

*Supplementary Material for*

## **C<sub>6</sub>H<sub>4</sub>S<sub>2</sub>AsCl: Description and Interpretation of an Incommensurately Modulated Molecular Crystal Structure**

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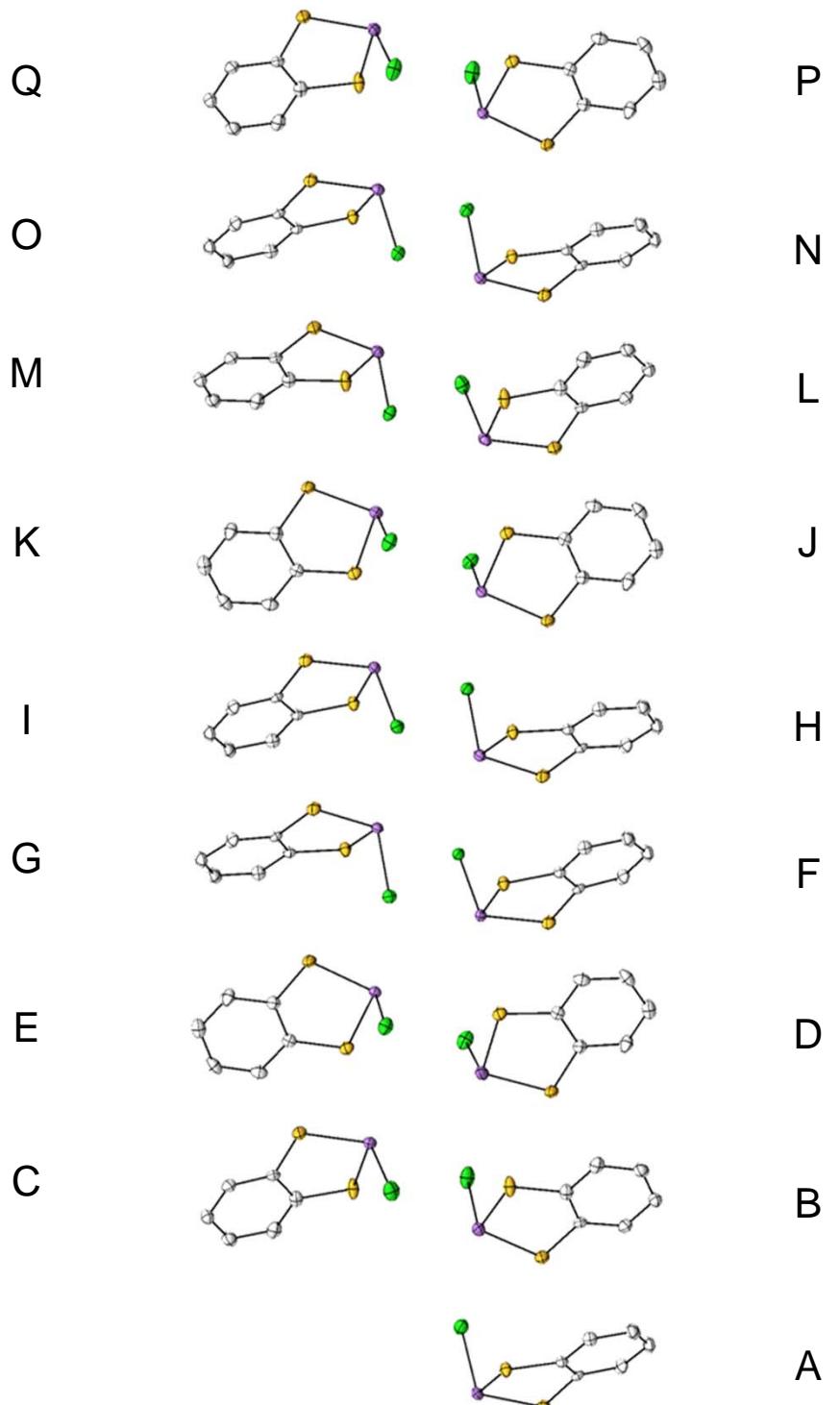
**Synopsis:** A modulated molecular structure has been refined in (3+1)-dimensional superspace and also as two different commensurate,  $Z' = 17$ , approximants. The incommensurate modulation found can be understood as relieving packing problems in several different directions.

1. Displacement ellipsoids resulting from the conventional, independent-atom refinements of approximants I and II (2 pp).
2. Reconstructed  $hk0$ ,  $h0l$ , and  $0kl$ , reciprocal-lattice slices for the basic cell. An enlargement of part of the  $hk0$  slice is also shown (4 pp).
3. Angles ( $^\circ$ ) between the dithiolate ( $S_2C_6$ ) planes and the plane  $(\bar{1}\bar{1}4)_{17}$  as calculated for the two approximants (1 pg).
4. Information about the additional refinements described in Sections 2.7 and 4.6 (4 pp.).
5. Information about CSD hits (2 pp).
6. Information about the energy calculations (4 pp).
7. Detailed input and output for the energy calculations (21 pp).
8. Two views comparing the results of the conventional, independent-atom refinements of approximants I and II. The first view is along  $[12\ 2\ \bar{5}]_{17} \parallel -\mathbf{c}^*_{\text{bas}}$ . The second view is the same as in Fig. 8 of the paper (2 pp).
9. Details of the interactions in clusters B and C (1 pg).

10. A plot of the variation in the  $(S_2C_6), (0\ 1\ 2)_{bas}$  angle with  $t$  as determined in the superspace refinement (1 pg).
11. Space-filling drawing showing the unique intermolecular interactions in the ribbon for approximant I (1 pg).
12. Incommensurate structures that could be archived in the Cambridge Structural Database but are not (2 pp).

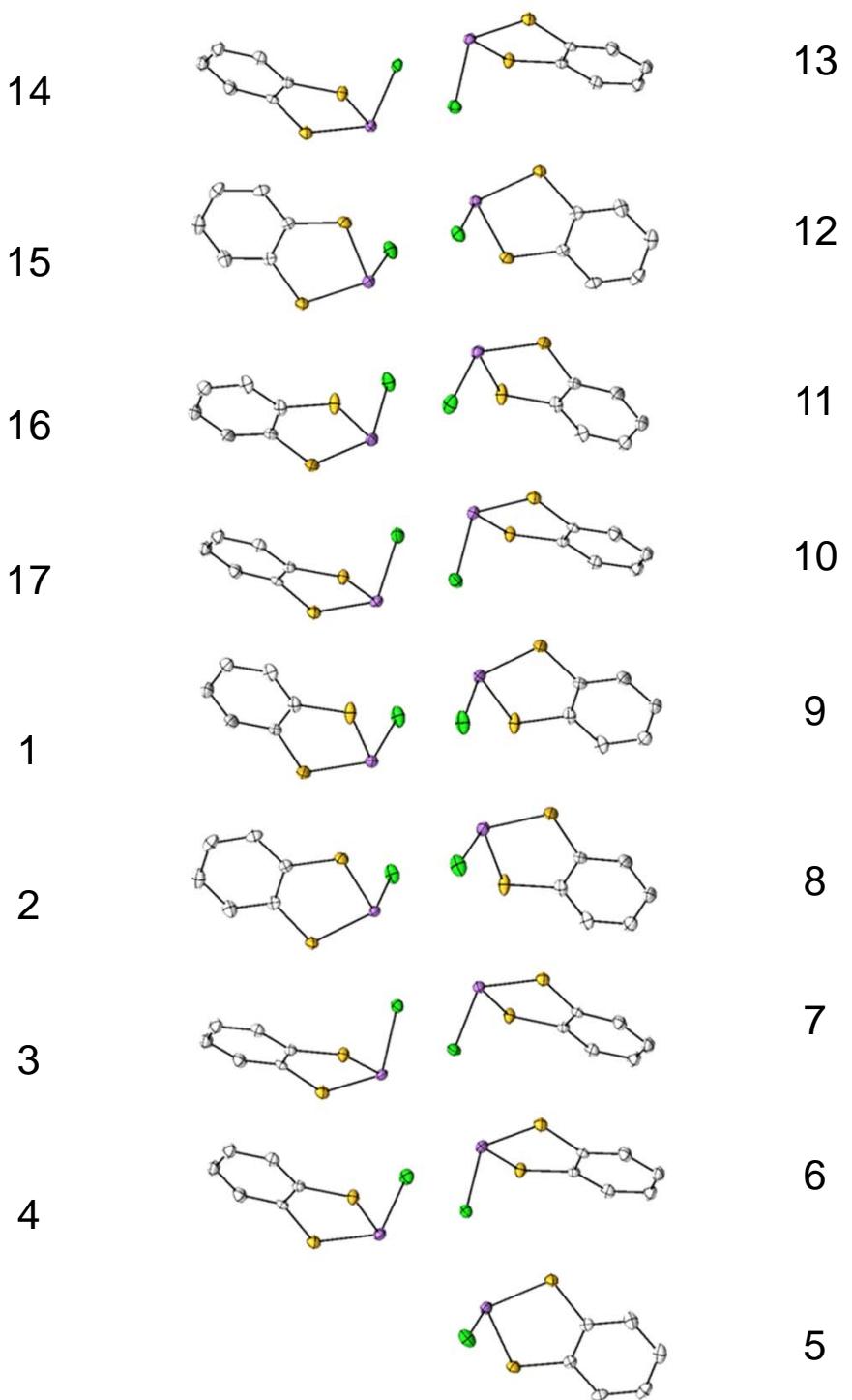
## 1-1. Displacement ellipsoids from the conventional independent-atom refinement of approximant I

The corresponding atomic ellipsoids in the following three groups of molecules were constrained to be the same: (A,F, G, H, I, N, O), (B, C, L, M, Q), (D, E, J, K, P).



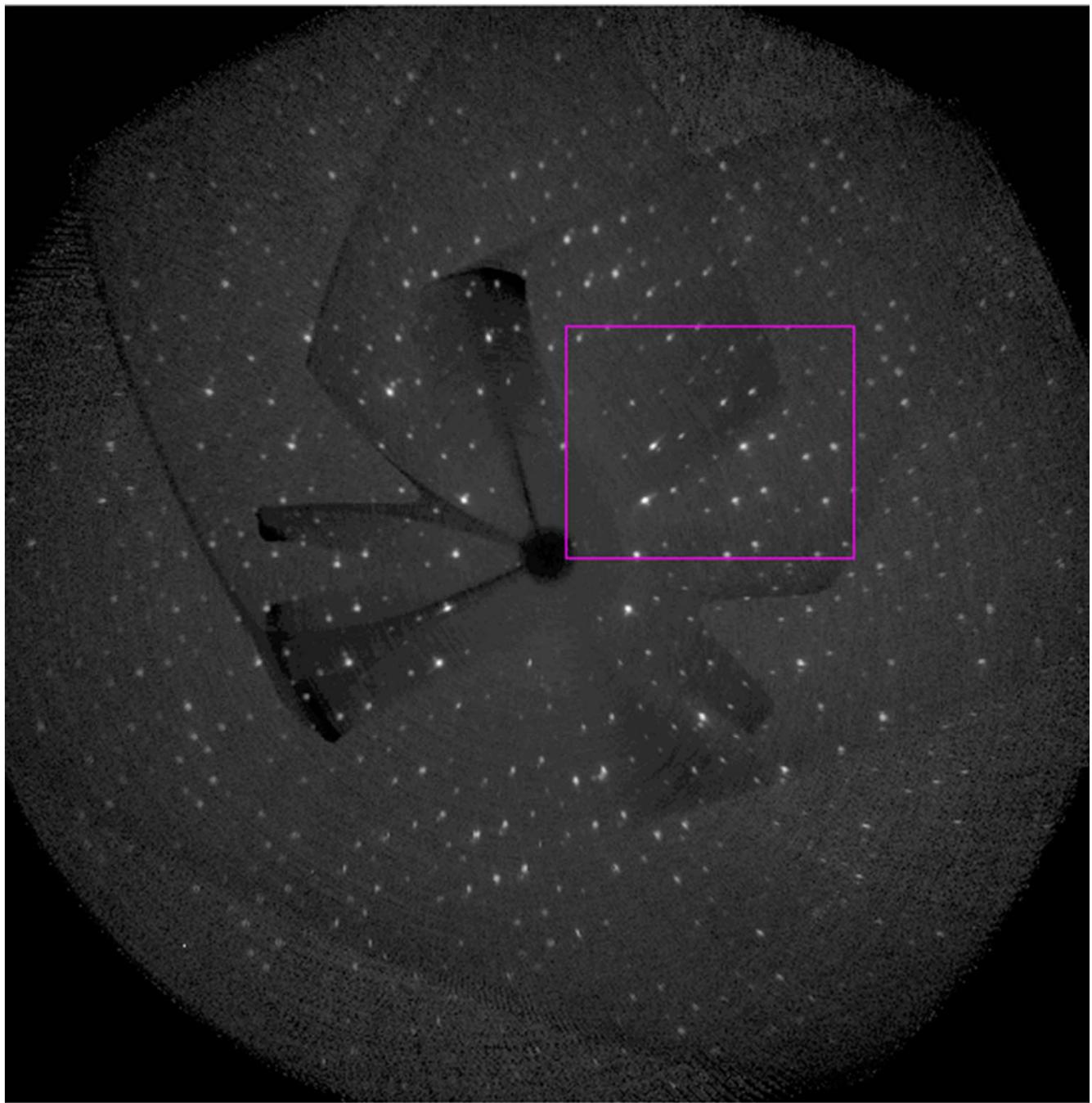
## 1-2. Displacement ellipsoids from the conventional independent-atom refinement of approximant II

The corresponding atomic ellipsoids in the following three groups of molecules were constrained to be the same: (3, 4, 6, 7, 10, 13, 14, 17), (1, 8, 9, 11, 16), (2, 5, 12, 15).



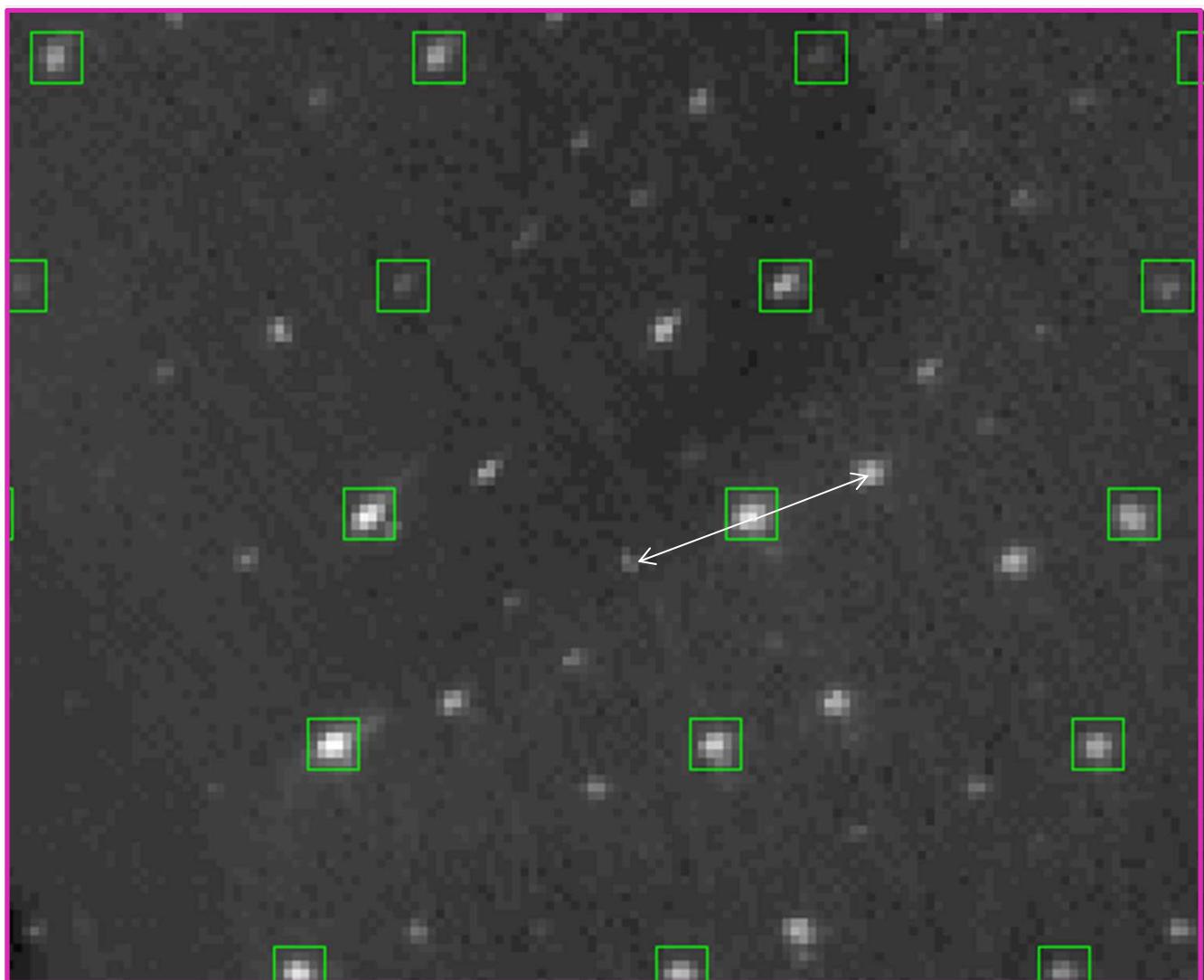
## **2-1. $hk0$ (basic cell)**

(A larger image of the marked rectangle is shown on  
the next page)

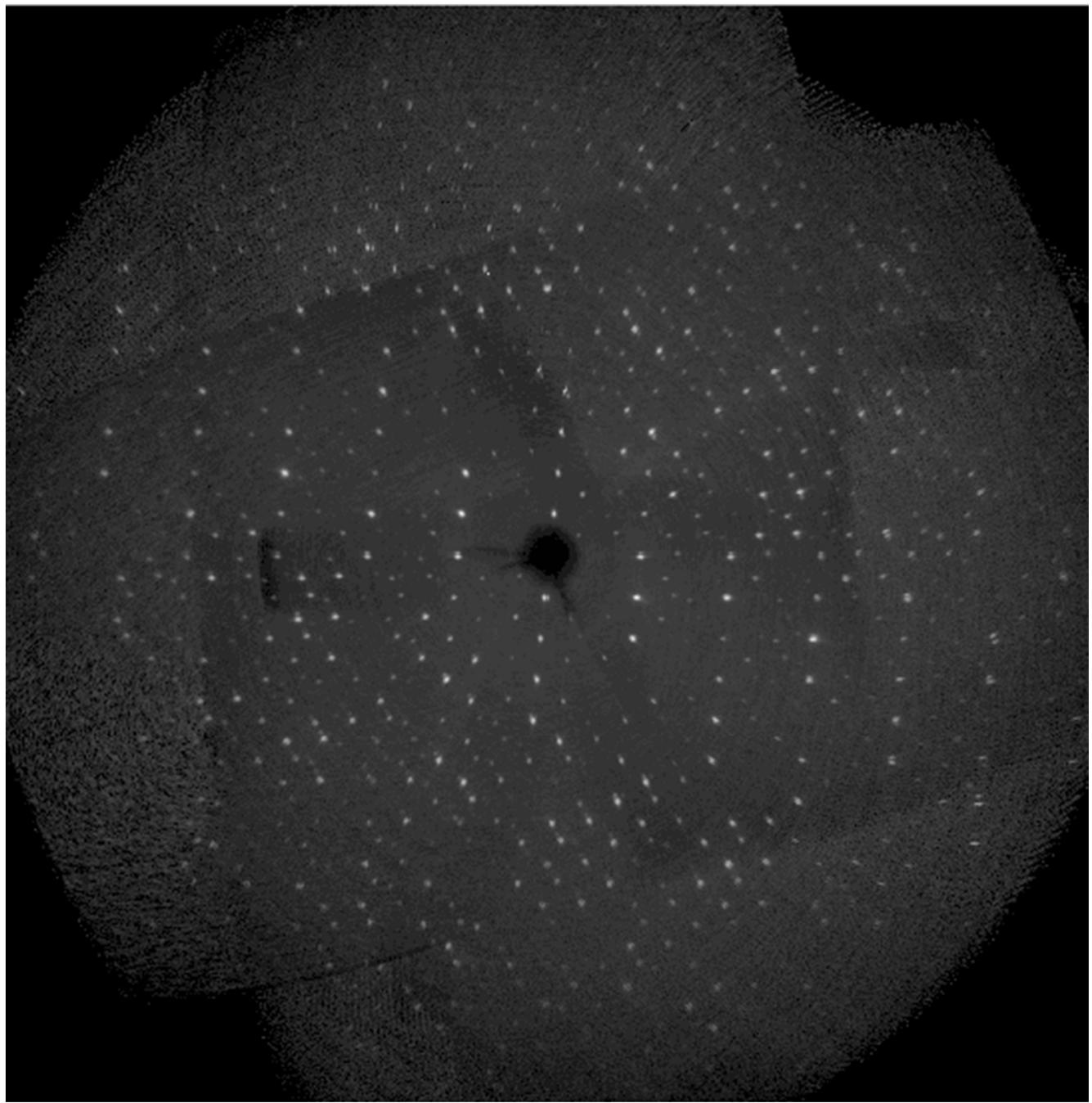


## 2-2. $hk0$ (basic cell)

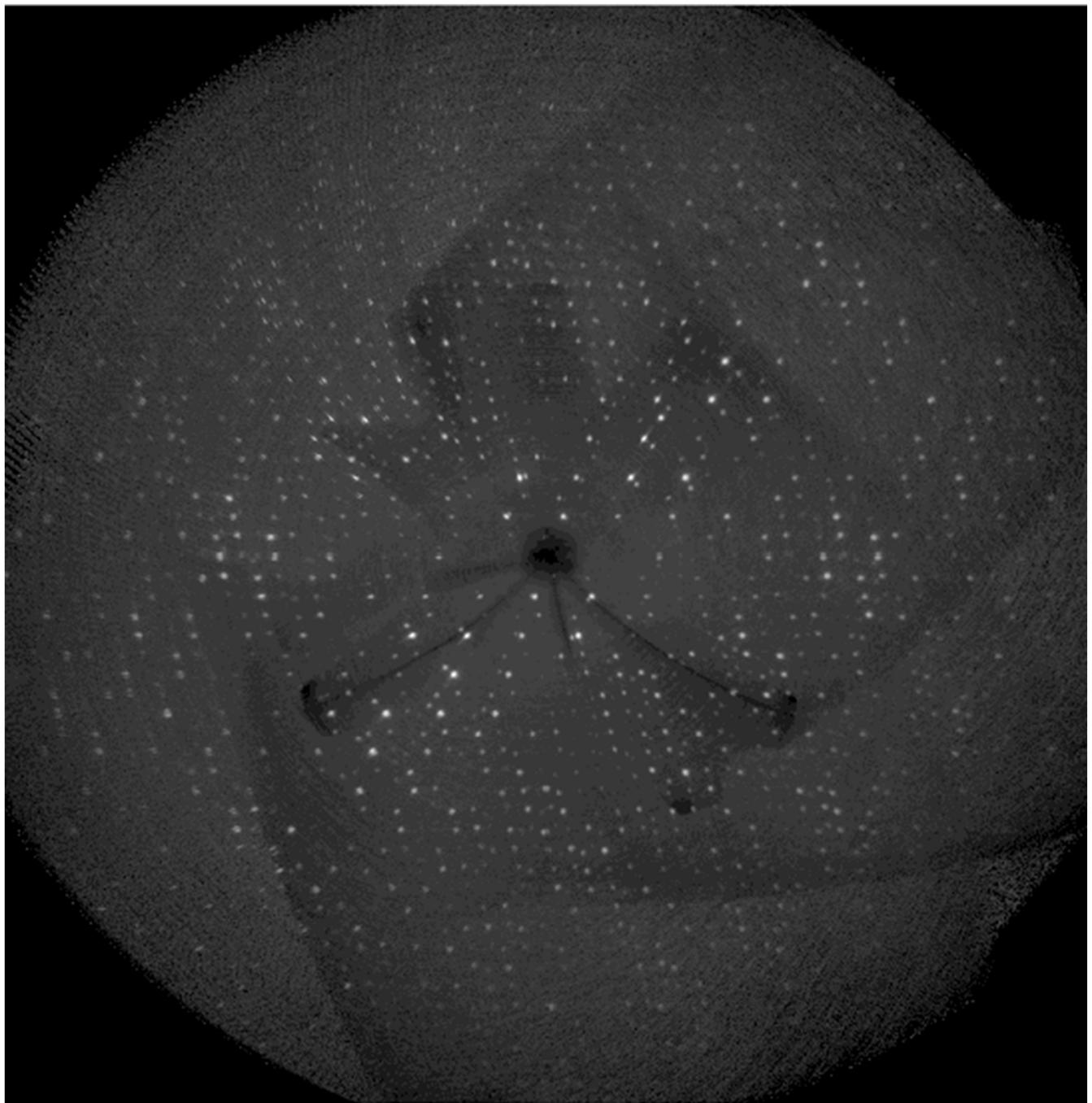
enlargement of the rectangle marked in the  $hk0$  slice of the basic cell (see previous page); main reflections are marked; the  $\pm q$  vectors are shown for one basic reflection.



## **2-3. $h0l$ (basic cell)**



## **2-4. $0kl$ (basic cell)**



**3. Angles ( $^{\circ}$ ) between the dithiolate ( $S_2C_6$ ) planes and the plane  $(\bar{1}\bar{1}4)_{17}$  as calculated for the two approximants.**

The molecules in dimers that can be well superposed are on the same line. The inversion centers are at the centers of the dimers in the outlined boxes. Because the crystallographic inversion centers are located in different places in the two structures a molecule in one approximant may correspond to two molecules in the other (e.g. A in approximant I corresponds to both molecules 17 and 10 in II).

approximant I		approximant II	
Dimer	Angles	Dimer	Angles
A … A	68, 68	17 … 10	68, 68
B … C	47, 51	16 … 11	53, 54
D … E	35, 31	15 … 12	32, 30
F … G	64, 67	14 … 13	63, 66
H … I	65, 61	13 … 14	66, 63
J … K	29, 29	12 … 15	30, 32
L … M	57, 60	11 … 16	54, 53
N … O	68, 67	10 … 17	68, 68
P … Q	36, 43	9 … 1	41, 47
Q … P	43, 36	8 … 2	39, 33
O … N	67, 68	7 … 3	66, 68
M … L	60, 57	6 … 4	63, 59
K … J	29, 29	5 … 5	28, 28
I … H	61, 65	4 … 6	59, 63
G … F	67, 64	3 … 7	68, 66
E … D	31, 35	2 … 8	33, 39
C … B	51, 47	1 … 9	47, 41
A … A	68, 68	17 … 10	68, 68

## 4. Information about Additional Conventional Refinements of Approximants I and II

Sections 2.7 and 4.6 discuss six refinements. All are conventional (*i.e.*, independent-atom) restrained refinements done with SHELXL97.

1. (a) Approximant I ( $t_0 = \frac{1}{2}$ ) using all data in the Eval15 data set.  
(b) Approximant II ( $t_0 = 0$ ) using all data in the Eval15 data set.
2. (a) Approximant I ( $t_0 = \frac{1}{2}$ ) using data from the Denzo set that are also in the Eval15 set.  
(b) Approximant II ( $t_0 = 0$ ) using data from the Denzo set that are also in the Eval15 set.  
(c) Approximant I ( $t_0 = \frac{1}{2}$ ) using data from the Eval15 set that are also in the Denzo set.  
(d) Approximant II ( $t_0 = 0$ ) using data from the Eval15 set that are also in the Denzo set.

All six refinements had convergence problems. Those problems were considerably worse when only the reflections present in both data sets were used, *i.e.*, in the last four refinements listed. The Denzo set has higher-order satellites but no reflections above  $\theta = 25^\circ$ . The Eval15 set has reflections above  $\theta = 25^\circ$  but no satellites above order 4. When the data above  $25^\circ$   $\theta$  and the higher-order reflections are both missing then convergence of even a restrained independent-atom refinement is a serious problem.

Information about the data sets:

Denzo data set: 48421 total reflections;  $R$  for averaging 0.052  
24396 unique reflections of which 8774 have  $I > 2\sigma(I)$   
Eval15 data set: 32057 total reflections;  $R$  for averaging 0.032  
16388 unique reflections of which 10864 have  $I > 2\sigma(I)$

The better  $R$  for averaging for the Eval15 set can be expected because there are fewer very weak reflections. The average value of  $\sigma(I)/I$  is 0.080 for the Denzo set and 0.045 for the Eval15 set.

For  $\theta \leq 25^\circ$  the indices of the reflections included in the two data sets are very similar. In both files almost all unique reflections appear twice, *i.e.*, as the members of Friedel pairs. In some cases (fewer than *ca.* 100) only one member of a pair occurs in the Denzo or in the Eval15 file. There are four reflections that appear in one file but not at all in the other.

There are 12731 unique reflections that are common to the two data sets. One reflection [*i.e.*, (0 -1 3)] was manually removed from the two sets because it was so obvious that its value in the Denzo set was very much too low.

The  $R$  factors for averaging to five the 12731 reflections are 0.035 for the Denzo set and 0.028 for the Eval15 set. This comparison indicates that the integration procedure in Eval15 gives more reliable intensities than does the integration procedure in Denzo.

A very conventional weighting scheme (WGHT 0.02 0) was applied in all refinements.

The following steps were taken to improve convergence:

1. In the refinements using all the data in the Eval15 data set the restraint SAME 0.015 was changed to SAME 0.005. This restraint is intended to keep corresponding bond lengths and bond angles in the 17 independent molecules similar. The value 0.015 (which was used for the refinements reported in Table 1) reflects our experience with the variation of bond lengths between the  $Z'$  independent molecules in a single structure and between the same molecule as found in different structures. Reducing the associated uncertainty from 0.015 to 0.005

strengthened that restraint. The uncertainty for the 1,3 distances that determine bond angles was the default, *i.e.*, double the uncertainty on the bond lengths.

2. In the refinements using the limited data sets (12731 unique reflections) the strengthened SAME restraint was insufficient; convergence could not be achieved without damping, even in the final cycles. The SHELXL DAMP instruction was used (“The diagonal elements of the least-squares matrix are multiplied by (1+damp/1000) before inversion; this is a version of the Marquardt (1963) algorithm.”) with the parameter set at 100 initially and reduced to 20 in the final cycles. This procedure resulted in a final  $|\langle \Delta/\sigma \rangle|_{\max}$  below 0.005. If the criterion for convergence were reduced less damping would be needed.

The only other restraint in the original SHELXL refinement of the full set of Denzo data was DELU 0.005, which was included as a rigid-bond restraint. This restraint was retained in the six new refinements.

A comparison of the Denzo and Eval15 refinements follows.

#### **Refinements using all data available:**

Data set	Denzo	Denzo	Eval15	Eval15
Approximant	I	II	I	II
No. of independent, unique and observed $[I > 2\sigma(I)]$ reflections	48421 24396 8774	48421 24396 8774	32057 16388 10864	32057 16388 10864
$R_{\text{int}}$	0.052	0.052	0.032	0.032
$ \langle \Delta/\sigma \rangle _{\max}$	0.002	0.002	0.003	0.006
$R[F^2 > 2\sigma(F^2)]$ ,	0.042	0.041	0.041	0.040
$wR(F^2)$ ,	0.107	0.104	0.086	0.085
$S$	1.06	1.04	1.36	1.35
$\Delta\rho_{\max}$ ,	+1.74	+1.40	+1.24	+1.11
$\Delta\rho_{\min} (\text{e } \text{\AA}^{-3})$	-1.57	-1.59	-0.89	-0.90

**Refinements using reflections common to the two data sets:**

Data set	Denzo	Denzo	Eval15	Eval15
Approximant	I	II	I	II
No. of independent, unique, and observed [ $I > 2\sigma(I)$ ] reflections	24890 12731 8160	24890 12731 8160	24890 12731 8966	24890 12731 8966
$R_{\text{int}}$	0.035	0.035	0.028	0.028
$ \langle \Delta/\sigma \rangle _{\max}$	0.002	0.003	0.002	0.003
$R[F^2 > 2\sigma(F^2)]$ , $wR(F^2)$ ,	0.036 0.084	0.036 0.083	0.036 0.079	0.035 0.078
$S$	1.17	1.15	1.40	1.39
$\Delta\rho_{\max}$ , $\Delta\rho_{\min}$ (e Å <sup>-3</sup> )	+1.02 -0.92	+0.96 -1.01	+1.05 -0.67	+0.94 -0.72

Overlays of the asymmetric units shows that atomic positions and displacement parameters for all refinements of the same approximant are, to the eye, indistinguishable.

Because convergence of the conventional (SHELXL) refinement of the Denzo data was significantly better for both approximants than refinement of the Eval15 data it seemed likely that the presence in the Denzo data set of higher-order (orders 5 – 8) satellites with measurable intensity explained the difference. We therefore worked out the satellite orders (assuming a commensurate, 17-fold modulation) for all the reflections present in the Denzo file but not in the Eval15 file. We found the following:

order 5: 5922 reflections of which 563 have  $I > 2\sigma(I)$  and 216 have  $I > 3\sigma(I)$ .

order 6: 5917 reflections of which 161 have  $I > 2\sigma(I)$  and 21 have  $I > 3\sigma(I)$ .

order 7: 5914 reflections of which 117 have  $I > 2\sigma(I)$  and 18 have  $I > 3\sigma(I)$ .

order 8: 5910 reflections of which 79 have  $I > 2\sigma(I)$  and 5 have  $I > 3\sigma(I)$ .

orders 5-8: 23663 reflections of which 920 have  $I > 2\sigma(I)$  and 260 have  $I > 3\sigma(I)$ .

Therefore 3.9% of the higher order satellites have  $I > 2\sigma(I)$  and 1.1% have  $I > 3\sigma(I)$ .

The information in that relatively small number of observable higher-order satellites seems to be sufficient to stabilize the refinement. The number of observable reflections may be small, but each of them is rich in information.

### **Summary**

There is no important difference between any of the conventional refinements.

The intensities as integrated with Eval15 are somewhat more reliable than the intensities as integrated with Denzo.

The higher-order satellites contain information that improves a conventional refinement. It is likely that this information would also improve a superspace refinement.

## 5. Information about CSD Hits

### Significant Hits:

CTRTAS	As	C1 S2	ALIJOU is the Sb analogue
CXTARS	As	C1 S2	ALIJIO is the Sb analogue
DAXLOD	As	C1 S2	
JUHNUV01	As	C1 S2	CLSSBP10 is the Sb analogue
JUHNUV02	As	C1 S2	(second polymorph) CLSSBP10 is the Sb analogue
NEJQAV	As	C1 S2	
NEQID	As	C1 S2	
PENCAN	As	C1 S2	CTTSTB is the Sb analogue
ALIJIO	Sb	C1 S2	CXTARS is the As analogue
ALIJOU	Sb	C1 S2	CTRTAS is the As analogue
CLSSBP10	Sb	C1 S2	JUHNUV is the As analogue
COXTSB	Sb	C1 S2	
CTTSTB	Sb	C1 S2	PENCAN is the As analogue
QENTAF	Sb	C1 S2	(the structure reported here is the As analogue)

### Rejected Hits:

JUHNUV	As	C1 S2	duplicate (less precise) of JUHNUV02
JUHPOR	As	C1 S2	cation composed of (SCCS)As attached to S of (SCCS)AsCl
CEDYIU	As	C1 S2	$\pi \cdots \pi$ stacking interactions prevent contacts to As
GOFFAJ	As	C1 S2	steric constraints prevent contacts to As (SCPhC=CPhCS dimer)
GOFFEN	As	C1 S2	steric constraints prevent contacts to As (SCPhPhCS dimer)
GOFFIR	As	C1 S2	steric constraints prevent contacts to As (SCPhCS dimer)
GOFFOX	As	C1 S2	steric constraints prevent contacts to As (SCPhCS dimer)
GOFFUD	As	C1 S2	steric constraints prevent contacts to As (SCPhCS dimer)
LUFTUC	As	C1 S2	steric constraints prevent contacts to As (SCPhCS dimer)
NESRAF	As	C1 S2	steric constraints prevent contacts to As (SCPhCS dimer)
NESREJ	As	C1 S2	steric constraints prevent contacts to As (SCPhCS dimer)
NESRIN	As	C1 S2	steric constraints prevent contacts to As (SCPhCS dimer)
TIRYAV	As	C1 S2	steric constraints prevent contacts to As (SCNaphthCS dimer)
TIRYEZ	As	C1 S2	steric constraints prevent contacts to As (SCPhCS dimer); Z'=6
TIRYID	As	C1 S2	steric constraints prevent contacts to As (SCPhCS dimer)
TIRYOJ	As	C1 S2	steric constraints prevent contacts to As (SCNaphthCS dimer)
WUQLUQ	As	C1 S2	steric constraints prevent contacts to As (cage)
WUQMAX	As	C1 S2	co-crystal with constrained molecular cage
SIPZEX	Sb	C1 S2	steric constraints prevent contacts to Sb (SCPhCS dimer)

### Hits for Cl<sub>2</sub>S Structures:

CUVGUW	As	Cl2 S	steric constraints prevent contacts to As (SCPhCS dimer)
CUVHAD	As	Cl2 S	steric constraints prevent contacts to As (SCPhCS dimer)
FUWXEB	As	Cl2 S	steric constraints prevent contacts to As (SCCPhCCS dimer)
LUFTOW	As	Cl2 S	
PAFNIU	Sb	Cl2 S	S bridges two Ir atoms
PAFQET	Sb	Cl2 S	S bridges two Rh atoms

PAPPES      Sb      Cl<sub>2</sub> S      S bridges two Ru atoms  
PAPPUI      Sb      Cl<sub>2</sub> S      S bridges two Ru atoms

## 6. Information about the energy calculations

Intermolecular energy calculations were carried out at the atom-atom level using the *AA-CLP* force field, recently developed to reproduce enthalpies of vaporization and sublimation for organic materials (Gavezzotti, 2011). The software was downloaded from the standard source of the *CLP* package, at <http://users.unimi.it/gavezzot>. An extension of parametrization for arsenic was applied (Gavezzotti, 2012). The *CLP* force field provides separate estimates of Coulombic-polarization, dispersion, and repulsion energies; however, atom-atom calculations using point charges for second-row elements notoriously underestimate Coulombic interactions but reproduce experimental quantities by compensation with the polarization term and a parallel reduction of the repulsion term. Most importantly, the *AA-CLP* calculation is very fast on a desktop computer, and the formulation has been shown to provide qualitative answers that parallel those obtained by the much more accurate *PIXEL* formulation (Gavezzotti, 2011), which cannot be used for a crystal structure with such a large  $Z'$ .

The coordinates of the asymmetric unit of approximant I were assumed for the construction of a model crystal including all molecule-molecule interactions up to a distance of 40 Å between centers of mass (22,349 molecule pairs). The lattice energy calculation provides (a) separate, detailed molecule-molecule energies between each single pair of molecules in the crystal,  $E_{jk}^i$ , where  $i$  denotes a molecule in the asymmetric unit ( $1 \leq i \leq 17$ ),  $j$  denotes another molecule in the asymmetric unit repeated by the  $k$ -th space-group symmetry operation plus translation;

- (b) cumulative interactions between molecules  $i$  and  $j$  in the whole crystal,  $E_j^i = \sum_k E_{jk}^i$ ;
- (c) total contribution to the lattice energy by molecule  $i$ ,  $E^i = \sum_j E_j^i$ ; and
- (d) total lattice-packing energy,  $E_{\text{latt}} = (1/17)(1/2)\sum_i E^i$ .

The total lattice-packing energy should compare with the experimental sublimation enthalpy, which is, however, unavailable for DTAsCl. Since sublimation enthalpies are often additive over fragments, an order-of-magnitude estimate can be obtained by adding the enthalpy of sublimation of benzene (45 kJ/mol) and about one-third of the enthalpy of sublimation of As<sub>4</sub>S<sub>3</sub> (85 kJ/mol) to get 80-85 kJ/mol (70-75 kJ/mol?), which is not far from the calculated values (see below). Tables of input and output to the calculation, including data from points (a) – (d) above, have been deposited as supplementary material.

For comparison, lattice energy calculations were carried out also on the  $\bar{P}\bar{1}$ ,  $Z' = 2$  basic cell using first molecular orientation A and then orientation B, but these calculations, as expected, led to unacceptably high energies.

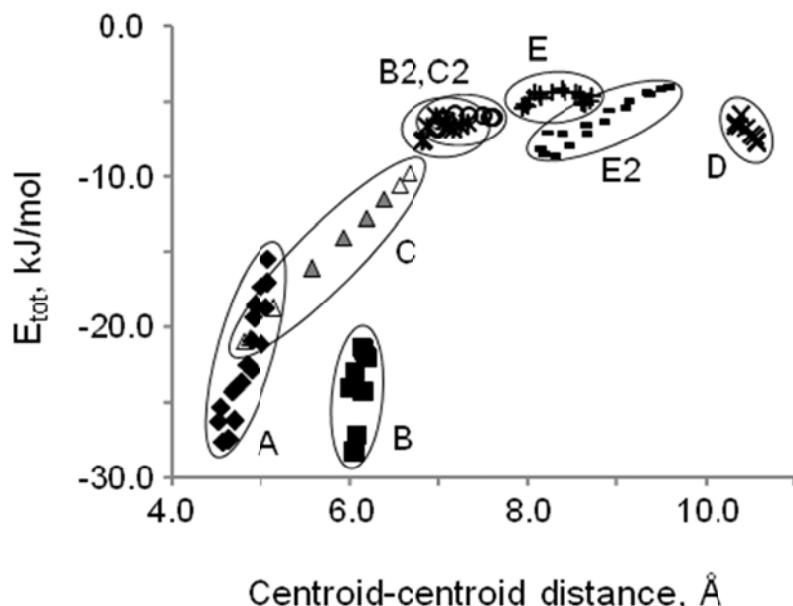
Energy contributions (Coulomb, polarization, and repulsive) in the DTAsCl crystal: total lattice energy and average/range of the contributions from each of the 17 molecules ( $i = 1 - 17$ ) in the asymmetric unit. Note that  $E_{\text{latt}} = (1/17) (1/2) \sum_i E^i$ .

	$E_{\text{Coul+Epol}}$ , kJ/mol	$E_{\text{disp}}$ , kJ/mol	$E_{\text{rep}}$ , kJ/mol	$E_{\text{tot}}$ , kJ/mol
$E_{\text{latt}} = \frac{1}{2} E_{\text{avg}}^i$	-9.5	-122	53.9	-77.5
range of $\frac{1}{2}E^i$	-7.5 – -11.5	-118 – -126	48 – 58	-74 – -80

Gavezzotti, A. (2012). Personal communication.

Gavezzotti, A. (2011). *New J. Chem.* **35**, 1360-1368.

A scatterplot showing the molecule-molecule interaction energies < -4.0 kJ/mol as a function of the distance between the mass-weighted molecular centroids. Each type of interaction is represented by a different symbol; the symbols of each type are surrounded by an ellipse. The designations of the groups are explained in the text. The groups that are more compact correspond to interactions that do not vary much with the structural modulation.



### Results of the Energy calculations

The energy calculations indicate (Table 1) that dispersion energy is, by far, the most important stabilizing factor, a result not unexpected given the chemical nature of the composing units. Main providers of dispersion are the polarizable ring  $\pi$ -system electrons, but the diffuse and polarizable As and Cl 3s and 3p electrons also contribute. A test calculation was carried out by *PIXEL* on a single molecule-molecule contact (molecules M and N at distance of 6.08 Å); the Coulomb-polarization energies were -6.8 kJ/mol by *AA* (the method described above) and -25.1 kJ/mol by *PIXEL*, while the dispersion energies were -29.3 kJ/mol by *AA* and -38.7 kJ/mol by *PIXEL*. The resulting approximate scaling factor of 3 – 4 between *AA* and *PIXEL* Coulomb-polarization is quite usual. Even considering this rescaling, dispersion remains predominant, which means that the crystals are correctly described as molecular.

A plot of the energy *vs.* centroid-centroid distance for pairs of molecules having interaction energies < -4.0 kJ/mol is shown in Fig. 1, in which contacts of the same type (17 or 9 unique depending on the location relative to the inversion centers) are enclosed in ellipses. The

most consistently favorable interactions (cluster B in Fig. 1; molecules adjacent along  $[12\ 2\ \bar{5}]_{17}$ ) lie within the gray parallelograms marked on Fig. 2. The next most favorable cluster (A) is composed of pairs of molecules adjacent in one half of the dimer ribbon (*i.e.*, adjacent along  $[1\ 3\ 1]_{17}$ ). The energies of the contacts in cluster A are more variable than those in B because the dominant dispersion interactions between the rings differ with their orientations, and because the aromatic rings in cluster A adopt a wider range of stacking/offset arrangements than those in cluster B (Figs. 1 and 2).

The third most favorable cluster (C; molecules also adjacent along  $[12\ 2\ \bar{5}]_{17}$ ) shows the most variation. This cluster is composed of pairs of molecules that sometimes have short S···S contacts (filled triangles). These S···S contacts are, however, in the middle of the cluster range rather than at the short end. The significance of the S···S contacts is therefore uncertain.

The remaining clusters shown do not add nearly as much to the overall stability of the structure as the three dominant clusters. The interactions in cluster D are between the “ends” of the molecules, *i.e.*, in the plane  $(\bar{1}\ \bar{1}\ 4)_{17} \parallel (0\ 1\ 2)_{\text{bas}}$  (Fig. 2). The interactions of cluster E are between molecules in the two halves of a ribbon but not within the same dimer. Clusters B2, C2, and E2 are variants of clusters B, C, and E, with the interacting molecules being offset by one along the ribbon axis; clusters B2 and C2 involve molecules adjacent along  $[10\ \bar{4}\ \bar{7}]_{17}$ .

These energy calculations, as often happens in crystals without strongly preferential directional forces (*e.g.*, without hydrogen bonds) cannot be easily reconciled with any atom-atom view and, as such, neither support nor contradict the idea that As···Cl and S···S interactions are structure determining. While the calculations suggest that segregation of As, Cl and S atoms is secondary to the prevailing drive towards inter-ring stacking with offset, this view is not supported by the wide range of ring orientations among the 17 independent molecules. The energetic estimates provided by the *AA* calculations do indicate, however, that the strongest interactions are within one half of a dimer ribbon and between that half ribbon and halves of the two closest ribbons. With the addition of inversion symmetry these strong interactions extend in three non-coplanar directions, which means that the calculations are consistent with the crystal morphology (blocks rather than plates or needles).

## 7. Detailed input and output for the energy calculations

### Input File to the Energy Calculations

```
#DTASCL01                                         0.0
0
12.3533   22.3789   26.6255      76.74      80.05      76.81
0.0
238
 1   0.12040   -0.07430   -0.02640   1   39   -0.1408
 2   0.13600    0.02880   -0.04020   1   42   -0.3122
 3   0.29570   -0.11770   -0.04970   1   34    0.4283
 4   0.13790   -0.10220    0.05750   1   34    0.4357
 5   0.35500   -0.12620    0.00810   1   12   -0.0616
 6   0.47090   -0.13970    0.00740   1   12   -0.3638
 7   0.51690   -0.15090    0.05340   1   12   -0.3617
 8   0.44770   -0.14790    0.09980   1   12   -0.3519
 9   0.33360   -0.13300    0.10070   1   12   -0.3603
10   0.28520   -0.12330    0.05530   1   12   -0.0598
11   0.52493   -0.14144   -0.02896   1   2    0.2887
12   0.60681   -0.16197    0.05297   1   2    0.2868
13   0.48385   -0.15738    0.13564   1   2    0.2859
14   0.28068   -0.12874    0.13701   1   2    0.2869
15   0.15580    0.09110    0.06680   2   39   -0.1318
16   0.19690    0.18570    0.02490   2   42   -0.3027
17   0.31420    0.02880    0.04550   2   34    0.4357
18   0.19670    0.08890    0.14530   2   34    0.4108
19   0.39070    0.02630    0.09580   2   12   -0.0529
20   0.50440   -0.00240    0.09210   2   12   -0.3713
21   0.56390   -0.00600    0.13230   2   12   -0.3536
22   0.51250    0.01830    0.17540   2   12   -0.3600
23   0.40190    0.04880    0.17890   2   12   -0.3631
24   0.34070    0.05200    0.13880   2   12   -0.0598
25   0.54476   -0.02141    0.05824   2   2    0.2887
26   0.65153   -0.02806    0.12996   2   2    0.2861
27   0.55977    0.01338    0.20715   2   2    0.2847
28   0.36361    0.06975    0.21204   2   2    0.2891
29   -0.06830    0.26070    0.07790   3   39   -0.1320
30   -0.08440    0.16290    0.12340   3   42   -0.2995
31   -0.24630    0.30910    0.08800   3   34    0.4258
32   -0.07480    0.25120   -0.00210   3   34    0.4238
33   -0.29400    0.29720    0.03270   3   12   -0.0599
34   -0.40810    0.31200    0.02750   3   12   -0.3673
35   -0.44560    0.30670   -0.01690   3   12   -0.3590
36   -0.37110    0.28530   -0.05710   3   12   -0.3612
37   -0.25830    0.26810   -0.05140   3   12   -0.3672
38   -0.21980    0.27340   -0.00680   3   12   -0.0527
39   -0.46797    0.32785    0.05871   3   2    0.2873
40   -0.53415    0.31941   -0.02032   3   2    0.2863
41   -0.40038    0.28210   -0.09216   3   2    0.2885
42   -0.19926    0.25030   -0.08202   3   2    0.2873
43   0.22610     0.26620    0.11760   4   39   -0.1431
44   0.25920     0.35060    0.05420   4   42   -0.3036
45   0.39200     0.20400    0.11320   4   34    0.4522
46   0.25260     0.29730    0.18750   4   34    0.4364
```

47	0.45380	0.22190	0.16080	4	12	-0.0641
48	0.56690	0.19610	0.16580	4	12	-0.3710
49	0.61520	0.20790	0.20420	4	12	-0.3639
50	0.55190	0.24400	0.23920	4	12	-0.3680
51	0.44190	0.27080	0.23400	4	12	-0.3631
52	0.39260	0.26140	0.19420	4	12	-0.0606
53	0.61589	0.16698	0.13944	4	2	0.2884
54	0.70296	0.18907	0.20733	4	2	0.2864
55	0.58959	0.25093	0.27059	4	2	0.2863
56	0.39358	0.29929	0.26096	4	2	0.2876
57	0.02780	0.44240	0.09910	5	39	-0.1429
58	-0.02060	0.36050	0.16150	5	42	-0.3038
59	-0.12420	0.51560	0.10900	5	34	0.4452
60	-0.02310	0.42080	0.03040	5	34	0.4236
61	-0.20640	0.50370	0.06640	5	12	-0.0512
62	-0.31650	0.53750	0.06600	5	12	-0.3718
63	-0.38200	0.53150	0.03140	5	12	-0.3515
64	-0.33980	0.49150	-0.00250	5	12	-0.3619
65	-0.23160	0.45710	-0.00240	5	12	-0.3679
66	-0.16370	0.46280	0.03240	5	12	-0.0644
67	-0.35022	0.56849	0.09304	5	2	0.2870
68	-0.46661	0.55823	0.03087	5	2	0.2862
69	-0.39173	0.48685	-0.02957	5	2	0.2854
70	-0.19951	0.42576	-0.02928	5	2	0.2880
71	0.30470	0.45690	0.14600	6	39	-0.1406
72	0.31010	0.56130	0.12220	6	42	-0.3054
73	0.48510	0.41690	0.12870	6	34	0.4375
74	0.31280	0.44240	0.23060	6	34	0.4291
75	0.53360	0.41370	0.18800	6	12	-0.0663
76	0.64840	0.40140	0.19110	6	12	-0.3599
77	0.68790	0.39450	0.23770	6	12	-0.3643
78	0.61260	0.40200	0.28210	6	12	-0.3557
79	0.49940	0.41650	0.28020	6	12	-0.3625
80	0.45920	0.42280	0.23300	6	12	-0.0606
81	0.70709	0.39724	0.15637	6	2	0.2870
82	0.77700	0.38331	0.23980	6	2	0.2874
83	0.64391	0.39629	0.31870	6	2	0.2852
84	0.44179	0.42300	0.31485	6	2	0.2891
85	0.06410	0.60630	0.19390	7	39	-0.1513
86	0.03930	0.50450	0.20550	7	42	-0.3215
87	-0.10500	0.65360	0.22180	7	34	0.4437
88	0.03790	0.63850	0.11120	7	34	0.4433
89	-0.17200	0.66810	0.16580	7	12	-0.0606
90	-0.28860	0.68650	0.17000	7	12	-0.3613
91	-0.34170	0.70140	0.12610	7	12	-0.3603
92	-0.27840	0.69710	0.07800	7	12	-0.3614
93	-0.16360	0.67710	0.07370	7	12	-0.3614
94	-0.10870	0.66390	0.11760	7	12	-0.0596
95	-0.33695	0.68903	0.20761	7	2	0.2883
96	-0.43170	0.71630	0.12895	7	2	0.2878
97	-0.31988	0.70964	0.04345	7	2	0.2860
98	-0.11640	0.67169	0.03635	7	2	0.2882
99	0.34540	0.62620	0.22280	8	39	-0.1384
100	0.37200	0.72780	0.20680	8	42	-0.3197
101	0.51340	0.57700	0.19450	8	34	0.4397
102	0.37520	0.59610	0.30410	8	34	0.4351
103	0.58240	0.56360	0.24970	8	12	-0.0614

104	0.69860	0.54240	0.24610	8	12	-0.3640
105	0.75260	0.52820	0.28950	8	12	-0.3552
106	0.69210	0.53580	0.33720	8	12	-0.3618
107	0.57720	0.55650	0.34150	8	12	-0.3639
108	0.52180	0.57090	0.29770	8	12	-0.0587
109	0.74625	0.53716	0.20880	8	2	0.2871
110	0.84214	0.51113	0.28643	8	2	0.2868
111	0.73482	0.52552	0.37123	8	2	0.2863
112	0.53028	0.56151	0.37899	8	2	0.2878
113	0.10660	0.78060	0.26320	9	39	-0.1494
114	0.10020	0.67640	0.29220	9	42	-0.3085
115	-0.07320	0.82250	0.27770	9	34	0.4408
116	0.09970	0.78900	0.17880	9	34	0.4374
117	-0.12180	0.82070	0.21980	9	12	-0.0624
118	-0.23660	0.83430	0.21690	9	12	-0.3587
119	-0.27400	0.83750	0.17090	9	12	-0.3575
120	-0.19930	0.82770	0.12670	9	12	-0.3654
121	-0.08560	0.81220	0.12930	9	12	-0.3630
122	-0.04590	0.80840	0.17610	9	12	-0.0622
123	-0.29557	0.84225	0.25085	9	2	0.2881
124	-0.36304	0.84781	0.16874	9	2	0.2853
125	-0.23051	0.83225	0.09026	9	2	0.2867
126	-0.02765	0.80306	0.09534	9	2	0.2887
127	0.38660	-0.20640	0.30960	10	39	-0.1369
128	0.43370	-0.12750	0.24440	10	42	-0.2955
129	0.53940	-0.27950	0.30330	10	34	0.4340
130	0.43390	-0.17920	0.37710	10	34	0.4291
131	0.61960	-0.26470	0.34580	10	12	-0.0533
132	0.72830	-0.29780	0.34820	10	12	-0.3626
133	0.79240	-0.28840	0.38180	10	12	-0.3589
134	0.74850	-0.24640	0.41470	10	12	-0.3666
135	0.64050	-0.21190	0.41210	10	12	-0.3715
136	0.57390	-0.22110	0.37800	10	12	-0.0673
137	0.76303	-0.33135	0.32340	10	2	0.2870
138	0.87779	-0.31389	0.38268	10	2	0.2859
139	0.79831	-0.24064	0.44220	10	2	0.2878
140	0.60742	-0.17773	0.43647	10	2	0.2887
141	0.19590	-0.03020	0.28510	11	39	-0.1350
142	0.15410	-0.10970	0.35140	11	42	-0.3011
143	0.04140	0.04070	0.28700	11	34	0.4342
144	0.15780	-0.06260	0.21800	11	34	0.4399
145	-0.03500	0.02060	0.24510	11	12	-0.0649
146	-0.14460	0.05210	0.24060	11	12	-0.3649
147	-0.20250	0.04110	0.20500	11	12	-0.3642
148	-0.15100	-0.00220	0.17390	11	12	-0.3662
149	-0.04110	-0.03310	0.17760	11	12	-0.3690
150	0.01870	-0.02310	0.21340	11	12	-0.0588
151	-0.18453	0.08533	0.26511	11	2	0.2883
152	-0.28750	0.06596	0.20122	11	2	0.2873
153	-0.19707	-0.01180	0.14665	11	2	0.2870
154	-0.00146	-0.06542	0.15225	11	2	0.2876
155	0.48160	-0.02050	0.32850	12	39	-0.1446
156	0.49120	0.08170	0.29250	12	42	-0.3035
157	0.66040	-0.06550	0.31630	12	34	0.4334
158	0.48760	-0.02070	0.41160	12	34	0.4276
159	0.70850	-0.05750	0.37270	12	12	-0.0603
160	0.82260	-0.07320	0.37660	12	12	-0.3570

161	0.86140	-0.07130	0.42110	12	12	-0.3589
162	0.78650	-0.05570	0.46390	12	12	-0.3681
163	0.67230	-0.04150	0.46090	12	12	-0.3633
164	0.63310	-0.04150	0.41510	12	12	-0.0548
165	0.88106	-0.08701	0.34420	12	2	0.2869
166	0.95049	-0.08192	0.42319	12	2	0.2864
167	0.81739	-0.05470	0.49919	12	2	0.2877
168	0.61383	-0.03044	0.49419	12	2	0.2884
169	0.24740	0.14150	0.35680	13	39	-0.1324
170	0.21450	0.04150	0.38310	13	42	-0.3146
171	0.08160	0.19530	0.38430	13	34	0.4240
172	0.21400	0.16230	0.27640	13	34	0.4259
173	0.01010	0.20590	0.33000	13	12	-0.0561
174	-0.10600	0.22860	0.33520	13	12	-0.3631
175	-0.16230	0.24000	0.29300	13	12	-0.3479
176	-0.10440	0.22990	0.24570	13	12	-0.3601
177	0.00930	0.20530	0.24050	13	12	-0.3619
178	0.06790	0.19310	0.28320	13	12	-0.0610
179	-0.15069	0.23703	0.37232	13	2	0.2877
180	-0.25191	0.25688	0.29677	13	2	0.2862
181	-0.14861	0.24140	0.21205	13	2	0.2851
182	0.05257	0.19557	0.20351	13	2	0.2882
183	0.52690	0.16010	0.39010	14	39	-0.1406
184	0.54730	0.26210	0.37910	14	42	-0.3148
185	0.69800	0.11470	0.36380	14	34	0.4355
186	0.55050	0.12800	0.47310	14	34	0.4403
187	0.76300	0.10340	0.42010	14	12	-0.0632
188	0.87880	0.08590	0.41780	14	12	-0.3604
189	0.92820	0.07240	0.46260	14	12	-0.3611
190	0.86350	0.07610	0.51030	14	12	-0.3609
191	0.74850	0.09350	0.51300	14	12	-0.3647
192	0.69720	0.10750	0.46800	14	12	-0.0585
193	0.92994	0.08291	0.38088	14	2	0.2880
194	1.01828	0.05877	0.46067	14	2	0.2859
195	0.90320	0.06536	0.54527	14	2	0.2869
196	0.69812	0.09627	0.55013	14	2	0.2876
197	0.28600	0.30870	0.44170	15	39	-0.1358
198	0.27800	0.20460	0.46040	15	42	-0.3060
199	0.10680	0.34930	0.46160	15	34	0.4307
200	0.27430	0.33010	0.35740	15	34	0.4233
201	0.05410	0.35460	0.40270	15	12	-0.0593
202	-0.06110	0.36730	0.40090	15	12	-0.3678
203	-0.10110	0.37670	0.35340	15	12	-0.3624
204	-0.02810	0.37110	0.30830	15	12	-0.3564
205	0.08600	0.35750	0.30970	15	12	-0.3614
206	0.12690	0.34790	0.35690	15	12	-0.0563
207	-0.11889	0.36983	0.43611	15	2	0.2894
208	-0.19035	0.38853	0.35170	15	2	0.2867
209	-0.06064	0.37741	0.27191	15	2	0.2867
210	0.14314	0.35433	0.27437	15	2	0.2886
211	0.56270	0.32370	0.48670	16	39	-0.1316
212	0.60910	0.41070	0.43140	16	42	-0.2996
213	0.71370	0.25230	0.47390	16	34	0.4375
214	0.61000	0.33730	0.55960	16	34	0.4055
215	0.79540	0.26040	0.51880	16	12	-0.0517
216	0.90660	0.22750	0.51700	16	12	-0.3746
217	0.96960	0.23030	0.55430	16	12	-0.3523



## Output File from the Energy Calculations

CLPCRY 26.4.2012 Coulomb-London-Pauli potentials  
charge,polarization,dispersion and repulsion coefficients  
0.410 235.000 650.000 77000.0

New structure #DTASCL01  
cell dimensions 12.3533 22.3789 26.6255 76.74 80.05 76.81

symmetry operations

1	1.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	1.0	0.00000	0.00000
0.00000											
2	-1.0	0.0	0.0	0.0	-1.0	0.0	0.0	0.0	-1.0	0.00000	0.00000
0.00000											

fragment,weight,charge+,- 1 250.59 0.8250 -0.8250  
fragment,weight,charge+,- 2 250.59 0.8180 -0.8180  
fragment,weight,charge+,- 3 250.59 0.8196 -0.8195  
fragment,weight,charge+,- 4 250.59 0.8353 -0.8353  
fragment,weight,charge+,- 5 250.59 0.8263 -0.8263  
fragment,weight,charge+,- 6 250.59 0.8263 -0.8263  
fragment,weight,charge+,- 7 250.59 0.8353 -0.8353  
fragment,weight,charge+,- 8 250.59 0.8293 -0.8295  
fragment,weight,charge+,- 9 250.59 0.8311 -0.8311  
fragment,weight,charge+,- 10 250.59 0.8251 -0.8252  
fragment,weight,charge+,- 11 250.59 0.8300 -0.8299  
fragment,weight,charge+,- 12 250.59 0.8243 -0.8243  
fragment,weight,charge+,- 13 250.59 0.8188 -0.8188  
fragment,weight,charge+,- 14 250.59 0.8299 -0.8299  
fragment,weight,charge+,- 15 250.59 0.8222 -0.8222  
fragment,weight,charge+,- 16 250.59 0.8175 -0.8175  
fragment,weight,charge+,- 17 250.59 0.8235 -0.8234

crystal density 2.045

fragment n. 1 dipole charge,module,moment e\*A 0.8250 0.4606  
0.3800  
components and module in Debye -0.4330 -1.7294 0.3913 1.8252

fragment n. 2 dipole charge,module,moment e\*A 0.8180 0.4170  
0.3411  
components and module in Debye -0.5190 -1.3558 0.7597 1.6385

fragment n. 3 dipole charge,module,moment e\*A 0.8196 0.4097  
0.3358  
components and module in Debye 0.3475 1.3539 -0.8049 1.6129

fragment n. 4 dipole charge,module,moment e\*A 0.8353 0.3825  
0.3195  
components and module in Debye -0.4212 -1.0250 1.0619 1.5348

fragment n. 5 dipole charge,module,moment e\*A 0.8263 0.4181  
0.3455  
components and module in Debye 0.4790 1.1113 -1.1354 1.6594

fragment n. 6 dipole charge,module,moment e\*A 0.8263 0.4233  
 0.3498 components and module in Debye -0.2998 -1.5854 0.4683 1.6801

fragment n. 7 dipole charge,module,moment e\*A 0.8353 0.4690  
 0.3918 components and module in Debye 0.5069 1.7816 -0.3316 1.8818

fragment n. 8 dipole charge,module,moment e\*A 0.8293 0.4716  
 0.3911 components and module in Debye -0.5433 -1.7639 0.3510 1.8787

fragment n. 9 dipole charge,module,moment e\*A 0.8311 0.4321  
 0.3591 components and module in Debye 0.2677 1.5956 -0.5981 1.7249

fragment n. 10 dipole charge,module,moment e\*A 0.8251 0.3983  
 0.3286 components and module in Debye -0.5242 -0.9825 1.1185 1.5784

fragment n. 11 dipole charge,module,moment e\*A 0.8300 0.4079  
 0.3385 components and module in Debye 0.5470 0.9427 -1.2067 1.6261

fragment n. 12 dipole charge,module,moment e\*A 0.8243 0.4315  
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fragment n. 13 dipole charge,module,moment e\*A 0.8188 0.4498  
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fragment n. 14 dipole charge,module,moment e\*A 0.8299 0.4748  
 0.3940 components and module in Debye -0.5429 -1.7891 0.2936 1.8926

fragment n. 15 dipole charge,module,moment e\*A 0.8222 0.4447  
 0.3656 components and module in Debye 0.3598 1.6719 -0.3991 1.7562

fragment n. 16 dipole charge,module,moment e\*A 0.8175 0.4167  
 0.3407 components and module in Debye -0.5094 -1.2039 0.9842 1.6363

fragment n. 17 dipole charge,module,moment e\*A 0.8235 0.3914  
 0.3223 components and module in Debye 0.3399 1.1890 -0.9312 1.5480  
 cell dipole components and total,Debye -0.0000 0.0000 0.0000 0.0000

vector for T-search,limit E and %R for print 40.0 3.0 0.90  
 cell translations on a, b, c 11 7 7  
 E(mol-mol) threshold for faulty structure 20.0

mol-mol Ens and short contacts, fr/fr, R, symm.op.,  
 T vec, ec,ed,er,et  
 3 4 6.059 1 -1.00 0.00 0.00 -4.4 -1.2 -22.5 5.2 -23.0

3	6	6.838	1	-1.00	0.00	0.00	2.4	-0.8	-13.3	4.0	-7.7
5	6	6.183	1	-1.00	0.00	0.00	-4.3	-1.2	-21.4	4.8	-22.0
5	8	7.174	1	-1.00	0.00	0.00	1.5	-0.7	-10.3	2.7	-6.9
7	8	6.055	1	-1.00	0.00	0.00	-5.7	-1.6	-30.9	9.9	-28.3
11	4	10.411	1	-1.00	0.00	0.00	-0.5	-0.7	-6.8	2.1	-5.9
11	12	6.134	1	-1.00	0.00	0.00	-4.2	-1.2	-20.9	4.8	-21.4
11	14	7.093	1	-1.00	0.00	0.00	2.0	-0.7	-10.8	3.1	-6.3
13	6	10.528	1	-1.00	0.00	0.00	-0.9	-0.7	-7.2	1.6	-7.2
13	14	6.084	1	-1.00	0.00	0.00	-5.3	-1.5	-29.3	8.9	-27.2
13	16	7.255	1	-1.00	0.00	0.00	1.3	-0.7	-9.6	2.3	-6.6
15	8	10.569	1	-1.00	0.00	0.00	-0.9	-0.7	-7.6	1.8	-7.4
15	16	6.192	1	-1.00	0.00	0.00	-4.2	-1.2	-21.5	4.8	-22.1
7	1	10.581	1	-1.00	1.00	0.00	-0.9	-0.8	-8.4	2.3	-7.7
7	10	7.129	1	-1.00	1.00	0.00	1.7	-0.7	-10.7	3.0	-6.7
9	2	10.470	1	-1.00	1.00	0.00	-1.0	-0.7	-6.9	1.7	-6.8
9	10	6.167	1	-1.00	1.00	0.00	-4.2	-1.2	-21.0	4.8	-21.6
9	12	6.845	1	-1.00	1.00	0.00	2.4	-0.8	-13.4	4.1	-7.6
17	10	10.363	1	-1.00	1.00	0.00	-0.8	-0.7	-7.1	2.2	-6.4
3	5	10.354	2	-1.00	1.00	0.00	-1.0	-0.7	-6.9	1.9	-6.6
5	3	10.354	2	-1.00	1.00	0.00	-1.0	-0.7	-6.9	1.9	-6.6
1	8	8.624	1	0.00	-1.00	0.00	0.1	-0.4	-6.8	2.0	-5.1
1	9	6.530	1	0.00	-1.00	0.00	1.5	-0.8	-14.7	3.4	-10.5
10	8	5.099	1	0.00	-1.00	0.00	-1.5	-1.2	-32.1	17.7	-17.1
11	9	4.852	1	0.00	-1.00	0.00	0.3	-1.4	-33.9	12.4	-22.6
1	2	4.893	1	0.00	0.00	0.00	-1.8	-1.5	-36.8	17.1	-22.9
1	10	9.458	1	0.00	0.00	0.00	-0.4	-0.3	-4.9	1.4	-4.2
1	11	7.200	1	0.00	0.00	0.00	2.0	-0.7	-10.0	2.7	-5.9
2	1	4.893	1	0.00	0.00	0.00	-1.8	-1.5	-36.8	17.1	-22.9
2	4	5.005	1	0.00	0.00	0.00	-1.1	-1.2	-31.0	15.8	-17.4
2	10	8.390	1	0.00	0.00	0.00	1.9	-0.4	-7.3	1.6	-4.2
2	11	5.134	1	0.00	0.00	0.00	0.8	-1.0	-25.4	6.9	-18.6
2	12	8.361	1	0.00	0.00	0.00	-0.5	-0.6	-13.8	7.7	-7.2
2	13	6.992	1	0.00	0.00	0.00	1.1	-0.6	-9.1	1.6	-6.9
3	4	7.272	1	0.00	0.00	0.00	-0.8	-0.2	-7.8	5.8	-3.0
3	5	4.924	1	0.00	0.00	0.00	-0.5	-1.2	-30.1	12.4	-19.4
3	11	7.974	1	0.00	0.00	0.00	2.3	-0.5	-9.7	2.7	-5.2
3	13	8.638	1	0.00	0.00	0.00	0.0	-0.4	-9.3	3.1	-6.6
4	2	5.005	1	0.00	0.00	0.00	-1.1	-1.2	-31.0	15.8	-17.4
4	3	7.272	1	0.00	0.00	0.00	-0.8	-0.2	-7.8	5.8	-3.0
4	6	4.776	1	0.00	0.00	0.00	1.1	-1.5	-35.3	12.1	-23.7
4	12	8.022	1	0.00	0.00	0.00	2.3	-0.4	-8.5	1.8	-4.8
4	13	5.557	1	0.00	0.00	0.00	0.4	-0.9	-21.8	6.4	-16.0
4	14	8.441	1	0.00	0.00	0.00	-1.0	-0.5	-10.5	4.0	-8.0
4	15	7.354	1	0.00	0.00	0.00	2.0	-0.7	-10.7	3.4	-6.0
5	3	4.924	1	0.00	0.00	0.00	-0.5	-1.2	-30.1	12.4	-19.4
5	7	5.071	1	0.00	0.00	0.00	-1.6	-1.3	-33.5	17.7	-18.8
5	13	8.609	1	0.00	0.00	0.00	1.2	-0.4	-7.8	2.5	-4.5
5	15	9.546	1	0.00	0.00	0.00	-0.5	-0.3	-4.9	1.6	-4.0
6	4	4.776	1	0.00	0.00	0.00	1.1	-1.5	-35.3	12.1	-23.7
6	8	4.555	1	0.00	0.00	0.00	0.9	-1.8	-44.7	20.2	-25.4
6	14	8.566	1	0.00	0.00	0.00	0.6	-0.4	-6.0	1.3	-4.4
6	15	6.659	1	0.00	0.00	0.00	1.4	-0.7	-13.2	2.8	-9.7
6	16	9.530	1	0.00	0.00	0.00	-0.5	-0.3	-4.7	1.3	-4.1
6	17	7.515	1	0.00	0.00	0.00	1.8	-0.7	-10.4	3.2	-6.0
7	5	5.071	1	0.00	0.00	0.00	-1.6	-1.3	-33.5	17.7	-18.8
7	9	4.524	1	0.00	0.00	0.00	1.6	-1.9	-45.8	19.8	-26.3
7	15	8.615	1	0.00	0.00	0.00	0.4	-0.4	-6.2	1.5	-4.7

7	17	8.644	1	0.00	0.00	0.00	-1.0	-0.5	-8.3	2.5	-7.2
8	6	4.555	1	0.00	0.00	0.00	0.9	-1.8	-44.7	20.2	-25.4
8	16	8.736	1	0.00	0.00	0.00	0.8	-0.4	-7.7	2.7	-4.6
8	17	5.920	1	0.00	0.00	0.00	0.7	-0.9	-19.1	5.2	-14.0
9	7	4.524	1	0.00	0.00	0.00	1.6	-1.9	-45.8	19.8	-26.3
9	17	8.082	1	0.00	0.00	0.00	2.2	-0.4	-7.6	1.5	-4.4
10	1	9.458	1	0.00	0.00	0.00	-0.4	-0.3	-4.9	1.4	-4.2
10	2	8.390	1	0.00	0.00	0.00	1.9	-0.4	-7.3	1.6	-4.2
10	12	4.901	1	0.00	0.00	0.00	-0.2	-1.3	-31.1	11.5	-21.0
11	1	7.200	1	0.00	0.00	0.00	2.0	-0.7	-10.0	2.7	-5.9
11	2	5.134	1	0.00	0.00	0.00	0.8	-1.0	-25.4	6.9	-18.6
11	3	7.974	1	0.00	0.00	0.00	2.3	-0.5	-9.7	2.7	-5.2
11	13	5.095	1	0.00	0.00	0.00	-1.0	-1.1	-30.8	17.4	-15.5
12	2	8.361	1	0.00	0.00	0.00	-0.5	-0.6	-13.8	7.7	-7.2
12	4	8.022	1	0.00	0.00	0.00	2.3	-0.4	-8.5	1.8	-4.8
12	10	4.901	1	0.00	0.00	0.00	-0.2	-1.3	-31.1	11.5	-21.0
12	14	4.569	1	0.00	0.00	0.00	1.3	-1.8	-43.4	16.2	-27.7
13	2	6.992	1	0.00	0.00	0.00	1.1	-0.6	-9.1	1.6	-6.9
13	3	8.638	1	0.00	0.00	0.00	0.0	-0.4	-9.3	3.1	-6.6
13	4	5.557	1	0.00	0.00	0.00	0.4	-0.9	-21.8	6.4	-16.0
13	5	8.609	1	0.00	0.00	0.00	1.2	-0.4	-7.8	2.5	-4.5
13	11	5.095	1	0.00	0.00	0.00	-1.0	-1.1	-30.8	17.4	-15.5
13	15	4.679	1	0.00	0.00	0.00	-0.1	-1.6	-40.9	18.4	-24.3
14	4	8.441	1	0.00	0.00	0.00	-1.0	-0.5	-10.5	4.0	-8.0
14	6	8.566	1	0.00	0.00	0.00	0.6	-0.4	-6.0	1.3	-4.4
14	12	4.569	1	0.00	0.00	0.00	1.3	-1.8	-43.4	16.2	-27.7
14	16	5.023	1	0.00	0.00	0.00	-2.1	-1.4	-35.2	17.5	-21.2
15	4	7.354	1	0.00	0.00	0.00	2.0	-0.7	-10.7	3.4	-6.0
15	5	9.546	1	0.00	0.00	0.00	-0.5	-0.3	-4.9	1.6	-4.0
15	6	6.659	1	0.00	0.00	0.00	1.4	-0.7	-13.2	2.8	-9.7
15	7	8.615	1	0.00	0.00	0.00	0.4	-0.4	-6.2	1.5	-4.7
15	13	4.679	1	0.00	0.00	0.00	-0.1	-1.6	-40.9	18.4	-24.3
15	17	4.703	1	0.00	0.00	0.00	1.1	-1.6	-37.9	12.3	-26.2
16	6	9.530	1	0.00	0.00	0.00	-0.5	-0.3	-4.7	1.3	-4.1
16	8	8.736	1	0.00	0.00	0.00	0.8	-0.4	-7.7	2.7	-4.6
16	14	5.023	1	0.00	0.00	0.00	-2.1	-1.4	-35.2	17.5	-21.2
17	6	7.515	1	0.00	0.00	0.00	1.8	-0.7	-10.4	3.2	-6.0
17	7	8.644	1	0.00	0.00	0.00	-1.0	-0.5	-8.3	2.5	-7.2
17	8	5.920	1	0.00	0.00	0.00	0.7	-0.9	-19.1	5.2	-14.0
17	9	8.082	1	0.00	0.00	0.00	2.2	-0.4	-7.6	1.5	-4.4
17	15	4.703	1	0.00	0.00	0.00	1.1	-1.6	-37.9	12.3	-26.2
1	3	4.634	2	0.00	0.00	0.00	1.4	-1.7	-40.6	13.4	-27.5
1	11	8.269	2	0.00	0.00	0.00	-0.9	-0.6	-12.2	4.9	-8.7
3	1	4.634	2	0.00	0.00	0.00	1.4	-1.7	-40.6	13.4	-27.5
11	1	8.269	2	0.00	0.00	0.00	-0.9	-0.6	-12.2	4.9	-8.7
8	1	8.624	1	0.00	1.00	0.00	0.1	-0.4	-6.8	2.0	-5.1
8	10	5.099	1	0.00	1.00	0.00	-1.5	-1.2	-32.1	17.7	-17.1
9	1	6.530	1	0.00	1.00	0.00	1.5	-0.8	-14.7	3.4	-10.5
9	11	4.852	1	0.00	1.00	0.00	0.3	-1.4	-33.9	12.4	-22.6
1	9	8.436	2	0.00	1.00	0.00	1.0	-0.4	-6.5	1.5	-4.4
2	7	8.721	2	0.00	1.00	0.00	0.3	-0.4	-8.0	3.1	-5.0
2	9	9.336	2	0.00	1.00	0.00	-0.5	-0.3	-4.8	1.1	-4.5
3	6	8.146	2	0.00	1.00	0.00	1.8	-0.4	-7.4	1.5	-4.5
3	7	6.168	2	0.00	1.00	0.00	1.2	-0.9	-18.1	5.1	-12.7
3	8	8.840	2	0.00	1.00	0.00	-0.9	-0.4	-7.0	1.9	-6.4
3	9	7.596	2	0.00	1.00	0.00	1.6	-0.7	-10.0	3.0	-6.1
4	5	8.004	2	0.00	1.00	0.00	2.2	-0.5	-9.7	2.7	-5.3

4	7	9.110	2	0.00	1.00	0.00	-0.1	-0.4	-6.2	1.7	-5.0
5	4	8.004	2	0.00	1.00	0.00	2.2	-0.5	-9.7	2.7	-5.3
5	5	4.772	2	0.00	1.00	0.00	1.8	-1.1	-30.7	9.0	-21.0
5	6	8.108	2	0.00	1.00	0.00	-0.8	-0.7	-16.5	9.8	-8.2
5	7	7.016	2	0.00	1.00	0.00	1.8	-0.6	-9.2	1.8	-6.3
6	3	8.146	2	0.00	1.00	0.00	1.8	-0.4	-7.4	1.5	-4.5
6	5	8.108	2	0.00	1.00	0.00	-0.8	-0.7	-16.5	9.8	-8.2
7	2	8.721	2	0.00	1.00	0.00	0.3	-0.4	-8.0	3.1	-5.0
7	3	6.168	2	0.00	1.00	0.00	1.2	-0.9	-18.1	5.1	-12.7
7	4	9.110	2	0.00	1.00	0.00	-0.1	-0.4	-6.2	1.7	-5.0
7	5	7.016	2	0.00	1.00	0.00	1.8	-0.6	-9.2	1.8	-6.3
8	3	8.840	2	0.00	1.00	0.00	-0.9	-0.4	-7.0	1.9	-6.4
9	1	8.436	2	0.00	1.00	0.00	1.0	-0.4	-6.5	1.5	-4.4
9	2	9.336	2	0.00	1.00	0.00	-0.5	-0.3	-4.8	1.1	-4.5
9	3	7.596	2	0.00	1.00	0.00	1.6	-0.7	-10.0	3.0	-6.1
15	17	6.882	2	0.00	1.00	1.00	2.7	-0.8	-13.4	4.8	-6.7
17	15	6.882	2	0.00	1.00	1.00	2.7	-0.8	-13.4	4.8	-6.7
17	17	6.014	2	0.00	1.00	1.00	-4.8	-1.3	-23.5	5.5	-24.1
1	7	10.581	1	1.00	-1.00	0.00	-0.9	-0.8	-8.4	2.3	-7.7
2	9	10.470	1	1.00	-1.00	0.00	-1.0	-0.7	-6.9	1.7	-6.8
10	7	7.129	1	1.00	-1.00	0.00	1.7	-0.7	-10.7	3.0	-6.7
10	9	6.167	1	1.00	-1.00	0.00	-4.2	-1.2	-21.0	4.8	-21.6
10	17	10.363	1	1.00	-1.00	0.00	-0.8	-0.7	-7.1	2.2	-6.4
12	9	6.845	1	1.00	-1.00	0.00	2.4	-0.8	-13.4	4.1	-7.6
4	3	6.059	1	1.00	0.00	0.00	-4.4	-1.2	-22.5	5.2	-23.0
4	11	10.411	1	1.00	0.00	0.00	-0.5	-0.7	-6.8	2.1	-5.9
6	3	6.838	1	1.00	0.00	0.00	2.4	-0.8	-13.3	4.0	-7.7
6	5	6.183	1	1.00	0.00	0.00	-4.3	-1.2	-21.4	4.8	-22.0
6	13	10.528	1	1.00	0.00	0.00	-0.9	-0.7	-7.2	1.6	-7.2
8	5	7.174	1	1.00	0.00	0.00	1.5	-0.7	-10.3	2.7	-6.9
8	7	6.055	1	1.00	0.00	0.00	-5.7	-1.6	-30.9	9.9	-28.3
8	15	10.569	1	1.00	0.00	0.00	-0.9	-0.7	-7.6	1.8	-7.4
12	11	6.134	1	1.00	0.00	0.00	-4.2	-1.2	-20.9	4.8	-21.4
14	11	7.093	1	1.00	0.00	0.00	2.0	-0.7	-10.8	3.1	-6.3
14	13	6.084	1	1.00	0.00	0.00	-5.3	-1.5	-29.3	8.9	-27.2
16	13	7.255	1	1.00	0.00	0.00	1.3	-0.7	-9.6	2.3	-6.6
16	15	6.192	1	1.00	0.00	0.00	-4.2	-1.2	-21.5	4.8	-22.1
1	2	6.153	2	1.00	0.00	0.00	-4.6	-1.3	-24.6	6.3	-24.3
1	4	6.991	2	1.00	0.00	0.00	2.6	-0.8	-12.2	4.4	-6.0
2	1	6.153	2	1.00	0.00	0.00	-4.6	-1.3	-24.6	6.3	-24.3
2	2	7.341	2	1.00	0.00	0.00	1.2	-0.6	-8.9	2.0	-6.4
4	1	6.991	2	1.00	0.00	0.00	2.6	-0.8	-12.2	4.4	-6.0
10	14	7.086	2	1.00	0.00	1.00	1.8	-0.6	-9.3	2.0	-6.2
10	15	8.143	2	1.00	0.00	1.00	-0.8	-0.6	-15.2	8.0	-8.6
10	16	4.853	2	1.00	0.00	1.00	1.4	-1.0	-29.1	8.2	-20.6
10	17	7.943	2	1.00	0.00	1.00	2.3	-0.5	-10.5	3.3	-5.4
11	14	9.300	2	1.00	0.00	1.00	-0.2	-0.3	-5.5	1.6	-4.4
11	16	8.153	2	1.00	0.00	1.00	2.1	-0.4	-8.3	1.8	-4.7
12	12	7.627	2	1.00	0.00	1.00	1.5	-0.7	-9.6	2.6	-6.1
12	13	9.071	2	1.00	0.00	1.00	-0.7	-0.4	-5.5	1.1	-5.4
12	14	6.359	2	1.00	0.00	1.00	1.6	-0.8	-16.7	4.5	-11.4
12	15	8.281	2	1.00	0.00	1.00	1.4	-0.4	-7.0	1.5	-4.4
13	12	9.071	2	1.00	0.00	1.00	-0.7	-0.4	-5.5	1.1	-5.4
13	14	8.662	2	1.00	0.00	1.00	0.2	-0.4	-7.7	2.7	-5.2
14	10	7.086	2	1.00	0.00	1.00	1.8	-0.6	-9.3	2.0	-6.2
14	11	9.300	2	1.00	0.00	1.00	-0.2	-0.3	-5.5	1.6	-4.4
14	12	6.359	2	1.00	0.00	1.00	1.6	-0.8	-16.7	4.5	-11.4

14	13	8.662	2	1.00	0.00	1.00	0.2	-0.4	-7.7	2.7	-5.2
15	10	8.143	2	1.00	0.00	1.00	-0.8	-0.6	-15.2	8.0	-8.6
15	12	8.281	2	1.00	0.00	1.00	1.4	-0.4	-7.0	1.5	-4.4
16	10	4.853	2	1.00	0.00	1.00	1.4	-1.0	-29.1	8.2	-20.6
16	11	8.153	2	1.00	0.00	1.00	2.1	-0.4	-8.3	1.8	-4.7
17	10	7.943	2	1.00	0.00	1.00	2.3	-0.5	-10.5	3.3	-5.4
8	16	6.974	2	1.00	1.00	1.00	1.5	-0.6	-9.4	1.8	-6.7
8	17	8.886	2	1.00	1.00	1.00	0.0	-0.4	-7.6	2.3	-5.6
9	16	8.177	2	1.00	1.00	1.00	-0.7	-0.7	-16.8	11.1	-7.1
16	8	6.974	2	1.00	1.00	1.00	1.5	-0.6	-9.4	1.8	-6.7
16	9	8.177	2	1.00	1.00	1.00	-0.7	-0.7	-16.8	11.1	-7.1
16	17	4.945	2	1.00	1.00	1.00	-1.0	-1.1	-30.5	14.0	-18.6
17	8	8.886	2	1.00	1.00	1.00	0.0	-0.4	-7.6	2.3	-5.6
17	16	4.945	2	1.00	1.00	1.00	-1.0	-1.1	-30.5	14.0	-18.6
17	17	7.283	2	1.00	1.00	1.00	-0.7	-0.2	-7.7	5.5	-3.1
12	16	10.400	2	2.00	0.00	1.00	-1.0	-0.7	-6.9	1.9	-6.7
14	14	10.592	2	2.00	0.00	1.00	-0.9	-0.8	-8.9	2.8	-7.8
16	12	10.400	2	2.00	0.00	1.00	-1.0	-0.7	-6.9	1.9	-6.7

56916 fragment pairs    22349 within cutoff    40.00

total frag-frag ec,ep,ed,er,etot

1	1	-2.9	-1.1	-33.2	31.7	-5.5
1	2	-6.9	-3.3	-70.5	31.5	-49.2
1	3	0.8	-2.2	-43.0	13.4	-31.0
1	4	2.3	-1.1	-13.4	4.4	-7.8
1	5	-0.5	-0.5	-1.8	0.0	-2.8
1	6	0.4	-0.4	-1.4	0.0	-1.4
1	7	-0.5	-1.3	-10.9	2.4	-10.2
1	8	0.4	-0.6	-7.3	2.0	-5.6
1	9	3.2	-1.9	-27.6	9.3	-17.1
1	10	-0.3	-0.6	-5.7	1.4	-5.2
1	11	1.1	-1.6	-22.9	7.6	-15.8
1	12	-0.3	-0.4	-1.5	0.0	-2.1
1	13	0.0	-0.4	-1.1	0.0	-1.5
1	14	0.1	-0.3	-0.6	0.0	-0.8
1	15	-0.0	-0.3	-0.4	0.0	-0.7
1	16	0.0	-0.3	-0.5	0.0	-0.8
1	17	-0.0	-0.3	-0.4	0.0	-0.7
2	2	1.3	-0.9	-9.8	2.0	-7.4
2	3	-2.7	-1.1	-32.4	31.4	-4.9
2	4	-0.5	-1.5	-32.0	15.8	-18.2
2	5	-1.0	-0.5	-2.6	0.0	-4.0
2	6	0.1	-0.4	-1.1	0.0	-1.4
2	7	0.3	-0.8	-9.2	3.1	-6.6
2	8	-0.1	-0.4	-1.3	0.0	-1.8
2	9	-1.1	-1.4	-13.4	2.8	-13.1
2	10	1.6	-0.6	-7.9	1.6	-5.3
2	11	0.9	-2.0	-34.6	14.3	-21.3
2	12	-0.6	-0.9	-14.5	7.7	-8.3
2	13	1.2	-0.9	-9.5	1.6	-7.6
2	14	0.6	-0.4	-1.2	0.0	-1.0
2	15	-0.5	-0.3	-0.7	0.0	-1.5
2	16	0.1	-0.3	-0.6	0.0	-0.7
2	17	-0.0	-0.3	-0.4	0.0	-0.7
3	3	-0.0	-0.4	-1.1	0.0	-1.5
3	4	-5.4	-1.7	-30.9	11.0	-27.1

3	5	-1.1	-2.2	-39.3	14.4	-28.2
3	6	4.2	-1.4	-21.3	5.6	-13.0
3	7	1.3	-1.8	-25.1	8.9	-16.7
3	8	-0.2	-0.7	-7.9	1.9	-7.0
3	9	1.4	-1.1	-10.9	3.0	-7.7
3	10	0.6	-0.3	-1.0	0.0	-0.8
3	11	2.2	-0.8	-10.7	2.7	-6.5
3	12	0.2	-0.3	-1.0	0.0	-1.2
3	13	-0.0	-0.7	-9.9	3.1	-7.5
3	14	-0.8	-0.3	-0.9	0.0	-2.1
3	15	0.5	-0.3	-0.9	0.0	-0.7
3	16	-0.2	-0.3	-0.5	0.0	-0.9
3	17	0.1	-0.3	-0.5	0.0	-0.7
4	4	0.6	-0.3	-0.8	0.0	-0.5
4	5	-0.2	-1.4	-41.7	36.2	-7.1
4	6	1.1	-1.9	-36.6	12.1	-25.3
4	7	-1.0	-0.8	-8.7	1.8	-8.6
4	8	-0.9	-0.5	-1.7	0.0	-3.1
4	9	0.1	-0.4	-1.3	0.0	-1.6
4	10	-0.4	-0.4	-0.9	0.0	-1.7
4	11	-0.0	-1.1	-8.7	2.1	-7.6
4	12	2.2	-0.7	-9.0	1.8	-5.6
4	13	0.6	-1.8	-29.3	11.1	-19.3
4	14	-1.0	-0.8	-11.1	4.0	-8.9
4	15	1.9	-1.0	-11.2	3.4	-6.9
4	16	-0.1	-0.4	-1.0	0.0	-1.4
4	17	0.2	-0.4	-1.1	0.0	-1.3
5	5	2.0	-2.1	-40.7	16.9	-23.9
5	6	-5.9	-2.3	-46.5	21.2	-33.5
5	7	0.3	-2.3	-43.4	19.4	-26.0
5	8	1.8	-1.1	-11.7	2.7	-8.4
5	9	-0.5	-0.5	-1.5	0.0	-2.5
5	10	0.2	-0.3	-0.7	0.0	-0.8
5	11	-0.2	-0.3	-0.8	0.0	-1.4
5	12	0.6	-0.3	-0.5	0.0	-0.2
5	13	1.1	-0.7	-8.3	2.5	-5.4
5	14	0.1	-0.3	-0.7	0.0	-0.8
5	15	-0.6	-0.6	-5.4	1.6	-5.0
5	16	-0.1	-0.3	-0.6	0.0	-0.9
5	17	-0.3	-0.4	-1.0	0.0	-1.6
6	6	-0.7	-0.4	-1.4	0.0	-2.5
6	7	-2.5	-1.2	-34.1	33.2	-4.6
6	8	1.0	-2.1	-45.7	20.2	-26.6
6	9	-0.4	-0.4	-2.3	0.0	-3.1
6	10	-0.2	-0.4	-1.2	0.0	-1.8
6	11	-0.2	-0.4	-0.9	0.0	-1.4
6	12	-0.2	-0.3	-0.8	0.0	-1.3
6	13	-0.6	-1.1	-8.8	1.6	-8.9
6	14	0.3	-0.6	-6.4	1.3	-5.4
6	15	2.4	-1.5	-19.8	7.2	-11.7
6	16	-0.9	-0.6	-5.5	1.3	-5.6
6	17	2.2	-1.1	-11.4	3.2	-7.1
7	7	-0.3	-0.3	-0.9	0.0	-1.5
7	8	-6.3	-2.0	-40.0	19.0	-29.4
7	9	1.5	-2.2	-46.6	19.8	-27.5
7	10	1.7	-1.0	-11.3	3.0	-7.6
7	11	-0.3	-0.5	-1.4	0.0	-2.2

7	12	0.6	-0.3	-0.8	0.0	-0.5
7	13	0.1	-0.4	-1.2	0.0	-1.4
7	14	0.5	-0.3	-0.6	0.0	-0.3
7	15	0.2	-0.6	-6.7	1.5	-5.7
7	16	0.4	-0.4	-1.5	0.0	-1.4
7	17	-1.7	-0.8	-9.3	2.5	-9.3
8	8	0.4	-0.3	-0.8	0.0	-0.8
8	9	-3.0	-1.1	-33.2	33.3	-3.9
8	10	-1.2	-1.5	-32.9	17.7	-17.9
8	11	-0.8	-0.4	-2.3	0.1	-3.4
8	12	-0.6	-0.4	-0.9	0.0	-1.9
8	13	0.4	-0.4	-1.3	0.0	-1.3
8	14	-0.6	-0.4	-1.2	0.0	-2.2
8	15	0.1	-1.2	-9.8	1.8	-9.0
8	16	2.0	-1.3	-17.6	4.5	-12.3
8	17	1.1	-2.1	-33.8	11.8	-23.1
9	9	0.2	-0.3	-0.7	0.0	-0.8
9	10	-5.1	-1.6	-29.2	11.1	-24.8
9	11	0.2	-1.8	-34.8	12.4	-24.0
9	12	2.6	-1.0	-14.0	4.1	-8.3
9	13	-0.5	-0.4	-1.1	0.0	-2.0
9	14	1.2	-0.4	-1.3	0.0	-0.5
9	15	-1.0	-0.4	-1.6	0.0	-3.0
9	16	-0.1	-1.0	-17.5	11.1	-7.5
9	17	2.2	-0.7	-8.6	1.5	-5.6
10	10	0.2	-0.3	-0.7	0.0	-0.8
10	11	-2.4	-1.0	-32.3	34.3	-1.3
10	12	-0.4	-1.7	-32.4	11.5	-22.9
10	13	-0.6	-0.5	-2.9	0.1	-3.9
10	14	1.4	-1.1	-10.6	2.0	-8.3
10	15	-0.9	-1.0	-16.4	8.0	-10.3
10	16	1.2	-2.0	-38.9	15.9	-23.9
10	17	1.9	-1.5	-19.5	5.5	-13.5
11	11	-0.0	-0.3	-0.8	0.0	-1.2
11	12	-4.9	-1.7	-29.6	11.1	-25.1
11	13	-1.2	-1.4	-31.7	17.4	-16.9
11	14	1.7	-1.3	-17.0	4.7	-11.8
11	15	0.0	-0.4	-1.4	0.0	-1.8
11	16	2.3	-0.7	-8.9	1.8	-5.5
11	17	0.3	-0.3	-0.8	0.0	-0.9
12	12	1.6	-1.0	-10.5	2.7	-7.2
12	13	-3.3	-1.4	-37.7	32.8	-9.6
12	14	3.6	-3.5	-66.8	24.7	-42.0
12	15	0.8	-0.8	-9.1	1.5	-7.5
12	16	-0.9	-1.2	-9.5	1.9	-9.6
12	17	-0.4	-0.4	-1.2	0.0	-2.0
13	13	0.0	-0.3	-1.0	0.0	-1.3
13	14	-6.0	-2.3	-45.9	20.4	-33.9
13	15	0.5	-1.9	-41.8	18.4	-24.9
13	16	1.2	-1.0	-10.8	2.3	-8.3
13	17	0.2	-0.5	-1.7	0.0	-2.0
14	14	-0.2	-1.2	-11.0	2.8	-9.6
14	15	-3.2	-1.2	-34.1	33.1	-5.4
14	16	-1.9	-1.8	-36.7	17.5	-22.9
14	17	-1.0	-0.5	-2.8	0.1	-4.2
15	15	0.8	-0.4	-1.1	0.0	-0.7
15	16	-5.5	-1.7	-30.6	11.9	-26.0

15	17	3.7	-2.7	-52.3	17.0	-34.2
16	16	-0.6	-0.4	-2.3	0.0	-3.3
16	17	-3.2	-2.1	-62.1	44.7	-22.7
17	17	-5.4	-1.7	-31.8	11.0	-27.8

#DTASCL01 Ec,Ep,Ed,Er,Ecd,Et -1.4 -8.1 -121.9 53.9 -0.0  
-77.5

per molecule in asymm.unit

#DTASCL01 DHs=-U-2RT exp,%D 77.5 0.0 0.0 2RT 0.0 E(Dp) -0.0  
per molecule in asymm.unit

#DTASCL01 Cell dipole module, cell dip E/molecule 0.0000 -0.0

end of data stream

structures read and written 1 1

writing data on ddf,distance density functions  
species indicators, rmin, n.counts, count density

2	2	2.10	1854	1.36	not significant
2	12	2.85	2340	1.79	not significant
2	34	2.80	813	0.62	not significant
2	39	3.10	423	0.33	not significant
2	42	2.80	410	0.31	not significant
12	12	3.35	4062	3.25	not significant
12	34	3.30	1103	0.88	not significant
12	39	3.70	665	0.56	not significant
12	42	3.45	660	0.53	not significant
34	34	3.35	530	0.42	not significant
34	39	3.60	226	0.19	not significant
34	42	3.40	238	0.19	not significant
39	39	3.80	154	0.13	not significant
39	42	3.30	85	0.07	not significant
42	42	3.85	174	0.15	not significant

### Calculated Energies per Molecule in kJ/mol

Molecule	<b>E<sub>Coulomb</sub></b>	<b>E<sub>polarization</sub></b>	<b>E<sub>dispersion</sub></b>	<b>E<sub>repulsive</sub></b>	<b>E<sub>total</sub></b>
1 (A)	-3.1	-16.6	-242.2	103.7	-158.2
2 (Q)	-0.1	-16.1	-238.7	97.3	-157.4
3 (P)	-6.3	-15.8	-245.1	112.9	-153.7
4 (O)	-0.8	-16.3	-243.3	105.4	-155.0
5 (N)	-5.2	-16.7	-248.9	110.6	-160.1
6 (M)	-6.9	-16.1	-244.0	111.3	-155.7
7 (L)	0.6	-16.3	-239.8	99.8	-155.3
8 (K)	-1.3	-16.0	-239.6	108.5	-148.1
9 (J)	-2.7	-15.8	-244.5	112.1	-150.8
10 (I)	0.9	-16.6	-245.6	108.4	-153.0
11 (H)	-6.5	-16.5	-249.4	115.0	-157.7
12 (G)	-5.7	-17.0	-251.7	114.6	-159.5
13 (F)	0.1	-16.5	-245.2	106.9	-154.6
14 (E)	-4.3	-16.1	-247.2	114.9	-152.5
15 (D)	-0.5	-16.2	-239.4	103.7	-152.0
16 (C)	0.9	-15.9	-237.3	95.4	-157.5
17 (B)	-7.3	-16.0	-241.7	111.8	-153.0

**Calculated Energies per Molecule Pair in kJ/mol**

(Totals summed over all fragment-fragment interactions in the crystal).

Mol 1	Mol 2	E <sub>Coulomb</sub>	E <sub>polarization</sub>	E <sub>dispersion</sub>	E <sub>repulsive</sub>	E <sub>total</sub>
1	1	-2.9	-1.1	-33.2	31.7	-5.5
1	2	-0.0	-0.3	-0.4	0.0	-0.7
1	3	0.0	-0.3	-0.5	0.0	-0.8
1	4	-0.0	-0.3	-0.4	0.0	-0.7
1	5	0.1	-0.3	-0.6	0.0	-0.8
1	6	0.0	-0.4	-1.1	0.0	-1.5
1	7	-0.3	-0.4	-1.5	0.0	-2.1
1	8	1.1	-1.6	-22.9	7.6	-15.8
1	9	-0.3	-0.6	-5.7	1.4	-5.2
1	10	3.2	-1.9	-27.6	9.3	-17.1
1	11	0.4	-0.6	-7.3	2.0	-5.6
1	12	-0.5	-1.3	-10.9	2.4	-10.2
1	13	0.4	-0.4	-1.4	0.0	-1.4
1	14	-0.5	-0.5	-1.8	0.0	-2.8
1	15	2.3	-1.1	-13.4	4.4	-7.8
1	16	0.8	-2.2	-43.0	13.4	-31.0
1	17	-6.9	-3.3	-70.5	31.5	-49.2
2	2	-5.4	-1.7	-31.8	11.0	-27.8
2	3	-3.2	-2.1	-62.1	44.7	-22.7
2	4	3.7	-2.7	-52.3	17.0	-34.2
2	5	-1.0	-0.5	-2.8	0.1	-4.2
2	6	0.2	-0.5	-1.7	0.0	-2.0
2	7	-0.4	-0.4	-1.2	0.0	-2.0
2	8	0.3	-0.3	-0.8	0.0	-0.9
2	9	1.9	-1.5	-19.5	5.5	-13.5

2	10	2.2	-0.7	-8.6	1.5	-5.6
2	11	1.1	-2.1	-33.8	11.8	-23.1
2	12	-1.7	-0.8	-9.3	2.5	-9.3
2	13	2.2	-1.1	-11.4	3.2	-7.1
2	14	-0.3	-0.4	-1.0	0.0	-1.6
2	15	0.2	-0.4	-1.1	0.0	-1.3
2	16	0.1	-0.3	-0.5	0.0	-0.7
2	17	-0.0	-0.3	-0.4	0.0	-0.7
3	3	-0.6	-0.4	-2.3	0.0	-3.3
3	4	-5.5	-1.7	-30.6	11.9	-26.0
3	5	-1.9	-1.8	-36.7	17.5	-22.9
3	6	1.2	-1.0	-10.8	2.3	-8.3
3	7	-0.9	-1.2	-9.5	1.9	-9.6
3	8	2.3	-0.7	-8.9	1.8	-5.5
3	9	1.2	-2.0	-38.9	15.9	-23.9
3	10	-0.1	-1.0	-17.5	11.1	-7.5
3	11	2.0	-1.3	-17.6	4.5	-12.3
3	12	0.4	-0.4	-1.5	0.0	-1.4
3	13	-0.9	-0.6	-5.5	1.3	-5.6
3	14	-0.1	-0.3	-0.6	0.0	-0.9
3	15	-0.1	-0.4	-1.0	0.0	-1.4
3	16	-0.2	-0.3	-0.5	0.0	-0.9
3	17	0.1	-0.3	-0.6	0.0	-0.7
4	4	0.8	-0.4	-1.1	0.0	-0.7
4	5	-3.2	-1.2	-34.1	33.1	-5.4
4	6	0.5	-1.9	-41.8	18.4	-24.9
4	7	0.8	-0.8	-9.1	1.5	-7.5
4	8	0.0	-0.4	-1.4	0.0	-1.8
4	9	-0.9	-1.0	-16.4	8.0	-10.3

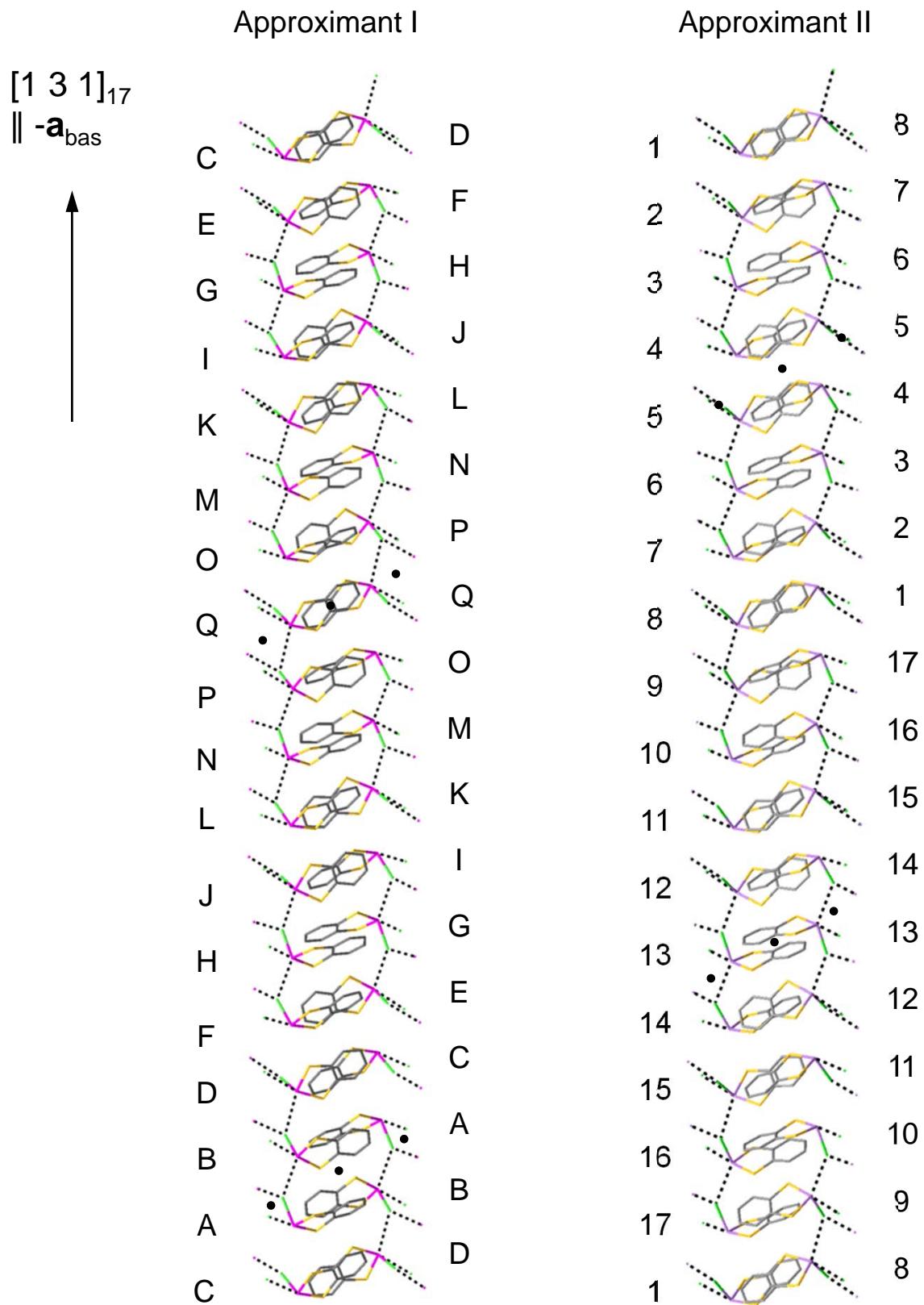
4	10	-1.0	-0.4	-1.6	0.0	-3.0
4	11	0.1	-1.2	-9.8	1.8	-9.0
4	12	0.2	-0.6	-6.7	1.5	-5.7
4	13	2.4	-1.5	-19.8	7.2	-11.7
4	14	-0.6	-0.6	-5.4	1.6	-5.0
4	15	1.9	-1.0	-11.2	3.4	-6.9
4	16	0.5	-0.3	-0.9	0.0	-0.7
4	17	-0.5	-0.3	-0.7	0.0	-1.5
5	5	-0.2	-1.2	-11.0	2.8	-9.6
5	6	-6.0	-2.3	-45.9	20.4	-33.9
5	7	3.6	-3.5	-66.8	24.7	-42.0
5	8	1.7	-1.3	-17.0	4.7	-11.8
5	9	1.4	-1.1	-10.6	2.0	-8.3
5	10	1.2	-0.4	-1.3	0.0	-0.5
5	11	-0.6	-0.4	-1.2	0.0	-2.2
5	12	0.5	-0.3	-0.6	0.0	-0.3
5	13	0.3	-0.6	-6.4	1.3	-5.4
5	14	0.1	-0.3	-0.7	0.0	-0.8
5	15	-1.0	-0.8	-11.1	4.0	-8.9
5	16	-0.8	-0.3	-0.9	0.0	-2.1
5	17	0.6	-0.4	-1.2	0.0	-1.0
6	6	0.0	-0.3	-1.0	0.0	-1.3
6	7	-3.3	-1.4	-37.7	32.8	-9.6
6	8	-1.2	-1.4	-31.7	17.4	-16.9
6	9	-0.6	-0.5	-2.9	0.1	-3.9
6	10	-0.5	-0.4	-1.1	0.0	-2.0
6	11	0.4	-0.4	-1.3	0.0	-1.3
6	12	0.1	-0.4	-1.2	0.0	-1.4
6	13	-0.6	-1.1	-8.8	1.6	-8.9

6	14	1.1	-0.7	-8.3	2.5	-5.4
6	15	0.6	-1.8	-29.3	11.1	-19.3
6	16	-0.0	-0.7	-9.9	3.1	-7.5
6	17	1.2	-0.9	-9.5	1.6	-7.6
7	7	1.6	-1.0	-10.5	2.7	-7.2
7	8	-4.9	-1.7	-29.6	11.1	-25.1
7	9	-0.4	-1.7	-32.4	11.5	-22.9
7	10	2.6	-1.0	-14.0	4.1	-8.3
7	11	-0.6	-0.4	-0.9	0.0	-1.9
7	12	0.6	-0.3	-0.8	0.0	-0.5
7	13	-0.2	-0.3	-0.8	0.0	-1.3
7	14	0.6	-0.3	-0.5	0.0	-0.2
7	15	2.2	-0.7	-9.0	1.8	-5.6
7	16	0.2	-0.3	-1.0	0.0	-1.2
7	17	-0.6	-0.9	-14.5	7.7	-8.3
8	8	-0.0	-0.3	-0.8	0.0	-1.2
8	9	-2.4	-1.0	-32.3	34.3	-1.3
8	10	0.2	-1.8	-34.8	12.4	-24.0
8	11	-0.8	-0.4	-2.3	0.1	-3.4
8	12	-0.3	-0.5	-1.4	0.0	-2.2
8	13	-0.2	-0.4	-0.9	0.0	-1.4
8	14	-0.2	-0.3	-0.8	0.0	-1.4
8	15	-0.0	-1.1	-8.7	2.1	-7.6
8	16	2.2	-0.8	-10.7	2.7	-6.5
8	17	0.9	-2.0	-34.6	14.3	-21.3
9	9	0.2	-0.3	-0.7	0.0	-0.8
9	10	-5.1	-1.6	-29.2	11.1	-24.8
9	11	-1.2	-1.5	-32.9	17.7	-17.9
9	12	1.7	-1.0	-11.3	3.0	-7.6

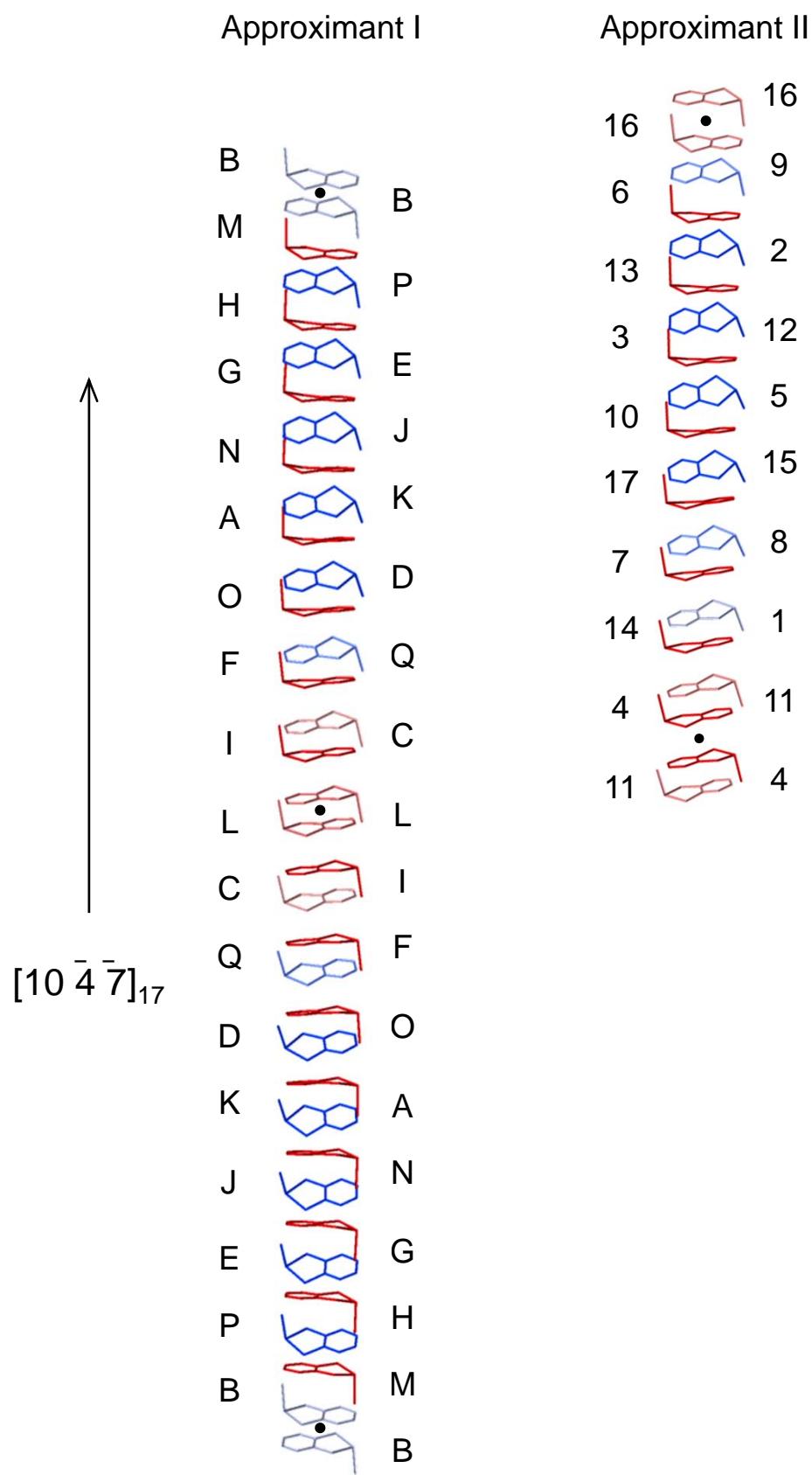
9	13	-0.2	-0.4	-1.2	0.0	-1.8
9	14	0.2	-0.3	-0.7	0.0	-0.8
9	15	-0.4	-0.4	-0.9	0.0	-1.7
9	16	0.6	-0.3	-1.0	0.0	-0.8
9	17	1.6	-0.6	-7.9	1.6	-5.3
10	10	0.2	-0.3	-0.7	0.0	-0.8
10	11	-3.0	-1.1	-33.2	33.3	-3.9
10	12	1.5	-2.2	-46.6	19.8	-27.5
10	13	-0.4	-0.4	-2.3	0.0	-3.1
10	14	-0.5	-0.5	-1.5	0.0	-2.5
10	15	0.1	-0.4	-1.3	0.0	-1.6
10	16	1.4	-1.1	-10.9	3.0	-7.7
10	17	-1.1	-1.4	-13.4	2.8	-13.1
11	11	0.4	-0.3	-0.8	0.0	-0.8
11	12	-6.3	-2.0	-40.0	19.0	-29.4
11	13	1.0	-2.1	-45.7	20.2	-26.6
11	14	1.8	-1.1	-11.7	2.7	-8.4
11	15	-0.9	-0.5	-1.7	0.0	-3.1
11	16	-0.2	-0.7	-7.9	1.9	-7.0
11	17	-0.1	-0.4	-1.3	0.0	-1.8
12	12	-0.3	-0.3	-0.9	0.0	-1.5
12	13	-2.5	-1.2	-34.1	33.2	-4.6
12	14	0.3	-2.3	-43.4	19.4	-26.0
12	15	-1.0	-0.8	-8.7	1.8	-8.6
12	16	1.3	-1.8	-25.1	8.9	-16.7
12	17	0.3	-0.8	-9.2	3.1	-6.6
13	13	-0.7	-0.4	-1.4	0.0	-2.5
13	14	-5.9	-2.3	-46.5	21.2	-33.5
13	15	1.1	-1.9	-36.6	12.1	-25.3

13	16	4.2	-1.4	-21.3	5.6	-13.0
13	17	0.1	-0.4	-1.1	0.0	-1.4
14	14	2.0	-2.1	-40.7	16.9	-23.9
14	15	-0.2	-1.4	-41.7	36.2	-7.1
14	16	-1.1	-2.2	-39.3	14.4	-28.2
14	17	-1.0	-0.5	-2.6	0.0	-4.0
15	15	0.6	-0.3	-0.8	0.0	-0.5
15	16	-5.4	-1.7	-30.9	11.0	-27.1
15	17	-0.5	-1.5	-32.0	15.8	-18.2
16	16	-0.0	-0.4	-1.1	0.0	-1.5
16	17	-2.7	-1.1	-32.4	31.4	-4.9
17	17	1.3	-0.9	-9.8	2.0	-7.4

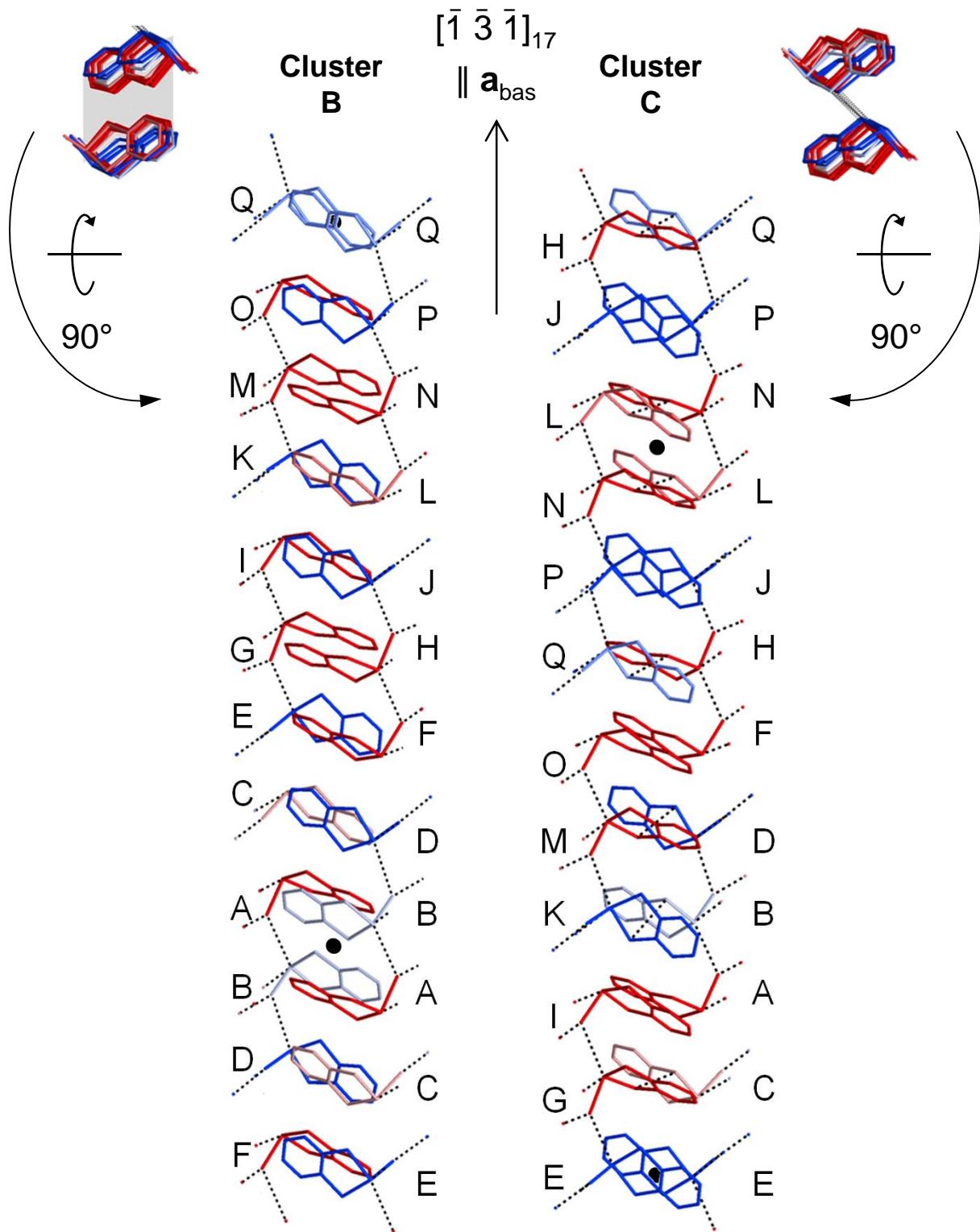
## 8-1. View of the modulation down $[12\ 2\ -5]_{17} \parallel -c^*_{\text{bas}}$



## 8-2. Another view of the modulation



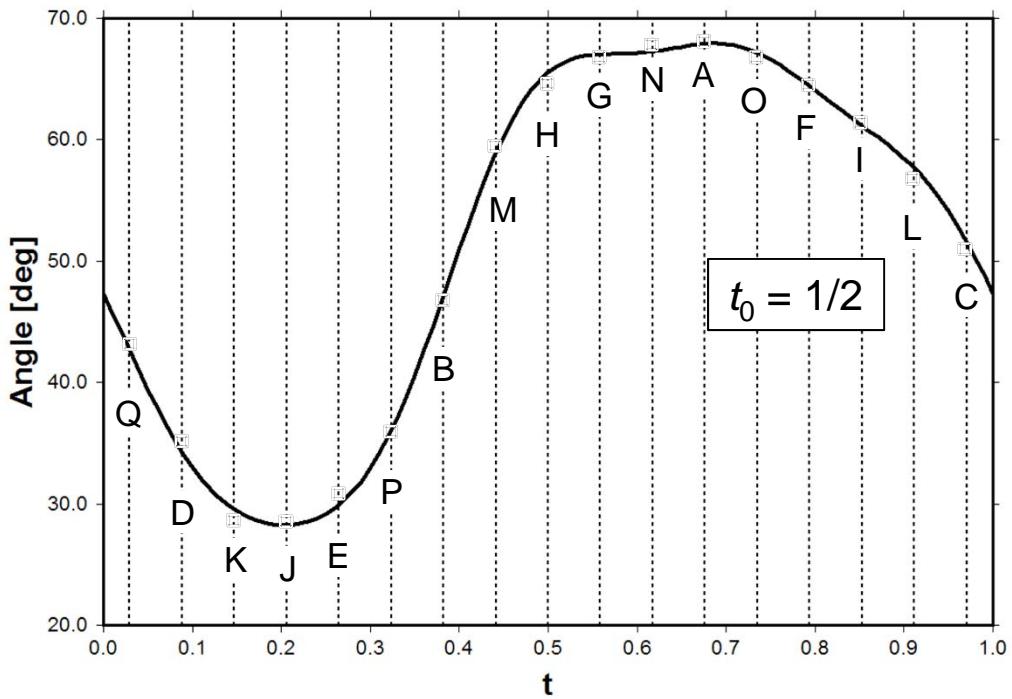
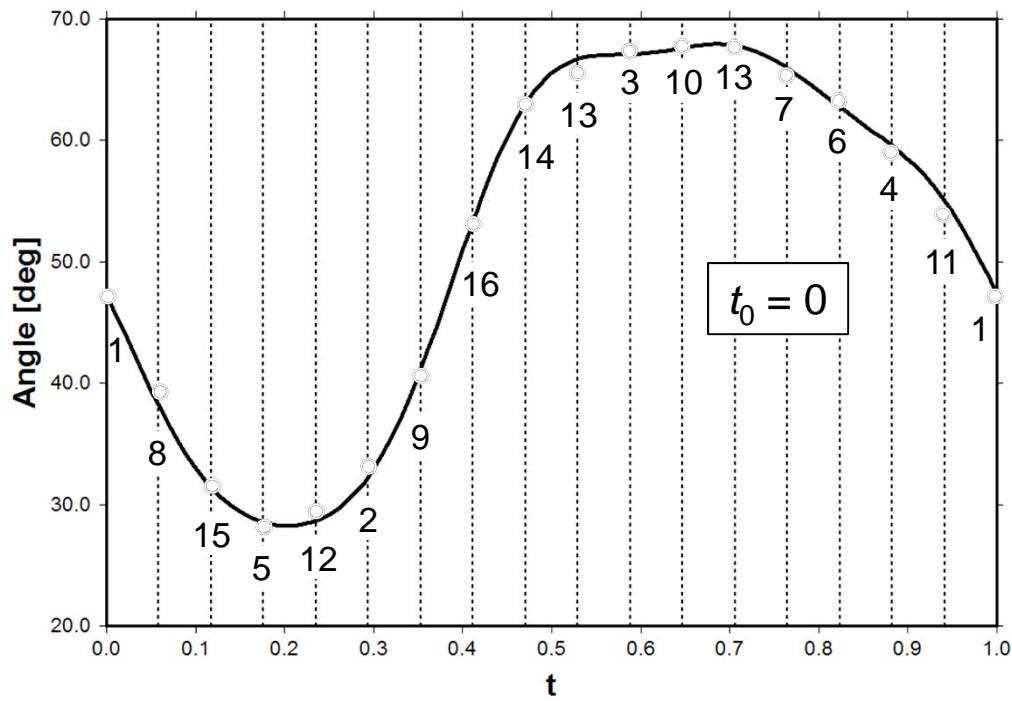
## 9. Details of the interactions in clusters B and C



**10. Variation in the  $(S_2C_6), (0\ 1\ 2)_{bas}$  angle with  $t$  as determined in the superspace refinement.**

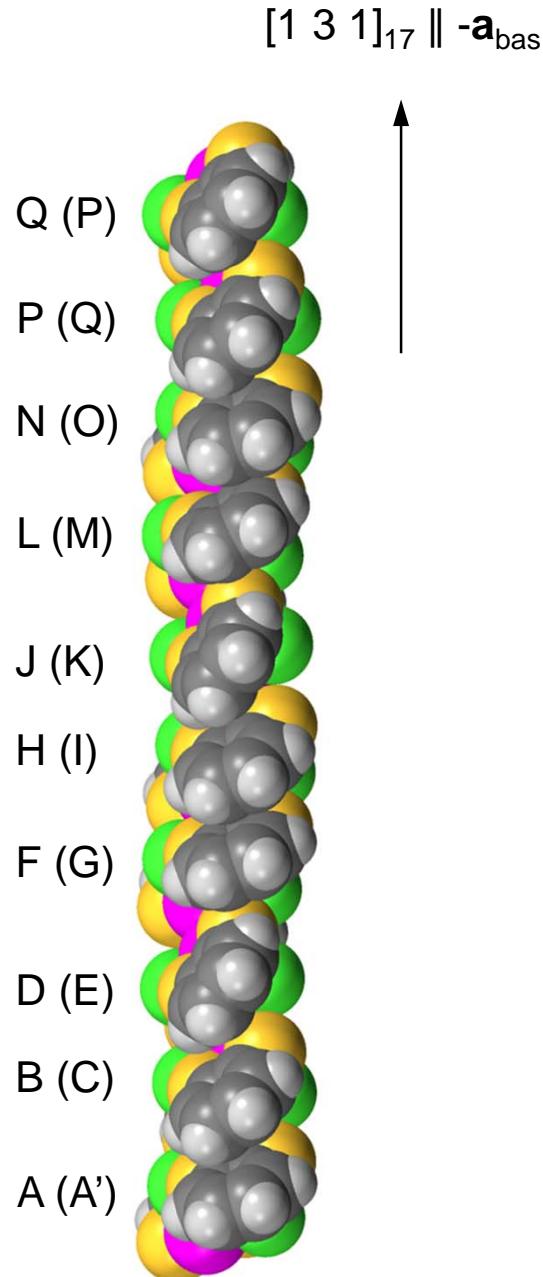
Dotted lines are drawn at intervals of  $t/17$  for  $t_0 = 0$  and  $t_0 = 1/2$ .

The individual values of the angle determined in the conventional refinements are superimposed.



**11. Space-filling drawing showing the unique intermolecular interactions in the ribbon for approximant I.**

Note that the C<sub>6</sub> rings are not all in good contact along the dimer ribbon (*i.e.*, along [1 3 1]<sub>17</sub>). The labels in parentheses designate molecules that are largely hidden.



## **12. Incommensurate structures that could be archived in the Cambridge Structural Database but are not**

List of incommensurate structures that are molecular or that have large ions and that seem not to be archived in the Cambridge Structural Database.. The list does not include layered perovskites containing ammonium ions or incommensurate urea inclusion complexes, of which there are many examples (see Schönleber, 2011).

Wagner, T. & Schönleber, A. (2009). *Acta Cryst.* **B65**, 249-268.

*A non-mathematical introduction to the superspace description of modulated structures*  
 $\text{C}_{19}\text{H}_{27}\text{NO}_3\text{Si}$

Damay, F., Rodríguez-Carvajal, J., André, D., Dunstetter, F. & Szwarc, H. (2008). *Acta Cryst.* . **B64**, 589-595.

*Orientational ordering in the low-temperature stable phases of deuterated thiophene*  
 $\text{C}_4\text{D}_4\text{S}$

Rodriguez, S. M. B., Palatinus, L., Petříček, V. & Chapuis, G. (2006). *Acta Cryst.* **B62**, 1043-1050.

*Growth-induced incommensurability observed in the organic co-crystal hexamethylenetetramine resorcinol*

$\text{C}_6\text{H}_{12}\text{N}_4 \cdot \text{C}_6\text{H}_6\text{O}_2$

Zuniga, F.J.; Palatinus, L.; Cabildo, P.; Claramunt, R.M. (2006). *Z. Kristallogr.* **221**, 281-287.  
*The molecular structure of 2-phenylbenzimidazole: a new example of incommensurate modulated intramolecular torsion*

$\text{C}_{13}\text{H}_{10}\text{N}_2$

Guiblin, N., Fuhrer, C. A., Häner, R., Stoeckli-Evans, H., Schenk, K. & Chapuis, G. (2006).  
*Acta Cryst.* **B62**, 506–512.

*The incommensurately modulated structure of a tricyclic natural-product-like compound of empirical formula  $\text{C}_{22}\text{H}_{20}\text{O}_3$*   
 $\text{C}_{22}\text{H}_{20}\text{O}_3$

Schönleber A. & Chapuis, G. (2004). *Acta Cryst.* **B60**, 108-120.

*Quininium (*R*)-mandelate, a structure with large Z' described as an incommensurately modulated structure in (3+1)-dimensional superspace*

$\text{C}_{20}\text{H}_{25}\text{N}_2\text{O}_2^+ \cdot \text{C}_8\text{H}_7\text{O}_3^-$

(solved in superspace approximations with  $Z' = 15$  and 18).

Bussien Gaillard, V., Chapuis, G., Dusek, M. & Petříček, V. (1998). *Acta Cryst.* **A54**, 31-43.  
*Hexamethylenetetramine Sebacate, an Incommensurate Structure with Large Nonsinusoidal Modulations: Comparison of Two Refinement Strategies*

$\text{C}_6\text{H}_{12}\text{N}_4 \cdot \text{C}_{10}\text{H}_{14}\text{O}$

Bussien Gaillard, V., Paciorek, W., Schenk, K. & Chapuis, G. (1996). *Acta Cryst.* **B52**, 1036-1047.

*Hexamethylenetetramine Suberate, a Strongly Anharmonic Modulated Structure*



A commensurate approximation ( $Z' = 1$ ) is archived in the CSD as TIPWAQ/TIPWAQ01 (123 K and RT). For TIPWAQ01 the entry under CCDC Notes is “Minimum, maximum and average bonds given in paper”. The word “incommensurate” does not occur in either entry.

Speziali, N. L. & Chapuis, G. (1991). *Acta Cryst.* **B47**, 757-766.

*Phase Transitions in  $N(\text{CH}_3)_4\text{HSO}_4$ : a Novel Compound with an Incommensurate Phase*



A commensurate approximation ( $Z' = 1$ ) for the structure at 215 K is archived in the CSD as JITNOP01. There is no indication that the structure is incommensurate. (JITNOP and JITNOP02 are the commensurate phases at higher and lower temperatures. Paper says that a full description of the incommensurate structure will be published elsewhere).

Zuñiga, J., Madariaga, G., Paciorek, W. A., Pérez-Mato, J. M., Ezpeleta, J. M. & Etxebarria, I. (1989). *Acta Cryst.* **B45**, 566-576.

*Modulated structure of thiourea*



There are 20 THIOUR $nn$  structures in the CSD but none of them corresponds to this reference.

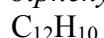
Petříček, V., Coppens, P. & Becker, P. (1985). *Acta Cryst.* **A41**, 478-483.

*Structure analysis of displacively modulated molecular crystals*

(three crystals already in the literature: biphenyl, phenothiazine-TCNQ, and [bis(ethylenedithio)-TTF] $_2\text{I}_3$ )

Baudour, J.L. & Sanquer, M. (1983). *Acta Cryst.* **B39**, 75-84.

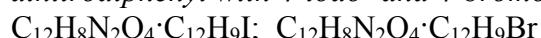
*Structural phase transitions in polyphenyls. VIII. The modulated structure of phase III of biphenyl (T=20K) from neutron diffraction data.*



Average structure in CSD as BIPHEN07. There is no mention of any modulation.

James, R. W.; Saunder, D. H. (1947). Proc. Roy. Soc. A **190**, 518-533.

*Some apparent periodic errors in the crystal lattice of the molecular complexes of 4,4'-dinitrodiphenyl with 4-iodo- and 4-bromodiphenyl*



James, R. W.; Saunder, D. H. (1948). *Acta Cryst.* **1**, 81-83.

*Periodic errors in the crystal lattices of some molecular complexes of 4,4'-dinitrodiphenyl*

