H22	.0760	-.0548	.0803	H21	.1224	-.0467	.0674	.455
H23	-.1929	-.0663	.0892	H22	-.1478	-.1035	.1000	.524
H24	-.3339	.0993	.1677	H23	-.2825	.0527	.1955	.712
H25	-.2062	.2815	.2451	H24	-.1376	.2622	.2585	.611
H26	.0665	.2999	.2410	H25	.1325	.3183	.2268	.631
H27	.4975	.8519	.0970	H20	.4599	.8998	.1255	.712
H28	.5563	.7587	.1729	H19	.5185	.7969	.2215	.895
						r.m.s.d.(A)=		.742

TITL Erk 3A Polymorph Predictor, #24 in P21/c, #54 of 5 space groups

	REFERENCE			TARGET		
Matrix code (Det)	655565556	1.		655545556	-1.	
Origin shift	.0000	.0000	.0000	-.5000	.5000	.0000

New cell dimensions, A,deg:			Dev
a	8.2510	8.5531	.3021
b	8.9640	9.2111	.2471
c	15.0870	15.0606	-.0264
alpha	90.00	90.00	.00
beta	91.21	88.08	-3.13
gamma	90.00	90.00	.00

Atom	x	y	z	Atom	x	y	z	Dev,A
S1	.3065	.1271	.1571	S1	.2955	.1306	.1442	.219
O2	.3553	.0380	.2313	O3	.3446	.0502	.2189	.235
O3	.3571	.0691	.0714	O2	.3707	.0550	.0719	.172
N4	.3651	.2887	.1764	N4	.3666	.2891	.1617	.221
N5	.4200	.5264	.1396	N5	.4234	.5298	.1431	.068
N6	.4991	.7682	.1249	N22	.4854	.7686	.1443	.314
C7	.3407	.3998	.1170	C12	.3507	.4102	.1125	.143
C8	.4149	.6559	.0945	C16	.4138	.6603	.1040	.149
C9	.3232	.6610	.0209	C15	.3294	.6782	.0264	.185
C10	.2441	.5393	-.0042	C14	.2539	.5566	-.0092	.193
C11	.2508	.4045	.0434	C13	.2645	.4215	.0341	.238
C12	.0989	.1234	.1598	C6	.0927	.1131	.1515	.165
C13	.0199	.0139	.1141	C11	.0195	-.0080	.1134	.200
C14	-.1371	.0087	.1195	C10	-.1444	-.0224	.1190	.290
C15	-.2216	.1066	.1666	C9	-.2353	.0840	.1632	.241
C16	-.1470	.2142	.2119	C8	-.1633	.2046	.2019	.222
C17	.0127	.2249	.2096	C7	.0005	.2190	.1960	.236
H18	.4960	.5240	.1830	H25	.4856	.5229	.1949	.199
H19	.3149	.7483	-.0122	H23	.3246	.7775	-.0032	.309
H20	.1809	.5430	-.0560	H24	.1931	.5659	-.0662	.278
H21	.1937	.3210	.0236	H21	.2110	.3328	.0085	.289
H22	.0760	-.0548	.0803	H20	.0857	-.0858	.0817	.294
H23	-.1929	-.0663	.0892	H19	-.1982	-.1097	.0909	.398
H24	-.3339	.0993	.1677	H28	-.3543	.0739	.1669	.288
H25	-.2062	.2815	.2451	H18	-.2303	.2817	.2341	.263
H26	.0665	.2999	.2410	H17	.0524	.3067	.2242	.287
H27	.4975	.8519	.0970	H27	.4708	.8670	.1235	.477

H28	.5563	.7587	.1729	H26	.5450	.7497	.1965	.377
						r.m.s.d.(A)=		.262

TITL Erk 3A Polymorph Predictor, #24 in P21/c, #54 of 5 space groups

	REFERENCE			TARGET		
Matrix code (Det)	655565556	1.		655545556	-1.	
Origin shift	.0000	.0000	.0000	-.5000	.5000	.0000

New cell dimensions, A,deg:			Dev
a	8.2510	8.5531	.3021
b	8.9640	9.2111	.2471
c	15.0870	15.0606	-.0264
alpha	90.00	90.00	.00
beta	91.21	88.08	-3.13
gamma	90.00	90.00	.00

Atom	x	y	z	Atom	x	y	z	Dev,A
S1	.3065	.1271	.1571	S1	.2955	.1306	.1442	.219
O2	.3553	.0380	.2313	O3	.3446	.0502	.2189	.235
O3	.3571	.0691	.0714	O2	.3707	.0550	.0719	.172
N4	.3651	.2887	.1764	N4	.3666	.2891	.1617	.221
N5	.4200	.5264	.1396	N5	.4234	.5298	.1431	.068
N6	.4991	.7682	.1249	N22	.4854	.7686	.1443	.314
C7	.3407	.3998	.1170	C12	.3507	.4102	.1125	.143
C8	.4149	.6559	.0945	C16	.4138	.6603	.1040	.149
C9	.3232	.6610	.0209	C15	.3294	.6782	.0264	.185
C10	.2441	.5393	-.0042	C14	.2539	.5566	-.0092	.193
C11	.2508	.4045	.0434	C13	.2645	.4215	.0341	.238
C12	.0989	.1234	.1598	C6	.0927	.1131	.1515	.165
C13	.0199	.0139	.1141	C11	.0195	-.0080	.1134	.200
C14	-.1371	.0087	.1195	C10	-.1444	-.0224	.1190	.290
C15	-.2216	.1066	.1666	C9	-.2353	.0840	.1632	.241
C16	-.1470	.2142	.2119	C8	-.1633	.2046	.2019	.222
C17	.0127	.2249	.2096	C7	.0005	.2190	.1960	.236
						r.m.s.d.(A)=		.213

TITL Hofmann VI minimized

	REFERENCE			TARGET		
Matrix code (Det)	655565556	1.		655565556	1.	
Origin shift	.0000	.0000	.0000	-.5000	.0000	-.5000

New cell dimensions, A,deg:			dp/p(%)
a	8.2510	8.3006	.6012
b	8.9640	8.7999	-1.8303
c	15.0870	15.0033	-.5546
alpha	90.00	90.00	.00
beta	91.21	90.46	-.83
gamma	90.00	90.00	.00

Atom	x	y	z	Atom	x	y	z	Dev,A
S1	.3065	.1271	.1571	S28	.3002	.1106	.1559	.156
O2	.3553	.0380	.2313	O26	.3486	.0191	.2298	.179
O3	.3571	.0691	.0714	O27	.3507	.0526	.0691	.160
N4	.3651	.2887	.1764	N21	.3584	.2750	.1755	.134
N5	.4200	.5264	.1396	N22	.4131	.5176	.1391	.097
N6	.4991	.7682	.1249	N23	.4917	.7641	.1248	.071
C7	.3407	.3998	.1170	C2	.3343	.3889	.1164	.111
C8	.4149	.6559	.0945	C3	.4081	.6500	.0943	.077
C9	.3232	.6610	.0209	C4	.3171	.6561	.0209	.067
C10	.2441	.5393	-.0042	C6	.2385	.5324	-.0043	.077
C11	.2508	.4045	.0434	C8	.2451	.3945	.0430	.101
C12	.0989	.1234	.1598	C10	.0939	.1068	.1599	.153
C13	.0199	.0139	.1141	C11	.0155	-.0042	.1141	.165
C14	-.1371	.0087	.1195	C13	-.1406	-.0096	.1205	.165
C15	-.2216	.1066	.1666	C15	-.2247	.0896	.1688	.157
C16	-.1470	.2142	.2119	C17	-.1506	.1987	.2143	.145
C17	.0127	.2249	.2096	C19	.0081	.2097	.2110	.142
H18	.4960	.5240	.1830	H1	.4885	.5147	.1822	.104
H19	.3149	.7483	-.0122	H5	.3089	.7454	-.0120	.056
H20	.1809	.5430	-.0560	H7	.1758	.5367	-.0559	.070
H21	.1937	.3210	.0236	H9	.1884	.3097	.0231	.110
H22	.0760	-.0548	.0803	H12	.0713	-.0738	.0794	.173
H23	-.1929	-.0663	.0892	H14	-.1960	-.0856	.0901	.174

H24	-.3339	.0993	.1677	H16	-.3363	.0822	.1707	.160
H25	-.2062	.2815	.2451	H18	-.2095	.2669	.2484	.142
H26	.0665	.2999	.2410	H20	.0615	.2857	.2425	.135
H27	.4975	.8519	.0970	H24	.4902	.8497	.0971	.064
H28	.5563	.7587	.1729	H25	.5485	.7539	.1726	.078
						r.m.s.d.(A)=		.128

TITL Mooy VI MinimizedExperimental

	REFERENCE			TARGET		
Matrix code (Det)	655565556	1.		655565556	1.	
Origin shift	.0000	.0000	.0000	-.5000	.0000	-.5000

New cell dimensions, A,deg:			Dev
a	8.2510	8.6530	.4020
b	8.9640	9.1970	.2330
c	15.0870	14.4540	-.6330
alpha	90.00	90.00	.00
beta	91.21	84.31	-6.90
gamma	90.00	90.00	.00

Atom	x	y	z	Atom	x	y	z	Dev,A
S1	.3065	.1271	.1571	S28	.2788	.1130	.1602	.269
O2	.3553	.0380	.2313	O26	.3293	.0259	.2465	.327
O3	.3571	.0691	.0714	O27	.3765	.0486	.0709	.248
N4	.3651	.2887	.1764	N21	.3461	.2823	.1771	.170
N5	.4200	.5264	.1396	N22	.4128	.5220	.1510	.182
N6	.4991	.7682	.1249	N23	.4857	.7668	.1351	.186
C7	.3407	.3998	.1170	C2	.3400	.4025	.1245	.113
C8	.4149	.6559	.0945	C3	.4113	.6503	.1054	.171
C9	.3232	.6610	.0209	C4	.3305	.6631	.0268	.110
C10	.2441	.5393	-.0042	C6	.2542	.5407	-.0035	.088
C11	.2508	.4045	.0434	C8	.2610	.4104	.0454	.107
C12	.0989	.1234	.1598	C10	.0804	.0958	.1558	.302
C13	.0199	.0139	.1141	C11	.0216	-.0317	.1193	.421
C14	-.1371	.0087	.1195	C13	-.1382	-.0471	.1146	.512
C15	-.2216	.1066	.1666	C15	-.2392	.0652	.1456	.513
C16	-.1470	.2142	.2119	C17	-.1810	.1915	.1834	.558
C17	.0127	.2249	.2096	C19	-.0213	.2070	.1885	.462
H18	.4960	.5240	.1830	H1	.4702	.5148	.2053	.397
H19	.3149	.7483	-.0122	H5	.3282	.7594	-.0079	.165
H20	.1809	.5430	-.0560	H7	.1951	.5464	-.0611	.142
H21	.1937	.3210	.0236	H9	.2094	.3208	.0245	.134
H22	.0760	-.0548	.0803	H12	.0947	-.1139	.0958	.607
H23	-.1929	-.0663	.0892	H14	-.1812	-.1398	.0881	.675
H24	-.3339	.0993	.1677	H16	-.3553	.0549	.1406	.601
H25	-.2062	.2815	.2451	H18	-.2549	.2727	.2069	.716
H26	.0665	.2999	.2410	H20	.0202	.2999	.2156	.553
H27	.4975	.8519	.0970	H24	.4828	.8578	.1010	.146
H28	.5563	.7587	.1729	H25	.5412	.7625	.1904	.286
						r.m.s.d.(A)=		.379

TITL Scheraga minimized experimental structure TARGET3

	REFERENCE			TARGET		
Matrix code (Det)	655565556	1.		655565556	1.	
Origin shift	.0000	.0000	.0000	-.5000	.0000	-.5000

New cell dimensions, A,deg:			dp/p(%)
a	8.2510	9.1700	11.1380
b	8.9640	10.4280	16.3320
c	15.0870	13.0010	*******
alpha	90.00	90.00	.00
beta	91.21	92.22	1.11
gamma	90.00	90.00	.00

Atom	x	y	z	Atom	x	y	z	Dev,A
S1	.3065	.1271	.1571	S11	.2054	.0467	.1941	1.296
O2	.3553	.0380	.2313	O11	.2219	-.0305	.2843	1.548
O3	.3571	.0691	.0714	O12	.2593	-.0125	.1009	1.243
N4	.3651	.2887	.1764	N12	.2758	.1789	.2200	1.464
N5	.4200	.5264	.1396	N13	.3643	.3733	.1806	1.670
N6	.4991	.7682	.1249	N14	.4705	.5697	.1686	2.038

C7	.3407	.3998	.1170	C17	.2811	.2730	.1487	1.412
C8	.4149	.6559	.0945	C18	.3864	.4817	.1273	1.770
C9	.3232	.6610	.0209	C19	.3203	.4923	.0347	1.647
C10	.2441	.5393	-.0042	C20	.2384	.3960	-.0001	1.392
C11	.2508	.4045	.0434	C21	.2165	.2830	.0563	1.230
C12	.0989	.1234	.1598	C14	.0203	.0663	.1786	.925
C13	.0199	.0139	.1141	C15	-.0558	-.0206	.1202	.747
C14	-.1371	.0087	.1195	C16	-.1969	-.0077	.1124	.551
C15	-.2216	.1066	.1666	C11	-.2677	.0872	.1579	.457
C16	-.1470	.2142	.2119	C12	-.1957	.1730	.2155	.586
C17	.0127	.2249	.2096	C13	-.0522	.1646	.2271	.854
H18	.4960	.5240	.1830	H17	.4228	.3652	.2371	1.839
H19	.3149	.7483	-.0122	H19	.3315	.5658	-.0048	1.778
H20	.1809	.5430	-.0560	H20	.1931	.4034	-.0651	1.364
H21	.1937	.3210	.0236	H21	.1583	.2172	.0293	1.056
H22	.0760	-.0548	.0803	H13	-.0088	-.0869	.0871	.810
H23	-.1929	-.0663	.0892	H12	-.2506	-.0670	.0733	.544
H24	-.3339	.0993	.1677	H11	-.3686	.0933	.1492	.397
H25	-.2062	.2815	.2451	H16	-.2456	.2384	.2476	.543
H26	.0665	.2999	.2410	H15	-.0003	.2242	.2672	1.013
H27	.4975	.8519	.0970	H18B	.4861	.6397	.1357	2.131
H28	.5563	.7587	.1729	H18A	.5105	.5579	.2288	2.141
						r.m.s.d.(A)=		1.337

TITL Schmidt VI minimized experimental

	REFERENCE			TARGET		
Matrix code (Det)	655565556	1.		655565556	1.	
Origin shift	.0000	.0000	.0000	.0000	.0000	.0000

New cell dimensions, A,deg:			dp/p(%)
a	8.2510	8.2576	.0800
b	8.9640	8.9015	-.6972
c	15.0870	14.8969	-1.2600
alpha	90.00	90.00	.00
beta	91.21	95.03	4.19
gamma	90.00	90.00	.00

Atom	x	y	z	Atom	x	y	z	Dev,A
S1	.3065	.1271	.1571	S1	.2903	.0794	.1538	.448
O2	.3553	.0380	.2313	O2	.3801	-.0023	.2268	.422
O3	.3571	.0691	.0714	O1	.2857	.0133	.0653	.773
N4	.3651	.2887	.1764	N1	.3680	.2442	.1606	.464
N5	.4200	.5264	.1396	N2	.4042	.4861	.1168	.509
N6	.4991	.7682	.1249	N3	.4719	.7276	.0872	.698
C7	.3407	.3998	.1170	C7	.3219	.3546	.1012	.489
C8	.4149	.6559	.0945	C11	.3806	.6092	.0620	.690
C9	.3232	.6610	.0209	C10	.2722	.6054	-.0108	.793
C10	.2441	.5393	-.0042	C9	.1823	.4746	-.0281	.839
C11	.2508	.4045	.0434	C8	.2051	.3519	.0269	.644
C12	.0989	.1234	.1598	C1	.0882	.0996	.1808	.395
C13	.0199	.0139	.1141	C6	-.0407	.0373	.1287	.595
C14	-.1371	.0087	.1195	C5	-.1975	.0625	.1501	.846
C15	-.2216	.1066	.1666	C4	-.2296	.1484	.2237	.939
C17	.0127	.2249	.2096	C2	.0587	.1841	.2554	.848
C16	-.1470	.2142	.2119	C3	-.0989	.2085	.2766	1.029
H18	.4960	.5240	.1830	H72	.4875	.4924	.1705	.344
H19	.3149	.7483	-.0122	H10	.2526	.6899	-.0587	.992
H20	.1809	.5430	-.0560	H9	.1008	.4622	-.0849	1.056
H21	.1937	.3210	.0236	H8	.1376	.2556	.0103	.765
H22	.0760	-.0548	.0803	H6	-.0178	-.0298	.0741	.807
H23	-.1929	-.0663	.0892	H5	-.2907	.0158	.1076	1.136
H24	-.3339	.0993	.1677	H4	-.3481	.1666	.2397	1.246
H25	-.2062	.2815	.2451	H3	-.1238	.2725	.3322	1.441
H26	.0665	.2999	.2410	H2	.1575	.2354	.2912	1.183
H27	.4975	.8519	.0970	H74	.4624	.8232	.0506	.782
H28	.5563	.7587	.1729	H73	.5508	.7219	.1429	.557
						r.m.s.d.(A)=		.831

TITL Van Eijck VI Prediction closest to the experimental structure, rank 340

	REFERENCE			TARGET		
Matrix code (Det)	655565556	1.		655545556	-1.	
Origin shift	.0000	.0000	.0000	-.5000	1.0000	.0000

New cell dimensions, A,deg:					Dev
a		8.2510		8.4082	.1572
b		8.9640		9.1789	.2149
c		15.0870		14.2427	-.8443
alpha		90.00		90.00	.00
beta		91.21		91.53	.32
gamma		90.00		90.00	.00

Atom	x	y	z	Atom	x	y	z	Dev,A
S1	.3065	.1271	.1571	S12	.3119	.0846	.1572	.388
O2	.3553	.0380	.2313	O14	.3685	.0054	.2381	.330
O3	.3571	.0691	.0714	O13	.3428	.0111	.0706	.540
N4	.3651	.2887	.1764	N15	.3735	.2511	.1611	.415
N5	.4200	.5264	.1396	N27	.4108	.4946	.1285	.339
N6	.4991	.7682	.1249	N24	.4610	.7415	.1102	.450
C7	.3407	.3998	.1170	C16	.3388	.3627	.1086	.359
C8	.4149	.6559	.0945	C23	.3841	.6224	.0805	.444
C9	.3232	.6610	.0209	C21	.2798	.6224	.0074	.537
C10	.2441	.5393	-.0042	C19	.1985	.4889	-.0206	.638
C11	.2508	.4045	.0434	C17	.2266	.3646	.0286	.465
C12	.0989	.1234	.1598	C11	.1037	.0944	.1688	.296
C13	.0199	.0139	.1141	C7	.0044	.0015	.1160	.174
C14	-.1371	.0087	.1195	C3	-.1608	.0086	.1250	.215
C15	-.2216	.1066	.1666	C1	-.2261	.1091	.1866	.298
C16	-.1470	.2142	.2119	C5	-.1274	.2016	.2398	.451
C17	.0127	.2249	.2096	C9	.0376	.1938	.2311	.468
H18	.4960	.5240	.1830	H28	.4897	.4949	.1837	.270
H19	.3149	.7483	-.0122	H22	.2568	.7216	-.0314	.605
H20	.1809	.5430	-.0560	H20	.1156	.4893	-.0799	.804
H21	.1937	.3210	.0236	H18	.1653	.2661	.0077	.596
H22	.0760	-.0548	.0803	H8	.0566	-.0760	.0688	.300
H23	-.1929	-.0663	.0892	H4	-.2383	-.0629	.0846	.384
H24	-.3339	.0993	.1677	H2	-.3534	.1152	.1934	.439
H25	-.2062	.2815	.2451	H6	-.1793	.2787	.2873	.654
H26	.0665	.2999	.2410	H10	.1151	.2646	.2719	.681
H27	.4975	.8519	.0970	H26	.4394	.8390	.0787	.560
H28	.5563	.7587	.1729	H25	.5336	.7388	.1672	.273
						r.m.s.d.(A)=		.469

TITL Williams VI observed relaxed with W99 force field

	REFERENCE			TARGET		
Matrix code (Det)	655565556	1.		655565556	1.	
Origin shift	.0000	.0000	.0000	-.5000	.0000	-.5000

New cell dimensions, A,deg:				dp/p(%)
a	8.2510	8.3508		1.2095
b	8.9640	9.0410		.8590
c	15.0870	14.6710		-2.7573
alpha	90.00	90.00		.00
beta	91.21	89.85		-1.49
gamma	90.00	90.00		.00

Atom	x	y	z	Atom	x	y	z	Dev,A
S1	.3065	.1271	.1571	S11	.3005	.1240	.1603	.075
O2	.3553	.0380	.2313	O11	.3448	.0397	.2384	.139
O3	.3571	.0691	.0714	O12	.3584	.0640	.0737	.059
N4	.3651	.2887	.1764	N12	.3534	.2861	.1783	.104
N5	.4200	.5264	.1396	N13	.4054	.5211	.1373	.134
N6	.4991	.7682	.1249	N14	.4796	.7616	.1193	.191
C7	.3407	.3998	.1170	C17	.3316	.3932	.1152	.099
C8	.4149	.6559	.0945	C18	.4012	.6475	.0889	.159
C9	.3232	.6610	.0209	C19	.3163	.6478	.0123	.184
C10	.2441	.5393	-.0042	C20	.2427	.5247	-.0125	.181
C11	.2508	.4045	.0434	C21	.2485	.3932	.0386	.126
C12	.0989	.1234	.1598	C14	.0953	.1166	.1609	.070
C13	.0199	.0139	.1141	C15	.0232	.0047	.1148	.088
C14	-.1371	.0087	.1195	C16	-.1321	-.0031	.1188	.115
C15	-.2216	.1066	.1666	C11	-.2214	.0943	.1647	.115
C16	-.1470	.2142	.2119	C12	-.1535	.2041	.2104	.108
C17	.0127	.2249	.2096	C13	.0041	.2176	.2096	.097
H18	.4960	.5240	.1830	H17	.4774	.5220	.1829	.156
H19	.3149	.7483	-.0122	H19	.3084	.7373	-.0251	.222
H20	.1809	.5430	-.0560	H20	.1812	.5250	-.0693	.255
H21	.1937	.3210	.0236	H21	.1926	.3040	.0179	.175

H22	.0760	-.0548	.0803	H13	.0860	-.0674	.0800	.141
H23	-.1929	-.0663	.0892	H12	-.1860	-.0839	.0865	.173
H24	-.3339	.0993	.1677	H11	-.3382	.0845	.1647	.145
H25	-.2062	.2815	.2451	H16	-.2195	.2747	.2445	.126
H26	.0665	.2999	.2410	H15	.0558	.2984	.2429	.094
H27	.4975	.8519	.0970	H18B	.4783	.8471	.0879	.212
H28	.5563	.7587	.1729	H18A	.5349	.7549	.1717	.181
						r.m.s.d.(A)=		.148