Supporting Information for

Synthesis and crystal structure of 2-(anthracen-9-yl)-1-(*tert*-butyldimethylsilyl)-3,6-dihydro-1λ⁴,2λ⁴-azaborinine

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Abbreviations

ATR	Attenuated total reflection
COSY	Correlation spectroscopy
DFT	Density Functional Theory
ESI	Electrospray ionization
HMBC	Heteronuclear multiple-bond correlation spectroscopy
HR	High resolution
HSQC	Heteronuclear single-quantum correlation spectroscopy
FT-IR	Fourier-transform infrared spectroscopy
m (NMR)	Multiplet (NMR)
NBO	Natural Bond Orbital
NLMO	Natural Localized Molecular Orbital
NMR	Nuclear magnetic resonance
NPA	Natural Population Analysis
s (NMR)	Singlet (NMR)
t (NMR)	Triplet
TMS	Tetramethylsilane

General Methods and Materials

Unless stated otherwise, all syntheses were carried out under standard Schlenk conditions under an atmosphere of nitrogen or argon. If necessary, reactions were carried out in a nitrogen-flushed glovebox from Inert Innovative Technology Inc. or reagents were prepared and stored there. All used glassware was heated under a vacuum below 0.1 mbar and flushed with inert gas at least three times before use. Syringes were flushed with inert gas at least three times before use. NMR tubes were dried in an oven at 110 °C for at least 2 h before use.

NMR Spectroscopy

^{1}H (601 MHz), $^{13}C\{^{1}H\}$ (151 MHz), $^{11}B\{^{1}H\}$ (193 MHz) and $^{29}Si\{^{1}H\}$ (119 MHz) NMR spectra were recorded at 298 K on a Bruker AVANCE NEO 600 spectrometer (Bruker BioSpin, Rheinstetten, Germany). The chemical shifts (δ) are given in parts per million (ppm). NMR spectra were referenced against tetramethylsilane, the residual solvent signals (^{1}H, $CDCl_3$: 7.26 ppm) or the solvent itself ($^{13}C\{^{1}H\}$, $CDCl_3$: 77.16 ppm). The assignment of signals was performed using two-dimensional NMR experiments such as $^{1}H/^{1}H$ COSY, $^{1}H/^{13}C\{^{1}H\}$ HSQC and $^{1}H/^{13}C$ HMBC. The positions of hydrogen and carbon atoms are labelled with numbers to simplify their assignment.

Mass Spectrometry

High-resolution ESI mass spectra were recorded on a Bruker Impact II (Bruker Daltonics, Bremen, Germany).

IR Spectroscopy

IR spectra were recorded on a Thermo Scientific Nicolet FT-IR Spectrometer System spectrometer with an ATR unit, equipped with a diamond window. The resolution was 4 cm^{-1}. The absorption bands are reported in cm^{-1}.

Melting Points

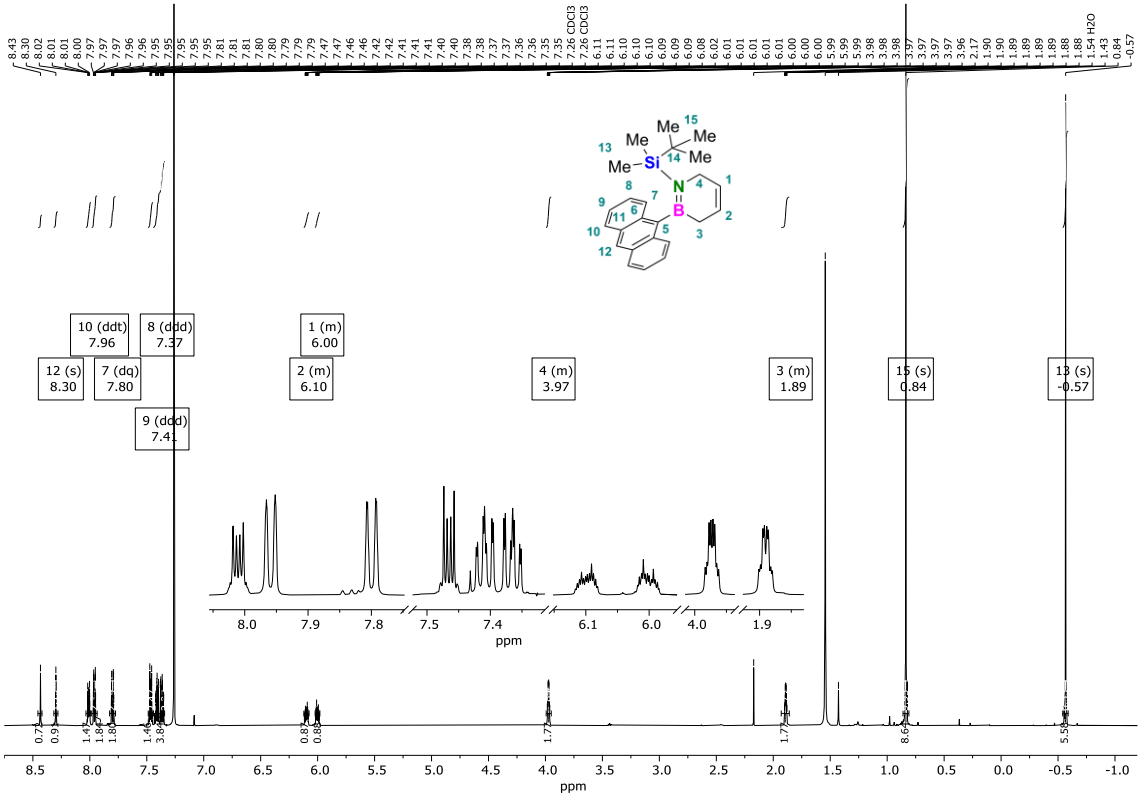
Melting points were measured on a Büchi M-560 Melting Point (Büchi, Flawil, Switzerland) device.

Computational Analysis

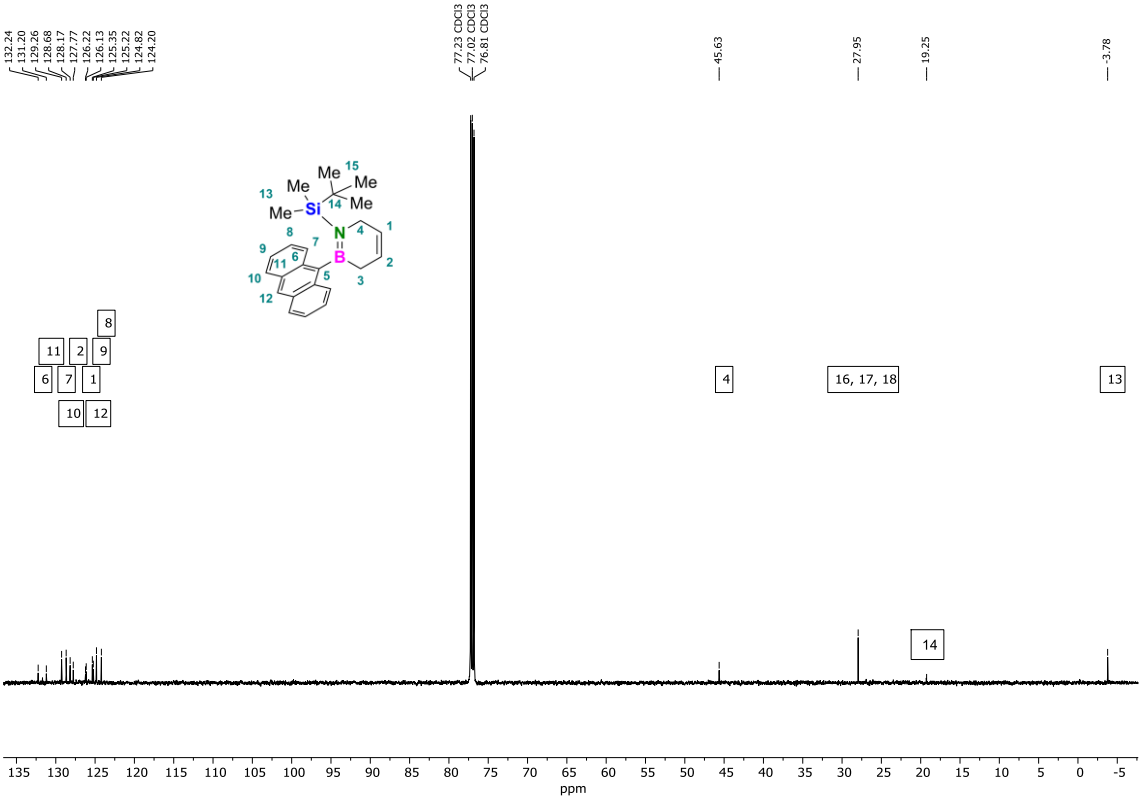
A geometry optimization based on density functional theory (DFT) was performed using Q-Chem 5.4.0 (Epifanovsky et al., 2021). The structure was optimized at the B3LYP/6-31G* level of theory (Becke, 1993; Francl et al., 1982; Hariharan et al., 1973; Hehre et al., 1972; Stephens et al., 1994). A natural bond orbital (NBO) analysis of the optimized structure was performed using the NBO 5.0 program package (Glendening et al., 2001). To determine bond orders, a natural population analysis (NPA) of the calculated natural localized molecular orbitals (NLMOs) was performed.

NMR Spectra

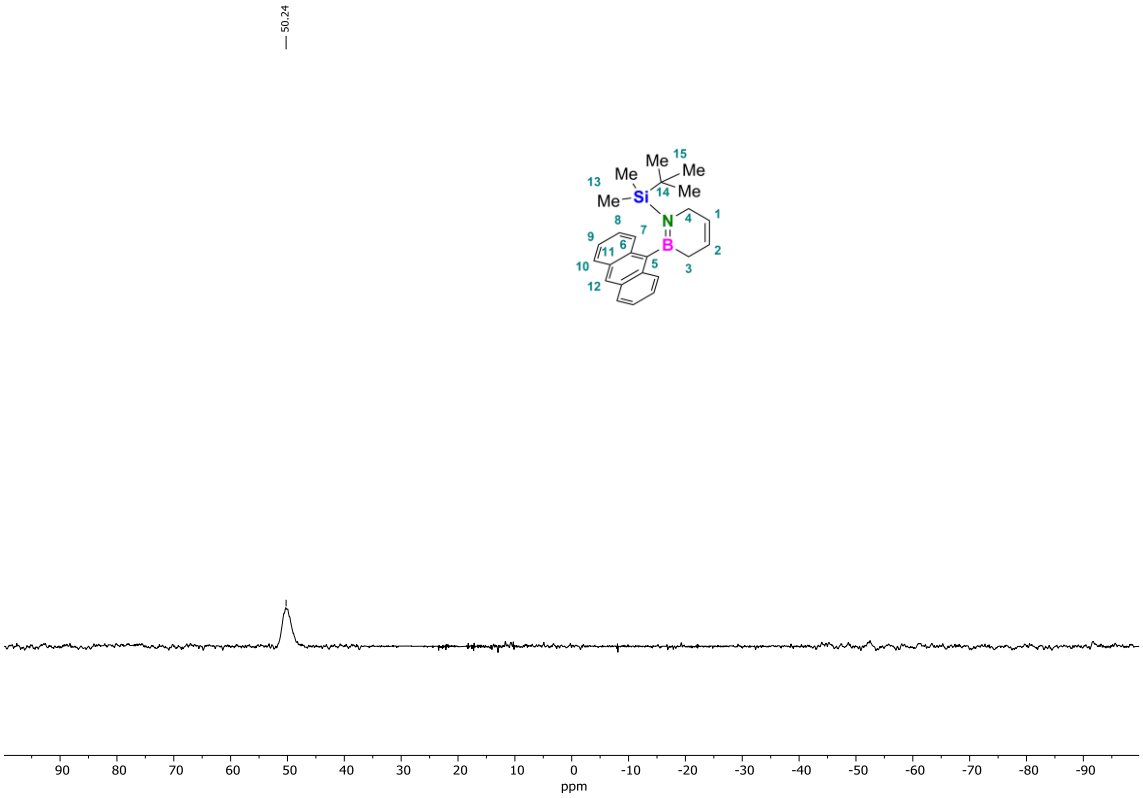
^{1}H NMR [600 MHz, $CDCl_3$, δ (ppm)]:



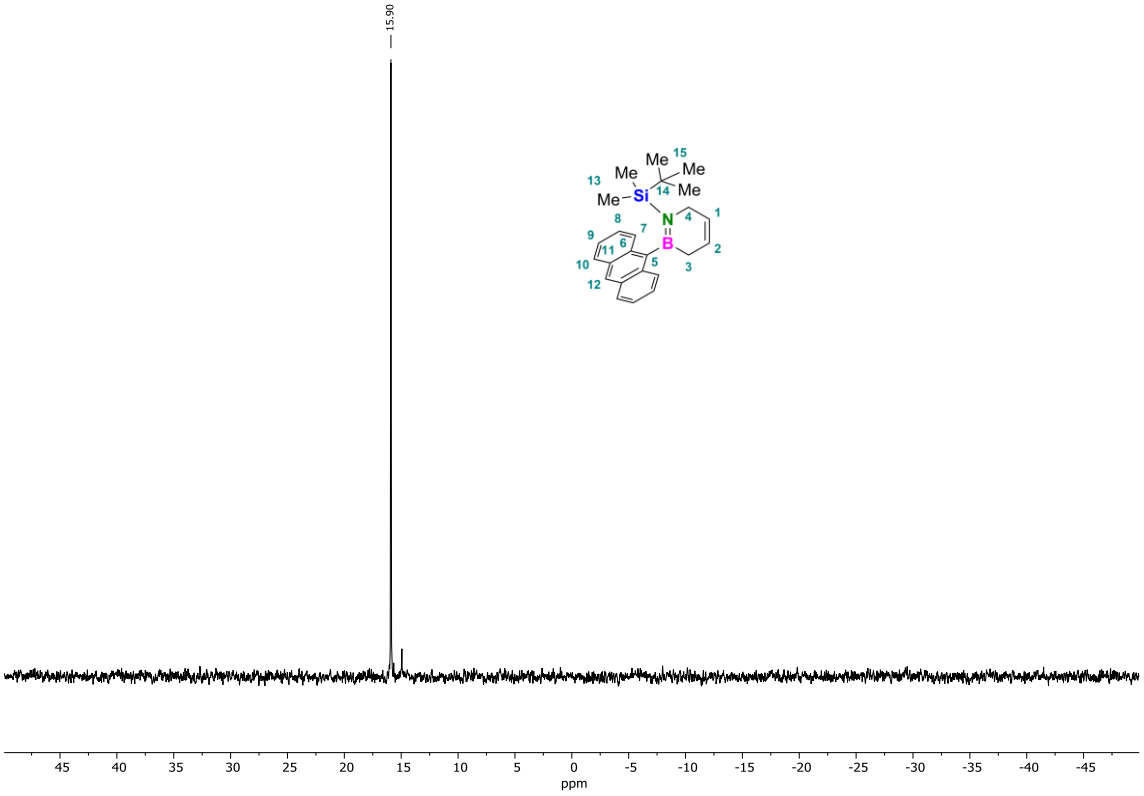
^{13}C{^{1}H} NMR [151 MHz, $CDCl_3$, δ (ppm)]:



$^{11}B\{^{1}H\}$ NMR [160 MHz, $CDCl_3$, δ (ppm)]:



$^{29}Si\{^{1}H\}$ NMR [119 MHz, $CDCl_3$, δ (ppm)]:



Platon Output

PLATON(V-301021)-Run for: gliesep200207_0maP b c a R = 0.04 TIME: sday, 31 August 2023

Crystal Data

Input Cell (Lattice Type: P) - Temp = 100K			Reduced Cell (Acta Cryst.(1976),A32,297-298)			
a = 13.3292(6) Angstrom	alpha =	90 Degree	a = 11.137	alpha =	90.00	V = 4245.0
b = 11.1365(5)	beta =	90	b = 13.329	beta =	90.00	
c = 28.5973(12)	gamma =	90	c = 28.597	gamma =	90.00	
V = 4245.0(3) Cubic-Angstrom	d(100) =	13.3292 Angstrom	Niggli Values			
	d(010) =	11.1365	124.022	177.668	817.806	
Lambda(MoKa) = 0.71073 Angstrom	d(001) =	28.5973	0.000	0.000	0.000	

Orthogonalization Matrices

(See e.g. J.D.Dunitz, Xray Analysis and Structure Determination of Organic Molecules, Cornell Univ. Press, 1979, P236)

$$\begin{pmatrix} XO \\ YO \\ ZO \end{pmatrix} = \begin{pmatrix} 13.32920 & 0 & 0 \\ 0 & 11.13650 & 0 \\ 0 & 0 & 28.59730 \end{pmatrix} \begin{pmatrix} X \\ Y \\ Z \end{pmatrix} , \quad \begin{pmatrix} X \\ Y \\ Z \end{pmatrix} = \begin{pmatrix} 0.07502 & 0 & 0 \\ 0 & 0.08979 & 0 \\ 0 & 0 & 0.03497 \end{pmatrix} \begin{pmatrix} XO \\ YO \\ ZO \end{pmatrix}$$

Orthogonal Axes AO, BO and CO are defined as: AO // A, CO // C*, BO // CO X AO

Space Group Symmetry

(See e.g. G. Burns & A.M. Glazer, Space Groups for Solid State Scientists, Academic Press, 1990 or Int. Tables A)

Space Group H-M: Pbca Laue: mmm
Space Group Hall: -P 2ac 2ab [Schoenflies: D2h^15]
Lattice Type: oP, Centric, Orthorhombic, Multiplicity: 8(4), No: 61

Non-Sohnke - No Absolute Structure

Nr	***** Symmetry Operation(s) *****		
1	X ,	Y ,	Z
2	1/2 - X ,	- Y ,	1/2 + Z
3	1/2 + X ,	1/2 - Y ,	- Z
4	- X ,	1/2 + Y ,	1/2 - Z
5	- X ,	- Y ,	- Z
6	1/2 + X ,	Y ,	1/2 - Z
7	1/2 - X ,	1/2 + Y ,	Z
8	X ,	1/2 - Y ,	1/2 + Z

(1:19-Rule Rounded) Coordinates of Unique Residue(s) Identified. Standard Deviations in the Last Digit are in Parentheses.

```
          Site    = Site Symmetry; SSN = Site Symmetry Number; SSOF = SHELX Site Occupation Factor (= S.O.F / SSN).
*******   Move    = Transformation on Input Data: N.IJK (N = SymOp, IJK = Translation) i.e. 1.555 = nomove
SYMBOLS:  Type    = D/A = Potential Donor or Acceptor atom, D-H = H on Donor atom, MET = Metal.
*******   El Type = AK = Alkali Metal, AE = Alkaline Earth, HL = Halogen, AN = Actinide, LN = Lanthanide, TR = Transition Element.
          ARU     = Asymmetric Residue Unit encoded as sklm.nn, with s = symmetry op, klm = translation, nn = residue #.
          RESIDUE = collection of ARU's constituting an isolated unit (= molecule, ion).
          FLAGS   : d = determined, c = calculated, R = riding G = group
```

Atom Types :	C	H	B	N	Si
Cov.Rad(Ang):	0.68	0.35	0.83	0.68	1.20
Atom Volume :	13.87	5.08	13.24	11.80	37.30
Atom Number :	6	1	5	7	14
Atom Weight :	12.010	1.008	10.81	14.01	28.09
Scat.Fact.f0:	5.999	1.000	4.999	6.995	13.998
Scat.Fact.f':	0.003	0.000	0.001	0.006	0.082
Scat.Fact.f":	0.002	0.000	0.001	0.003	0.070
Mu/Rho(MoKa):	0.58	0.37	0.37	0.84	6.65
Elem. Type :	--	--	--	--	--

Sources - Cov. Radii : Manual Cambridge Crystallographic Data Base
- Atom Volume: D.W.M. Hofmann (2002). Acta Cryst. B58, 489-493
- Atomic Wt. : SHELXL NOMOVE
- Scat. Fact.: SHELXL (International Tables)
- mu/rho : International Tables C, Table 4.2.4.2, 193-199 - [Multiply by Atom Weight and 1.66054 for Barns/atom values]

Flags	Label	Fractional Coordinates (x,y,z)	Orthogonal Coordinates (XO,YO,ZO)	Site	SSN	SSOF	=	S.O.F	Move	Type
d	Si1	0.64414(3) 0.53526(3) 0.67676(2)	8.5859(4) 5.9609(3) 19.3535(6)	1	1	1	=	1	-	-
d	N1	0.59622(8) 0.46229(9) 0.62665(4)	7.9471(11) 5.1483(10) 17.9205(11)	1	1	1	=	1	-	D/A
d	C1	0.48884(10) 0.41613(12) 0.55382(5)	6.5158(13) 4.6342(13) 15.8378(14)	1	1	1	=	1	-	-
d	C2	0.48012(10) 0.29143(12) 0.57271(5)	6.3996(13) 3.2455(13) 16.3780(14)	1	1	1	=	1	-	-
d	C3	0.54188(11) 0.25311(12) 0.60593(5)	7.2228(15) 2.8188(13) 17.3280(14)	1	1	1	=	1	-	-
d	C4	0.62300(10) 0.33186(11) 0.62535(5)	8.3041(13) 3.6958(12) 17.8833(14)	1	1	1	=	1	-	-
d	C5	0.61517(11) 0.69869(12) 0.67683(5)	8.1997(15) 7.7810(13) 19.3555(14)	1	1	1	=	1	-	-
d	C6	0.78352(10) 0.52013(13) 0.67616(6)	10.4437(13) 5.7924(14) 19.3363(17)	1	1	1	=	1	-	-
d	C7	0.58707(11) 0.46528(13) 0.73184(5)	7.8252(15) 5.1816(14) 20.9286(14)	1	1	1	=	1	-	-
d	C8	0.47669(12) 0.43301(16) 0.72304(6)	6.3539(16) 4.8222(18) 20.6770(17)	1	1	1	=	1	-	-
d	C9	0.64271(14) 0.35359(15) 0.74992(6)	8.5668(19) 3.9378(17) 21.4457(17)	1	1	1	=	1	-	-
d	C10	0.59141(18) 0.55923(17) 0.77124(6)	7.883(2) 6.2279(19) 22.0554(17)	1	1	1	=	1	-	-
d	C11	0.52126(9) 0.64751(11) 0.58088(4)	6.9480(12) 7.2110(12) 16.6116(11)	1	1	1	=	1	-	-
d	C12	0.59392(9) 0.71475(11) 0.55610(4)	7.9165(12) 7.9598(12) 15.9030(11)	1	1	1	=	1	-	-
d	C13	0.68530(10) 0.66195(12) 0.53987(4)	9.1345(13) 7.3718(13) 15.4388(11)	1	1	1	=	1	-	-
d	C14	0.75406(10) 0.72648(12) 0.51500(5)	10.0510(13) 8.0904(13) 14.7276(14)	1	1	1	=	1	-	-
d	C15	0.73675(11) 0.84979(13) 0.50489(5)	9.8203(15) 9.4637(14) 14.4385(14)	1	1	1	=	1	-	-
d	C16	0.65239(10) 0.90463(12) 0.52065(5)	8.6958(13) 10.0744(13) 14.8892(14)	1	1	1	=	1	-	-
d	C17	0.57825(10) 0.84029(12) 0.54660(5)	7.7076(13) 9.3579(13) 15.6313(14)	1	1	1	=	1	-	-

d	C18	0.49112(10) 0.89607(12) 0.56257(5)	6.5462(13) 9.9791(13) 16.0880(14)	1	1	1	=	1	-	-
d	C19	0.41726(10) 0.83144(12) 0.58633(5)	5.5617(13) 9.2593(13) 16.7675(14)	1	1	1	=	1	-	-
d	C20	0.32658(11) 0.88722(13) 0.60194(5)	4.3530(15) 9.8805(14) 17.2139(14)	1	1	1	=	1	-	-
d	C21	0.25508(11) 0.82314(14) 0.62480(5)	3.4000(15) 9.1669(16) 17.8676(14)	1	1	1	=	1	-	-
d	C22	0.26936(10) 0.69877(14) 0.63369(5)	3.5904(13) 7.7819(16) 18.1218(14)	1	1	1	=	1	-	-
d	C23	0.35484(10) 0.64256(12) 0.61956(5)	4.7297(13) 7.1559(13) 17.7177(14)	1	1	1	=	1	-	-

d	C24	0.43227(9)	0.70565(11)	0.59506(4)	5.7618(12)	7.8585(12)	17.0171(11)	1	1	1	1	-	-
d	B1	0.53820(10)	0.50755(13)	0.58960(5)	7.1738(13)	5.6523(14)	16.8610(14)	1	1	1	1	-	-
cRU	H1A	0.42113	0.44547	0.54535	5.6133	4.9610	15.5954	1	1	1	1	-	-
cRU	H1B	0.52972	0.41418	0.52492	7.0607	4.6125	15.0114	1	1	1	1	-	-
cRU	H2	0.42991	0.23911	0.56084	5.7304	2.6628	16.0384	1	1	1	1	-	-
cRU	H3	0.53448	0.17382	0.61769	7.1243	1.9357	17.6641	1	1	1	1	-	-
cRU	H4A	0.63894	0.30496	0.65749	8.5166	3.3962	18.8026	1	1	1	1	-	-
cRU	H4B	0.68421	0.32166	0.60615	9.1199	3.5821	17.3341	1	1	1	1	-	-
cRU	H5A	0.63998	0.73506	0.64785	8.5304	8.1860	18.5267	1	1	1	1	-	-
cRU	H5B	0.64786	0.73690	0.70368	8.6354	8.2065	20.1235	1	1	1	1	-	-
cRU	H5C	0.54243	0.71021	0.67901	7.2302	7.9092	19.4177	1	1	1	1	-	-
cRU	H6A	0.80167	0.43486	0.67595	10.6856	4.8428	19.3302	1	1	1	1	-	-
cRU	H6B	0.81159	0.55850	0.70409	10.8178	6.2197	20.1350	1	1	1	1	-	-
cRU	H6C	0.81053	0.55910	0.64813	10.8036	6.2264	18.5348	1	1	1	1	-	-
cRU	H8A	0.44050	0.50444	0.71227	5.8714	5.6177	20.3691	1	1	1	1	-	-
cRU	H8B	0.44642	0.40382	0.75213	5.9504	4.4971	21.5089	1	1	1	1	-	-
cRU	H8C	0.47271	0.37019	0.69912	6.3008	4.1226	19.9930	1	1	1	1	-	-
cRU	H9A	0.63560	0.28808	0.72728	8.4721	3.2082	20.7981	1	1	1	1	-	-
cRU	H9B	0.61402	0.32894	0.77997	8.1844	3.6632	22.3052	1	1	1	1	-	-
cRU	H9C	0.71396	0.37255	0.75403	9.5165	4.1489	21.5631	1	1	1	1	-	-
cRU	H10A	0.66097	0.58525	0.77576	8.8102	6.5177	22.1848	1	1	1	1	-	-
cRU	H10B	0.56608	0.52371	0.80028	7.5454	5.8323	22.8860	1	1	1	1	-	-
cRU	H10C	0.54994	0.62855	0.76276	7.3302	6.9999	21.8129	1	1	1	1	-	-
cRU	H13	0.69848	0.57990	0.54657	9.3101	6.4581	15.6305	1	1	1	1	-	-
cRU	H14	0.81381	0.68882	0.50437	10.8474	7.6710	14.4237	1	1	1	1	-	-
cRU	H15	0.78434	0.89383	0.48708	10.4547	9.9542	13.9292	1	1	1	1	-	-
cRU	H16	0.64241	0.98750	0.51429	8.5629	10.9973	14.7074	1	1	1	1	-	-
cRU	H18	0.48185	0.97951	0.55720	6.4227	10.9083	15.9344	1	1	1	1	-	-
cRU	H20	0.31621	0.97033	0.59624	4.2148	10.8061	17.0507	1	1	1	1	-	-
cRU	H21	0.19527	0.86164	0.63489	2.6028	9.5956	18.1562	1	1	1	1	-	-
cRU	H22	0.21889	0.65452	0.64961	2.9177	7.2891	18.5772	1	1	1	1	-	-
cRU	H23	0.36331	0.55955	0.62612	4.8426	6.2314	17.9052	1	1	1	1	-	-

Ordered Structure — Unit Cell Contents (Based on Contents of Atom List, that may be Incomplete)

Resd	Site	X(cen)	Y(cen)	Z(cen)	Mol.Wt	S.O.F	Z	C	H	B	N	Si
1	1	0.550	0.608	0.619	371.39	1	8	24	30	1	1	1
	Unit Cell Weight =				2971.12			192	240	8	8	8
	Calculated Analysis (%) =							77.6	8.1	2.9	3.8	7.6

Moiety_Formula = C24 H30 B N Si

Sum_Formula = C24 H30 B N Si

Formula_Weight = 371.39 [Note: Based on SHELXL2014 Atomic Weights]

Formula_Z = 8

SpaceGroup_Z = 8 ===> Z' = 8 / 8 = 1.000

Calculated Density = 1.1622(1) g cm-3 [= Mg m-3]

F(000) = 1600.0 [1601.11]

mu(MoKa) = 1.19 cm-1 = 0.119 mm-1

** WARNING **
Please Check the Derived Crystal Data.
They may be Incorrect for Disordered,
Incomplete or Polymeric Structures.

Predicted Volume = 4381.0[4298.6] Ang**3, 298[100]K - (D.W.M. Hofmann (2002). Acta Cryst. B58, 489-493)

Note on F000: The first number is a pure electron count, the second number between [] is calculated from f,f' & f"

MOLSYM: Search for (additional) Molecular (Point Group) Symmetry - Hydrogen Atoms Excluded ! - Ordered Residues Only !

For Details on the Molecular Symmetry Determination see: T. Pilati & A. Forni, J.Appl.Cryst. (1998), 31, 503-504 & (2000), 33, 417.

For CSM (i.e. Continuous Symmetry Measure), see: H. Zabrodsky et al. (1993) JACS, 115, 8278-8289

***** Weighting Mode = ATOMIC *****

Resd 1 No Molecular Symmetry Within Tolerance = 0.80 Ang.
Resd 1 No Molecular Symmetry Within Tolerance = 0.80 Ang.

MOLSYM: Search for (additional) Molecular (Point Group) Symmetry - Hydrogen Atoms Excluded ! - Ordered Residues Only !

For Details on the Molecular Symmetry Determination see: T. Pilati & A. Forni, J.Appl.Cryst. (1998), 31, 503-504 & (2000), 33, 417.

For CSM (i.e. Continuous Symmetry Measure), see: H. Zabrodsky et al. (1993) JACS, 115, 8278-8289

***** Weighting Mode = UNIT *****

Resd 1 No Molecular Symmetry Within Tolerance = 0.80 Ang.
Resd 1 No Molecular Symmetry Within Tolerance = 0.80 Ang.

NONSYM Search for Additional (Non)Crystallographic Symmetry between Residues (Experimental)

- Residue numbers with opposite signs indicate potential enantiomeric pairs
- Hydrogen atoms omitted from the analysis
- Only residues with more than 6 atoms are analysed

RES#	Coords Center of Gravity			Main axes (hor)			EigenV	Asym	Angle a,b,c		
1	0.5487	0.6126	0.6168	0.425	0.642	0.638	3324	35.96	65	50	50
	7.3134	6.8220	17.6376	-0.892	0.177	0.417	2856	45.41	153	80	65
	Res.Mol.Wt. =	341.15		0.154	-0.746	0.648	1832	47.49	81	138	50

(An)isotropic, Equivalent and Main Axes Displacement Parameters - Unusual Values Marked with a # - [Optional Coordinate Split-up]

Atom	Label	U11 or Uiso	U22	U33	U23	U13	U12	Ueq(sUeq)	U1	U2	U3	U3/U1
1	Si1	0.01541(18)	0.01078(17)	0.01295(17)	-0.00092(13)	-0.00323(13)	-0.00045(13)	0.01305(10)	0.0097	0.0118	0.0176	1.81
		[0.6466	0.5354	0.6764] & [0.6417	0.5352	0.6771]						
2	N1	0.0150(5)	0.0087(5)	0.0127(5)	-0.0003(4)	-0.0005(4)	0.0004(4)	0.0121(3)	0.0087	0.0126	0.0151	1.75
		[0.5985	0.4625	0.6265] & [0.5940	0.4621	0.6268]						
3	C1	0.0204(7)	0.0136(6)	0.0152(6)	0.0009(5)	-0.0034(5)	-0.0005(5)	0.0164(4)	0.0129	0.0141	0.0222	1.71
		[0.4914	0.4157	0.5535] & [0.4863	0.4165	0.5541]						
4	C2	0.0200(7)	0.0127(6)	0.0224(7)	-0.0027(5)	-0.0023(5)	-0.0042(5)	0.0184(4)	0.0099	0.0215	0.0238	2.42
		[0.4769	0.2912	0.5739] & [0.4833	0.2916	0.5715]						
5	C3	0.0249(7)	0.0088(6)	0.0221(7)	0.0007(5)	-0.0014(5)	-0.0019(5)	0.0186(4)	0.0086	0.0215	0.0257	3.01
		[0.5468	0.2522	0.6055] & [0.5369	0.2540	0.6064]						
6	C4	0.0204(7)	0.0097(6)	0.0164(6)	-0.0009(5)	-0.0047(5)	0.0031(5)	0.0155(4)	0.0088	0.0135	0.0242	2.73
		[0.6272	0.3334	0.6248] & [0.6188	0.3303	0.6259]						
7	C5	0.0262(7)	0.0131(6)	0.0190(7)	-0.0036(5)	-0.0063(6)	-0.0001(5)	0.0194(4)	0.0108	0.0175	0.0300	2.79
		[0.6201	0.6996	0.6762] & [0.6102	0.6978	0.6775]						
8	C6	0.0174(7)	0.0185(7)	0.0349(8)	0.0005(6)	-0.0076(6)	-0.0013(5)	0.0236(4)	0.0143	0.0187	0.0378	2.64
		[0.7800	0.5208	0.6782] & [0.7870	0.5194	0.6741]						
9	C7	0.0302(8)	0.0196(7)	0.0125(6)	0.0005(5)	0.0000(5)	0.0011(6)	0.0208(4)	0.0125	0.0195	0.0303	2.43
		[0.5917	0.4660	0.7318] & [0.5824	0.4646	0.7318]						
10	C8	0.0264(8)	0.0412(10)	0.0256(8)	0.0085(7)	0.0092(6)	-0.0016(7)	0.0311(5)	0.0147	0.0332	0.0453	3.07
		[0.4776	0.4410	0.7237] & [0.4758	0.4250	0.7224]						
11	C9	0.0447(10)	0.0350(9)	0.0238(8)	0.0144(7)	0.0028(7)	0.0081(8)	0.0345(5)	0.0138	0.0366	0.0531	3.86
		[0.6485	0.3608	0.7506] & [0.6369	0.3464	0.7493]						
12	C10	0.0817(15)	0.0363(10)	0.0165(8)	-0.0064(7)	0.0059(9)	-0.0084(10)	0.0448(7)	0.0144	0.0361	0.0839	5.81
		[0.6038	0.5558	0.7715] & [0.5790	0.5626	0.7710]						
13	C11	0.0138(6)	0.0115(6)	0.0105(6)	-0.0001(5)	-0.0033(4)	-0.0009(5)	0.0119(3)	0.0084	0.0115	0.0160	1.91
		[0.5237	0.6468	0.5806] & [0.5188	0.6482	0.5812]						
14	C12	0.0149(6)	0.0115(6)	0.0114(6)	0.0004(5)	-0.0037(5)	-0.0008(5)	0.0126(3)	0.0091	0.0114	0.0174	1.92
		[0.5965	0.7141	0.5557] & [0.5913	0.7154	0.5565]						
15	C13	0.0177(6)	0.0132(6)	0.0150(6)	-0.0012(5)	-0.0005(5)	-0.0005(5)	0.0153(3)	0.0125	0.0156	0.0178	1.42
		[0.6869	0.6618	0.5398] & [0.6837	0.6621	0.5399]						
16	C14	0.0180(6)	0.0195(7)	0.0171(6)	-0.0027(5)	0.0020(5)	-0.0019(5)	0.0182(4)	0.0151	0.0167	0.0228	1.51
		[0.7530	0.7286	0.5148] & [0.7551	0.7244	0.5152]						
17	C15	0.0210(7)	0.0210(7)	0.0164(6)	0.0030(5)	0.0001(5)	-0.0092(6)	0.0195(4)	0.0109	0.0170	0.0305	2.80
		[0.7401	0.8449	0.5047] & [0.7334	0.8547	0.5050]						
18	C16	0.0212(7)	0.0133(6)	0.0193(7)	0.0046(5)	-0.0053(5)	-0.0048(5)	0.0179(4)	0.0104	0.0149	0.0285	2.75
		[0.6563	0.9014	0.5199] & [0.6485	0.9079	0.5214]						
19	C17	0.0173(6)	0.0122(6)	0.0144(6)	0.0009(5)	-0.0054(5)	-0.0028(5)	0.0146(3)	0.0097	0.0120	0.0222	2.28
		[0.5816	0.8386	0.5461] & [0.5749	0.8419	0.5471]						
20	C18	0.0204(7)	0.0112(6)	0.0187(7)	0.0009(5)	-0.0055(5)	0.0011(5)	0.0168(4)	0.0106	0.0146	0.0251	2.37
		[0.4950	0.8962	0.5619] & [0.4873	0.8959	0.5633]						
21	C19	0.0156(6)	0.0136(6)	0.0154(6)	-0.0010(5)	-0.0050(5)	0.0021(5)	0.0149(3)	0.0103	0.0132	0.0211	2.05

		[0.4200	0.8330	0.5858] & [0.4145	0.8298	0.5869]						
22	C20	0.0209(7)	0.0173(7)	0.0219(7)	-0.0020(5)	-0.0035(5)	0.0061(5)	0.0200(4)	0.0127	0.0193	0.0281	2.21
		[0.3296	0.8903	0.6014] & [0.3236	0.8841	0.6025]						
23	C21	0.0168(7)	0.0256(7)	0.0238(7)	-0.0042(6)	0.0002(6)	0.0059(6)	0.0221(4)	0.0134	0.0222	0.0306	2.29
		[0.2565	0.8280	0.6244] & [0.2536	0.8182	0.6252]						
24	C22	0.0160(7)	0.0259(7)	0.0202(7)	-0.0003(6)	0.0014(5)	-0.0021(6)	0.0207(4)	0.0152	0.0205	0.0264	1.73
		[0.2688	0.7022	0.6336] & [0.2699	0.6953	0.6337]						
25	C23	0.0177(6)	0.0159(6)	0.0162(6)	0.0008(5)	-0.0013(5)	-0.0014(5)	0.0166(3)	0.0151	0.0154	0.0192	1.27
		[0.3558	0.6418	0.6194] & [0.3539	0.6433	0.6197]						
26	C24	0.0136(6)	0.0130(6)	0.0126(6)	-0.0005(5)	-0.0036(5)	0.0001(5)	0.0131(3)	0.0094	0.0130	0.0168	1.78
		[0.4345	0.7061	0.5946] & [0.4300	0.7052	0.5955]						
27	B1	0.0116(6)	0.0116(6)	0.0124(6)	0.0005(5)	0.0016(5)	-0.0003(5)	0.0119(3)	0.0101	0.0118	0.0137	1.35
		[0.5392	0.5078	0.5899] & [0.5372	0.5073	0.5893]						
28	H1A	0.02000						0.02000				
29	H1B	0.02000						0.02000				
30	H2	0.02200						0.02200				
31	H3	0.02200						0.02200				
32	H4A	0.01900						0.01900				
33	H4B	0.01900						0.01900				
34	H5A	0.02900						0.02900				
35	H5B	0.02900						0.02900				
36	H5C	0.02900						0.02900				
37	H6A	0.03500						0.03500				
38	H6B	0.03500						0.03500				
39	H6C	0.03500						0.03500				
40	H8A	0.04700						0.04700				
41	H8B	0.04700						0.04700				
42	H8C	0.04700						0.04700				
43	H9A	0.05200						0.05200				
44	H9B	0.05200						0.05200				
45	H9C	0.05200						0.05200				
46	H10A	0.06700						0.06700				
47	H10B	0.06700						0.06700				
48	H10C	0.06700						0.06700				
49	H13	0.01800						0.01800				
50	H14	0.02200						0.02200				
51	H15	0.02300						0.02300				
52	H16	0.02200						0.02200				
53	H18	0.02000						0.02000				
54	H20	0.02400						0.02400				
55	H21	0.02700						0.02700				
56	H22	0.02500						0.02500				
57	H23	0.02000						0.02000				
U(i,j)-Average		0.0222	0.0172	0.0178	0.0004	-0.0016	-0.0006	0.0190	0.0170	0.0174	0.0228	1.34

==========

The Displacement Factor has the Form of Exp(-T)

where

T = 8*(pi**2)*Uiso*sin(theta/lambda)**2, for Isotropic Atoms,

T = 2*(pi**2)*(U11*(h*as)**2+U22*(k*bs)**2+U33*(l*cs)**2+2*U23*k*l*bs*cs+2*U13*h*l*as*cs+2*U12*h*k*as*bs),for Anisotr. Atoms

Ueq = 1/3 Sum(i,j) (Uij*as(i)*as(j)*a(i).a(j))

U1, U2, U3 are the three Main Axes Components of Uij

Reference U(eq): R.X. Fischer & E. Tillmanns, Acta Cryst. (1988). C44, 775-776

Ueq [or U(iso)] Averages per Element

	Non-H	C	H	B	N	Si
Average	0.0191	0.0199	0.0338	0.0119	0.0121	0.0131
Minimum	0.0119	0.0119	0.0180	0.0119	0.0121	0.0131

```
Maximum  0.0448 0.0448 0.0670 0.0119 0.0121 0.0131
Ratio    3.7647 3.7647 3.7222 1.0000 1.0000 1.0000
Number       27     24     30      1      1      1
```


V.Schomaker and K.N.Trueblood Rigid Body Motion Analysis, TLS - Model (Acta Cryst. (1968), B24, 63-76) - see also Dunitz, p244

Observed Vibration Tensor in Inertial System I(1) = L, I(2) = M, I(3) = N (Difference U(calc) - U(obs) in Parentheses)

Label	U(L,L)	U(L,M)	U(L,N)	U(M,M)	U(M,N)	U(N,N)	Ueq(obs)	Ueq(cal)
	U11	U12	U13	U22	U23	U33		
Si1	0.01215[0.00171]	-0.00147[0.00116]	-0.00015[0.00418]	0.01724[0.00733]	-0.00004[-.00151]	0.00975[0.00507]	0.0130	0.0178
	0.01541[0.00770]	-0.00045[0.00088]	-0.00323[-.00155]	0.01078[0.00724]	-0.00092[0.00170]	0.01295[-.00083]		
N1	0.01063[0.00168]	-0.00080[0.00131]	-0.00181[0.00155]	0.01460[0.00246]	-0.00144[0.00097]	0.01117[0.00153]	0.0121	0.0140
	0.01500[0.00169]	0.00040[-.00121]	-0.00050[-.00062]	0.00870[0.00370]	-0.00030[0.00071]	0.01270[0.00028]		
C1	0.01300[0.00395]	-0.00072[0.00099]	0.00011[-.00302]	0.02210[-.00301]	-0.00023[0.00034]	0.01410[-.00529]	0.0164	0.0149
	0.02040[-.00285]	-0.00050[-.00294]	-0.00340[0.00158]	0.01360[-.00263]	0.00090[-.00415]	0.01520[0.00113]		
C2	0.02006[-.00063]	-0.00041[-.00011]	-0.00471[-.00221]	0.02282[0.00044]	0.00177[-.00006]	0.01222[0.00177]	0.0184	0.0189
	0.02000[0.00096]	-0.00420[0.00011]	-0.00230[0.00105]	0.01270[-.00177]	-0.00270[0.00088]	0.02240[0.00239]		
C3	0.01424[0.00256]	-0.00064[0.00002]	-0.00640[-.00083]	0.02565[-.00236]	-0.00081[0.00223]	0.01591[0.00327]	0.0186	0.0198
	0.02490[-.00280]	-0.00190[-.00034]	-0.00140[0.00147]	0.00880[0.00241]	0.00070[0.00073]	0.02210[0.00386]		
C4	0.01198[0.00170]	-0.00507[0.00410]	-0.00109[-.00216]	0.02175[-.00123]	-0.00232[0.00278]	0.01277[0.00535]	0.0155	0.0174
	0.02040[-.00067]	0.00310[-.00323]	-0.00470[0.00390]	0.00970[0.00276]	-0.00090[0.00301]	0.01640[0.00373]		
C5	0.01813[-.00056]	-0.00366[0.00253]	-0.00118[0.00568]	0.02872[-.00258]	-0.00225[-.00168]	0.01145[-.00131]	0.0194	0.0179
	0.02620[-.00107]	-0.00010[0.00044]	-0.00630[0.00038]	0.01310[0.00479]	-0.00360[-.00026]	0.01900[-.00817]		
C6	0.02365[-.00648]	-0.00748[0.00191]	-0.00412[0.00780]	0.02660[0.00432]	0.00859[-.00435]	0.02055[-.00267]	0.0236	0.0220
	0.01740[0.00560]	-0.00130[0.00188]	-0.00760[-.00321]	0.01850[0.00242]	0.00050[0.00155]	0.03490[-.01284]		
C7	0.01614[-.00028]	0.00271[0.00114]	0.00251[0.00487]	0.02652[0.00750]	-0.00626[0.00057]	0.01964[0.00840]	0.0208	0.0260
	0.03020[0.00672]	0.00110[0.00114]	0.00000[-.00199]	0.01960[0.00863]	0.00050[0.00486]	0.01250[0.00027]		
C8	0.02830[-.01107]	0.00967[-.00199]	0.00414[-.00079]	0.02165[0.00594]	0.00189[-.00759]	0.04325[-.00909]	0.0311	0.0263
	0.02640[0.00813]	-0.00160[0.00283]	0.00920[-.00353]	0.04120[-.01273]	0.00850[-.00126]	0.02560[-.00962]		
C9	0.01531[-.00099]	0.00301[-.00050]	0.00559[0.00236]	0.03826[0.00557]	-0.00630[0.00344]	0.04993[-.01281]	0.0345	0.0318
	0.04470[-.00097]	0.00810[-.00511]	0.00280[-.00813]	0.03500[-.00275]	0.01440[-.00301]	0.02380[-.00452]		
C10	0.03838[-.01528]	0.01918[-.01464]	0.00077[0.01254]	0.06629[-.02057]	-0.02306[0.01087]	0.02983[0.00124]	0.0448	0.0333
	0.08170[-.03042]	-0.00840[0.01283]	0.00590[-.01001]	0.03630[0.00197]	-0.00640[0.00840]	0.01650[-.00617]		
C11	0.01078[0.00170]	-0.00050[0.00097]	0.00129[-.00093]	0.01588[-.00105]	0.00056[-.00118]	0.00914[-.00230]	0.0119	0.0114
	0.01380[0.00007]	-0.00090[-.00095]	-0.00330[0.00124]	0.01150[-.00093]	-0.00010[-.00216]	0.01050[-.00079]		
C12	0.01060[0.00184]	-0.00077[0.00177]	0.00105[-.00097]	0.01725[-.00070]	0.00068[-.00050]	0.00996[-.00261]	0.0126	0.0121
	0.01490[0.00001]	-0.00080[-.00200]	-0.00370[0.00120]	0.01150[-.00064]	0.00040[-.00191]	0.01140[-.00083]		
C13	0.01524[-.00030]	-0.00001[0.00229]	-0.00103[0.00009]	0.01744[-.00169]	-0.00124[0.00164]	0.01322[-.00153]	0.0153	0.0141
	0.01770[-.00225]	-0.00050[-.00250]	-0.00050[0.00068]	0.01320[0.00021]	-0.00120[0.00047]	0.01500[-.00148]		
C14	0.02190[-.00337]	0.00225[0.00220]	-0.00024[-.00248]	0.01661[0.00159]	-0.00093[0.00314]	0.01609[0.00372]	0.0182	0.0188
	0.01800[0.00041]	-0.00190[-.00247]	0.00200[0.00091]	0.01950[-.00138]	-0.00270[0.00474]	0.01710[0.00291]		
C15	0.01831[-.00073]	0.00825[-.00302]	0.00004[-.00381]	0.02347[0.00049]	0.00445[0.00020]	0.01661[0.00553]	0.0195	0.0212
	0.02100[0.00090]	-0.00920[0.00267]	0.00010[0.00105]	0.02100[-.00252]	0.00300[0.00190]	0.01640[0.00691]		
C16	0.01160[0.00275]	0.00098[0.00114]	-0.00179[-.00117]	0.02675[-.00069]	0.00481[-.00072]	0.01544[0.00029]	0.0179	0.0187
	0.02120[0.00059]	-0.00480[-.00082]	-0.00530[0.00192]	0.01330[0.00065]	0.00460[-.00138]	0.01930[0.00112]		
C17	0.01194[0.00089]	-0.00055[0.00055]	0.00022[-.00111]	0.02167[-.00036]	0.00250[-.00105]	0.01030[-.00114]	0.0146	0.0144
	0.01730[0.00062]	-0.00280[-.00046]	-0.00540[0.00102]	0.01220[-.00114]	0.00090[-.00128]	0.01440[-.00009]		
C18	0.01234[0.00217]	-0.00416[0.00097]	-0.00135[-.00003]	0.02369[-.00055]	0.00045[0.00011]	0.01427[-.00445]	0.0168	0.0158
	0.02040[-.00100]	0.00110[-.00211]	-0.00550[-.00032]	0.01120[-.00039]	0.00090[-.00268]	0.01870[-.00143]		

C19	0.01389[0.00285]	-0.00443[0.00082]	0.00139[-.00226]	0.01841[0.00075]	0.00026[-.00118]	0.01231[-.00107]	0.0149	0.0157
	0.01560[0.00189]	0.00210[-.00121]	-0.00500[0.00144]	0.01360[-.00104]	-0.00100[-.00218]	0.01540[0.00169]		
C20	0.01914[0.00441]	-0.00716[0.00017]	0.00038[-.00318]	0.02134[-.00063]	-0.00256[0.00065]	0.01962[-.00020]	0.0200	0.0212
	0.02090[-.00047]	0.00610[-.00160]	-0.00350[0.00164]	0.01730[-.00049]	-0.00200[-.00217]	0.02190[0.00454]		
C21	0.02738[0.00197]	-0.00553[-.00036]	0.00228[-.00611]	0.01566[0.00181]	-0.00175[-.00038]	0.02316[0.00504]	0.0221	0.0250
	0.01680[0.00338]	0.00590[-.00003]	0.00020[0.00314]	0.02560[-.00280]	-0.00420[0.00066]	0.02380[0.00823]		
C22	0.02433[0.00219]	0.00229[-.00380]	0.00200[-.00523]	0.01662[-.00185]	0.00262[-.00333]	0.02115[0.00627]	0.0207	0.0229
	0.01600[0.00188]	-0.00210[0.00490]	0.00140[0.00392]	0.02590[-.00303]	-0.00030[-.00096]	0.02020[0.00776]		
C23	0.01536[0.00378]	0.00063[-.00060]	-0.00001[-.00141]	0.01891[-.00445]	0.00091[-.00131]	0.01553[0.00189]	0.0166	0.0170
	0.01770[-.00209]	-0.00140[0.00154]	-0.00130[0.00328]	0.01590[0.00093]	0.00080[-.00208]	0.01620[0.00238]		
C24	0.01259[0.00248]	-0.00182[0.00093]	0.00146[-.00153]	0.01598[-.00053]	0.00084[-.00166]	0.01064[-.00071]	0.0131	0.0135
	0.01360[0.00123]	0.00010[-.00055]	-0.00360[0.00195]	0.01300[-.00052]	-0.00050[-.00207]	0.01260[0.00054]		
B1	0.01184[0.00103]	0.00091[0.00004]	-0.00096[0.00016]	0.01072[0.00404]	-0.00008[-.00044]	0.01304[-.00420]	0.0119	0.0122
	0.01160[0.00280]	-0.00030[-.00168]	0.00160[-.00240]	0.01160[-.00097]	0.00050[-.00207]	0.01240[-.00096]		

```
R1 = Sum(abs(U(obs)-U(calc)))/Sum(abs(U(obs)))     =   0.25200

R2 = Sqrt(Sum((U(obs)-U(calc))**2)/Sum(U(obs)**2)) =   0.27102

S  = Sqrt(Sum((U(obs)-U(calc))**2)/(6*N-NS*M))     =   0.00444

N  = Number of Atoms in Rigid Group                =        27

NS = Symmetry Factor                               =         1

M  = Number of Rigid-Body Parameters               =        20

     Largest abs(U(obs)-U(calc))                   =   0.02057

                                                    TLS-Mode
```

:: No TLS-Analysis for Residue Nr: 1, Because R > 0.25

Rigid-Body Model Libration Corrections for Bond Distances and "Hirshfeld Rigid-Bond" Test (Acta Cryst., 1976, A32, 239-244)

Bond		Bond Distance	Components of the Correction				MSDA from U(obs) Vibration Along the Interatomic Bond				Angle with Lib. Axes		
Atom(I)	Atom(J)	Obsd	Calcd	Del(L)	Del(M)	Del(N)	I to J	J to I	Difference	Sqrt(Diff)	L(1)	L(2)	L(3)
Si1	- N1	1.7669(12)	0	0	0	0	0.01008(17)	0.0118(5)	0.0017(5)	0.0412	0.00	0.00	0.00
Si1	- C5	1.8606(14)	0	0	0	0	0.01116(17)	0.0137(7)	0.0025(7)	0.0500	0.00	0.00	0.00
Si1	- C6	1.8655(14)	0	0	0	0	0.01551(17)	0.0178(7)	0.0023(8)	0.0480	0.00	0.00	0.00
Si1	- C7	1.9150(15)	0	0	0	0	0.01556(17)	0.0165(7)	0.0009(7)	0.0300	0.00	0.00	0.00
N1	- C4	1.4962(16)	0	0	0	0	0.0089(5)	0.0089(6)	0.0000(8)	0	0.00	0.00	0.00
N1	- B1	1.4053(18)	0	0	0	0	0.0125(5)	0.0132(6)	0.0007(8)	0.0265	0.00	0.00	0.00
C1	- C2	1.4946(19)	0	0	0	0	0.0134(6)	0.0154(7)	0.0020(9)	0.0447	0.00	0.00	0.00
C1	- B1	1.586(2)	0	0	0	0	0.0141(6)	0.0131(6)	0.0010(9)	0.0316	0.00	0.00	0.00
C2	- C3	1.328(2)	0	0	0	0	0.0213(7)	0.0210(7)	0.0003(9)	0.0173	0.00	0.00	0.00
C3	- C4	1.4989(19)	0	0	0	0	0.0170(7)	0.0159(6)	0.0011(9)	0.0332	0.00	0.00	0.00
C7	- C8	1.535(2)	0	0	0	0	0.0297(7)	0.0300(9)	0.0003(11)	0.0173	0.00	0.00	0.00
C7	- C9	1.538(2)	0	0	0	0	0.0201(7)	0.0227(9)	0.0026(11)	0.0510	0.00	0.00	0.00
C7	- C10	1.539(2)	0	0	0	0	0.0164(7)	0.0193(11)	0.0029(13)	0.0539	0.00	0.00	0.00
C11	- C12	1.4145(17)	0	0	0	0	0.0140(6)	0.0148(6)	0.0008(8)	0.0283	0.00	0.00	0.00
C11	- C24	1.4109(17)	0	0	0	0	0.0153(6)	0.0149(6)	0.0004(8)	0.0200	0.00	0.00	0.00
C11	- B1	1.5946(19)	0	0	0	0	0.0117(6)	0.0116(6)	0.0001(8)	0.0100	0.00	0.00	0.00
C12	- C13	1.4300(18)	0	0	0	0	0.0167(6)	0.0170(6)	0.0003(8)	0.0173	0.00	0.00	0.00

C12 - C17	1.4395(18)	0	0	0	0	0.0114(6)	0.0126(6)	0.0012(8)	0.0346	0.00	0.00	0.00
C13 - C14	1.3647(19)	0	0	0	0	0.0164(6)	0.0169(6)	0.0005(9)	0.0224	0.00	0.00	0.00
C14 - C15	1.422(2)	0	0	0	0	0.0212(6)	0.0225(7)	0.0013(9)	0.0361	0.00	0.00	0.00
C15 - C16	1.357(2)	0	0	0	0	0.0282(7)	0.0273(7)	0.0009(9)	0.0300	0.00	0.00	0.00
C16 - C17	1.4285(19)	0	0	0	0	0.0168(7)	0.0167(6)	0.0001(9)	0.0100	0.00	0.00	0.00
C17 - C18	1.3940(19)	0	0	0	0	0.0213(6)	0.0208(7)	0.0005(9)	0.0224	0.00	0.00	0.00
C18 - C19	1.3961(19)	0	0	0	0	0.0217(7)	0.0205(6)	0.0012(9)	0.0346	0.00	0.00	0.00
C19 - C20	1.430(2)	0	0	0	0	0.0160(6)	0.0172(7)	0.0012(9)	0.0346	0.00	0.00	0.00
C19 - C24	1.4369(18)	0	0	0	0	0.0132(6)	0.0130(6)	0.0002(8)	0.0141	0.00	0.00	0.00
C20 - C21	1.358(2)	0	0	0	0	0.0280(7)	0.0272(7)	0.0008(10)	0.0283	0.00	0.00	0.00
C21 - C22	1.421(2)	0	0	0	0	0.0253(7)	0.0263(7)	0.0010(10)	0.0316	0.00	0.00	0.00
C22 - C23	1.3614(19)	0	0	0	0	0.0193(7)	0.0191(6)	0.0002(9)	0.0141	0.00	0.00	0.00
C23 - C24	1.4317(18)	0	0	0	0	0.0165(6)	0.0161(6)	0.0004(8)	0.0200	0.00	0.00	0.00

Sqrt(Sum(DelIJ**2)/Nrb) = 0.0013

- Indicates bonds exceeding the 5.0 sigma test level

Test Matrix for Rigid-Body Vibrations - /Del(A,B)/ = /Z(A,B)**2 - Z(B,A)**2/ Should be Near Zero (Acta Cryst. A34, 1978, 828)

Atom-Atom	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27
1 Si1 -	0	-2	4	3	3	1	-3	-2	-1	1	2	3	2	2	2	3	1	1	0	0	1	1	2	5	4	1	3
2 N1 -	-2	0	1	0	1	0	2	1	0	3	5	2	1	1	4	6	1	0	2	1	2	2	3	7	5	1	-1
3 C1 -	4	3	0	-2	2	2	3	3	0	10	11	5	3	3	2	0	4	4	3	2	2	2	2	2	0	2	-1
4 C2 -	5	3	-1	0	0	2	0	3	2	13	14	3	0	0	2	4	1	2	1	2	1	1	0	6	1	1	2
5 C3 -	4	3	2	-1	0	-1	0	0	3	13	15	0	2	2	3	6	2	1	3	1	2	1	3	7	3	2	2
6 C4 -	3	-1	3	2	-1	0	2	1	1	5	11	2	2	0	0	3	1	2	2	1	3	3	4	9	6	3	3
7 C5 -	-2	3	5	6	5	4	0	1	1	5	3	4	6	8	6	9	11	7	7	5	7	5	6	6	3	7	2
8 C6 -	-2	3	5	6	5	3	3	0	2	3	2	7	7	11	12	10	11	11	9	7	6	3	2	2	2	5	3
9 C7 -	-2	3	5	5	4	3	3	3	0	0	-3	-3	4	3	2	3	3	2	2	3	5	4	2	1	4	5	0
10 C8 -	3	3	5	5	4	4	4	4	-2	0	3	0	9	6	0	2	5	7	8	12	14	15	12	9	14	13	8
11 C9 -	3	4	6	6	4	4	4	3	-2	3	0	2	5	3	1	3	2	3	2	4	5	5	4	3	7	6	5
12 C10 -	3	4	7	7	6	5	3	4	-2	2	2	0	14	10	3	4	10	10	13	19	28	35	41	41	32	25	5
13 C11 -	3	3	3	4	4	4	3	5	5	5	6	6	0	-1	2	1	2	1	0	1	1	1	2	1	3	0	0
14 C12 -	4	3	4	5	5	5	3	5	6	6	7	6	-1	0	0	1	3	1	-1	0	1	0	2	1	1	1	1
15 C13 -	4	4	4	5	5	4	4	4	6	6	7	7	2	-1	0	-1	1	1	2	1	1	0	3	2	1	1	6
16 C14 -	5	5	5	6	7	6	5	5	7	8	8	8	4	2	-1	0	-1	1	3	3	1	3	0	0	2	0	7
17 C15 -	6	6	6	7	8	7	5	6	8	9	9	8	4	3	2	-1	0	-1	2	1	1	2	0	0	4	2	1
18 C16 -	6	6	6	7	8	7	5	6	8	8	9	8	4	2	3	2	-1	0	0	0	1	0	3	3	0	0	0
19 C17 -	5	5	5	6	7	6	4	6	7	7	8	7	2	-1	2	3	2	-1	0	0	1	0	2	3	0	0	1
20 C18 -	6	5	5	7	7	7	4	7	7	7	8	7	3	2	4	4	4	2	-1	0	-1	0	3	4	2	0	1
21 C19 -	5	5	5	6	7	6	4	7	6	6	8	7	2	3	4	5	5	4	2	-1	0	-1	1	3	2	0	0
22 C20 -	6	6	6	7	8	7	5	8	7	6	8	7	4	4	6	6	6	5	4	2	-1	0	-1	1	0	0	1
23 C21 -	6	6	6	7	7	7	5	8	7	6	8	7	4	5	6	7	7	6	5	4	2	-1	0	-1	1	1	3
24 C22 -	5	5	5	6	6	6	5	7	6	5	7	6	4	5	6	7	7	6	5	4	3	2	-1	0	0	1	8
25 C23 -	4	4	4	4	5	5	4	6	5	4	6	5	2	4	5	6	6	6	4	4	2	3	2	-1	0	0	8
26 C24 -	4	4	4	5	5	5	3	6	5	5	7	6	-1	2	4	5	5	4	3	2	-1	2	3	2	-1	0	1
27 B1 -	3	-1	-2	3	3	2	3	4	4	4	5	5	-2	3	3	4	5	5	4	4	4	5	5	4	3	3	0

Remarks

- Upper Triangle Entries Represent /Del(A,B)/*1000 Values

- Lower Triangle Entries Represent Distances (A-B) Angstrom

- Negative Entries Indicate Bonded Atoms

Analysis of Bond Distance and Angle Values - Identification of Chiral Center(s) and Their (R/S)-Configuration (Cahn-Ingold-Prelog)

The Following Tests are done. Faults are Marked Under Note
-- V : Valency Check Fault for H, C
-- S : Bond Too Short
-- A : Unusual Bond Angle Values (PLEASE CHECK)

*** PLEASE NOTE: R/S ASSIGNMENTS ARE TENTATIVE *** (CIP Special rules NOT Implemented)
*** See Angew.Chem.Intern. Ed. Eng.,(1966),5,385 & (1982),21,567 for Authoritative Details for Special Cases

Flag	Label	- Connected to	(May be Incomplete for Polymeric Structures)						=A.N.G.L.E.S= nra	min	max	Aver	=B.O.N.D.S= min	max	nrb	tnr	Hyb	RS	Note
d	Si1	- N1	C5	C6	C7	-------	-------	-------	6	107	112	109.5	1.767	1.915	4	39	sp3		
d	N1	- Si1	C4	B1	-------	-------	-------	-------	3	112	130	120.0	1.405	1.767	3	38	sp2		
d	C1	- C2	B1	H1A	H1B	-------	-------	-------	6	108	113	109.4	0.990	1.586	4	30	sp3		
d	C2	- C1	C3	H2	-------	-------	-------	-------	3	120	121	120.0	0.950	1.495	3	32	sp2		
d	C3	- C2	C4	H3	-------	-------	-------	-------	3	119	122	120.0	0.950	1.499	3	33	sp2		
d	C4	- N1	C3	H4A	H4B	-------	-------	-------	6	108	114	109.4	0.990	1.499	4	35	sp3		
d	C5	- Si1	H5A	H5B	H5C	-------	-------	-------	6	109	109	109.5	0.980	1.861	4	36	sp3		
d	C6	- Si1	H6A	H6B	H6C	-------	-------	-------	6	109	109	109.5	0.980	1.866	4	36	sp3		
d	C7	- Si1	C8	C9	C10	-------	-------	-------	6	107	114	109.4	1.535	1.915	4	37	sp3		
d	C8	- C7	H8A	H8B	H8C	-------	-------	-------	6	109	109	109.5	0.980	1.535	4	34	sp3		
d	C9	- C7	H9A	H9B	H9C	-------	-------	-------	6	109	109	109.5	0.980	1.538	4	34	sp3		
d	C10	- C7	H10A	H10B	H10C	-------	-------	-------	6	109	109	109.5	0.980	1.539	4	34	sp3		
d	C11	- C12	C24	B1	-------	-------	-------	-------	3	118	122	120.0	1.411	1.595	3	28	sp2		
d	C12	- C11	C13	C17	-------	-------	-------	-------	3	117	122	120.0	1.415	1.439	3	19	sp2		
d	C13	- C12	C14	H13	-------	-------	-------	-------	3	119	122	120.0	0.950	1.430	3	26	sp2		
d	C14	- C13	C15	H14	-------	-------	-------	-------	3	120	120	120.0	0.950	1.422	3	15	sp2		
d	C15	- C14	C16	H15	-------	-------	-------	-------	3	120	120	120.0	0.950	1.422	3	23	sp2		
d	C16	- C15	C17	H16	-------	-------	-------	-------	3	119	121	120.0	0.950	1.429	3	18	sp2		
d	C17	- C12	C16	C18	-------	-------	-------	-------	3	119	122	120.0	1.394	1.439	3	27	sp2		
d	C18	- C17	C19	H18	-------	-------	-------	-------	3	119	121	120.0	0.950	1.396	3	20	sp2		
d	C19	- C18	C20	C24	-------	-------	-------	-------	3	119	122	120.0	1.396	1.437	3	27	sp2		
d	C20	- C19	C21	H20	-------	-------	-------	-------	3	119	121	120.0	0.950	1.430	3	18	sp2		
d	C21	- C20	C22	H21	-------	-------	-------	-------	3	120	120	120.0	0.950	1.421	3	23	sp2		
d	C22	- C21	C23	H22	-------	-------	-------	-------	3	120	120	120.0	0.950	1.421	3	15	sp2		
d	C23	- C22	C24	H23	-------	-------	-------	-------	3	119	122	120.0	0.950	1.432	3	26	sp2		
d	C24	- C11	C19	C23	-------	-------	-------	-------	3	118	121	120.0	1.411	1.437	3	19	sp2		
d	B1	- N1	C1	C11	-------	-------	-------	-------	3	118	123	120.0	1.405	1.595	3	12			
cRU	H1A	- C1	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.990	0.990	1	6			
cRU	H1B	- C1	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.990	0.990	1	6			
cRU	H2	- C2	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.950	0.950	1	7			
cRU	H3	- C3	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.950	0.950	1	8			
cRU	H4A	- C4	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.990	0.990	1	10			
cRU	H4B	- C4	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.990	0.990	1	10			

cRU	H5A	- C5	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.980	0.980	1	11			
cRU	H5B	- C5	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.980	0.980	1	11			
cRU	H5C	- C5	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.980	0.980	1	11			
cRU	H6A	- C6	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.980	0.980	1	11			

cRU	H6B	- C6	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.980	0.980	1	11
cRU	H6C	- C6	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.980	0.980	1	11
cRU	H8A	- C8	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.980	0.980	1	9
cRU	H8B	- C8	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.980	0.980	1	9
cRU	H8C	- C8	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.980	0.980	1	9
cRU	H9A	- C9	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.980	0.980	1	9
cRU	H9B	- C9	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.980	0.980	1	9
cRU	H9C	- C9	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.980	0.980	1	9
cRU	H10A	- C10	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.980	0.980	1	9
cRU	H10B	- C10	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.980	0.980	1	9
cRU	H10C	- C10	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.980	0.980	1	9
cRU	H13	- C13	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.950	0.950	1	2
cRU	H14	- C14	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.950	0.950	1	3
cRU	H15	- C15	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.950	0.950	1	1
cRU	H16	- C16	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.950	0.950	1	4
cRU	H18	- C18	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.950	0.950	1	5
cRU	H20	- C20	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.950	0.950	1	4
cRU	H21	- C21	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.950	0.950	1	1
cRU	H22	- C22	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.950	0.950	1	3
cRU	H23	- C23	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.950	0.950	1	2

Analysis of the IntraMolecular Geometry in Terms of Unique Molecule(s)/Ions, with Bond Criterium: d(i-j) < R(i) + R(j) + Tol

-- Tol = 0.40 Ang. for Normal Bonds + 0.70 for (Earth)alkali-NonMetal Contacts and adjusted by -.40 Ang. for Metal-Metal Distances
-- The Bond Distance and Angle su's have been Incremented to Include the Effect of the Unit-cell su.
(Rel.Error in Dist. 0.0000 Ang. , Abs. Angle Error 0.000 Deg.)
-- Bonds below with '>' or '<' Substituted for '-' have Distances that Deviate from Expected Values(Based on the hybridisations).

Bond Lengths (Angstrom). - (Bonds are ordered on the first label, left to right and top to bottom) - su in last digit in ().

Si1	-	N1	1.7669(12)	Si1	-	C5	1.8606(14)	Si1	-	C6	1.8655(14)	Si1	-	C7	1.9150(15)
N1	-	C4	1.4962(16)	N1	-	B1	1.4053(18)	C1	-	C2	1.4946(19)	C1	-	B1	1.586(2)
C2	-	C3	1.328(2)	C3	-	C4	1.4989(19)	C7	-	C8	1.535(2)	C7	-	C9	1.538(2)
C7	-	C10	1.539(2)	C11	-	C12	1.4145(17)	C11	-	C24	1.4109(17)	C11	-	B1	1.5946(19)
C12	-	C13	1.4300(18)	C12	-	C17	1.4395(18)	C13	-	C14	1.3647(19)	C14	-	C15	1.422(2)
C15	-	C16	1.357(2)	C16	-	C17	1.4285(19)	C17	-	C18	1.3940(19)	C18	-	C19	1.3961(19)
C19	-	C20	1.430(2)	C19	-	C24	1.4369(18)	C20	-	C21	1.358(2)	C21	-	C22	1.421(2)
C22	-	C23	1.3614(19)	C23	-	C24	1.4317(18)								
C1	-	H1A	0.99	C1	-	H1B	0.99	C2	-	H2	0.95	C3	-	H3	0.95
C4	-	H4A	0.99	C4	-	H4B	0.99	C5	-	H5A	0.98	C5	-	H5B	0.98
C5	-	H5C	0.98	C6	-	H6A	0.98	C6	-	H6B	0.98	C6	-	H6C	0.98
C8	-	H8A	0.98	C8	-	H8B	0.98	C8	-	H8C	0.98	C9	-	H9A	0.98
C9	-	H9B	0.98	C9	-	H9C	0.98	C10	-	H10A	0.98	C10	-	H10B	0.98
C10	-	H10C	0.98	C13	-	H13	0.95	C14	-	H14	0.95	C15	-	H15	0.95
C16	-	H16	0.95	C18	-	H18	0.95	C20	-	H20	0.95	C21	-	H21	0.95
C22	-	H22	0.95	C23	-	H23	0.95								

Bond/Valence Angles (Degrees) - (Angles are ordered on the middle label, left to right and top to bottom) - su in last digit in ().

N1	-	Si1	-	C5	112.07(6)	N1	-	Si1	-	C6	108.12(7)	N1	-	Si1	-	C7	109.65(6)
C5	-	Si1	-	C6	107.16(7)	C5	-	Si1	-	C7	108.35(7)	C6	-	Si1	-	C7	111.49(7)
Si1	-	N1	-	C4	112.36(9)	Si1	-	N1	-	B1	130.20(9)	C4	-	N1	-	B1	117.44(11)
C2	-	C1	-	B1	113.29(12)	C1	-	C2	-	C3	120.61(12)	C2	-	C3	-	C4	121.63(12)
N1	-	C4	-	C3	113.90(11)	Si1	-	C7	-	C8	109.94(10)	Si1	-	C7	-	C9	114.47(11)
Si1	-	C7	-	C10	108.10(11)	C8	-	C7	-	C9	109.15(13)	C8	-	C7	-	C10	108.37(14)
C9	-	C7	-	C10	106.60(13)	C12	-	C11	-	C24	118.47(11)	C12	-	C11	-	B1	119.92(11)
C24	-	C11	-	B1	121.51(11)	C11	-	C12	-	C13	121.88(11)	C11	-	C12	-	C17	120.62(11)
C13	-	C12	-	C17	117.50(11)	C12	-	C13	-	C14	121.65(12)	C13	-	C14	-	C15	120.36(13)
C14	-	C15	-	C16	120.11(13)	C15	-	C16	-	C17	121.34(13)	C12	-	C17	-	C16	119.00(12)
C12	-	C17	-	C18	119.46(12)	C16	-	C17	-	C18	121.54(12)	C17	-	C18	-	C19	121.15(12)
C18	-	C19	-	C20	121.59(12)	C18	-	C19	-	C24	119.28(12)	C20	-	C19	-	C24	119.13(12)
C19	-	C20	-	C21	120.99(13)	C20	-	C21	-	C22	120.28(13)	C21	-	C22	-	C23	120.48(13)
C22	-	C23	-	C24	121.53(13)	C11	-	C24	-	C19	120.97(11)	C11	-	C24	-	C23	121.43(11)
C19	-	C24	-	C23	117.59(11)	N1	-	B1	-	C1	118.97(12)	N1	-	B1	-	C11	123.12(11)
C1	-	B1	-	C11	117.89(11)														
C2	-	C1	-	H1A	109	C2	-	C1	-	H1B	109	B1	-	C1	-	H1A	109		

B1	-	C1	-	H1B	109	H1A	-	C1	-	H1B	108	C1	-	C2	-	H2	120		
C3	-	C2	-	H2	120	C2	-	C3	-	H3	119	C4	-	C3	-	H3	119		
N1	-	C4	-	H4A	109	N1	-	C4	-	H4B	109	C3	-	C4	-	H4A	109		
C3	-	C4	-	H4B	109	H4A	-	C4	-	H4B	108	Si1	-	C5	-	H5A	109		
Si1	-	C5	-	H5B	109	Si1	-	C5	-	H5C	109	H5A	-	C5	-	H5B	109		
H5A	-	C5	-	H5C	109	H5B	-	C5	-	H5C	109	Si1	-	C6	-	H6A	109		
Si1	-	C6	-	H6B	109	Si1	-	C6	-	H6C	109	H6A	-	C6	-	H6B	109		
H6A	-	C6	-	H6C	109	H6B	-	C6	-	H6C	109	C7	-	C8	-	H8A	109		
C7	-	C8	-	H8B	109	C7	-	C8	-	H8C	109	H8A	-	C8	-	H8B	109		
H8A	-	C8	-	H8C	109	H8B	-	C8	-	H8C	109	C7	-	C9	-	H9A	109		
C7	-	C9	-	H9B	109	C7	-	C9	-	H9C	109	H9A	-	C9	-	H9B	109		
H9A	-	C9	-	H9C	109	H9B	-	C9	-	H9C	109	C7	-	C10	-	H10A	109		
C7	-	C10	-	H10B	109	C7	-	C10	-	H10C	109	H10A	-	C10	-	H10B	109		
H10A	-	C10	-	H10C	109	H10B	-	C10	-	H10C	109	C12	-	C13	-	H13	119		
C14	-	C13	-	H13	119	C13	-	C14	-	H14	120	C15	-	C14	-	H14	120		
C14	-	C15	-	H15	120	C16	-	C15	-	H15	120	C15	-	C16	-	H16	119		
C17	-	C16	-	H16	119	C17	-	C18	-	H18	119	C19	-	C18	-	H18	119		
C19	-	C20	-	H20	120	C21	-	C20	-	H20	119	C20	-	C21	-	H21	120		
C22	-	C21	-	H21	120	C21	-	C22	-	H22	120	C23	-	C22	-	H22	120		
C22	-	C23	-	H23	119	C24	-	C23	-	H23	119								

Torsion/Dihedral Angles (Deg.) - Klyne & Prelog Convention (Dunitz, p241) - (Excl. Minor Disorder & Embedded Bond Angl. > 160. Deg.)

C5	Si1	N1	C4	177.56(9)	C5	Si1	N1	B1	-3.02(14)	C6	Si1	N1	C4	59.67(10)
C6	Si1	N1	B1	-120.90(12)	C7	Si1	N1	C4	-62.08(10)	C7	Si1	N1	B1	117.35(12)
N1	Si1	C7	C8	-37.56(12)	N1	Si1	C7	C9	85.70(12)	N1	Si1	C7	C10	-155.69(11)
C5	Si1	C7	C8	85.04(12)	C5	Si1	C7	C9	-151.70(11)	C5	Si1	C7	C10	-33.08(13)
C6	Si1	C7	C8	-157.27(10)	C6	Si1	C7	C9	-34.01(13)	C6	Si1	C7	C10	84.61(13)
Si1	N1	C4	C3	143.11(10)	B1	N1	C4	C3	-36.39(16)	Si1	N1	B1	C1	-168.86(9)
Si1	N1	B1	C11	12.59(19)	C4	N1	B1	C1	10.54(17)	C4	N1	B1	C11	-168.01(11)
B1	C1	C2	C3	-25.45(18)	C2	C1	B1	N1	20.11(17)	C2	C1	B1	C11	-161.26(11)
C1	C2	C3	C4	-0.7(2)	C2	C3	C4	N1	32.76(19)	C24	C11	C12	C13	-178.98(11)
C24	C11	C12	C17	1.46(17)	B1	C11	C12	C13	-2.48(17)	B1	C11	C12	C17	177.96(11)
C12	C11	C24	C19	-2.56(17)	C12	C11	C24	C23	178.93(11)	B1	C11	C24	C19	-179.00(11)
B1	C11	C24	C23	2.49(18)	C12	C11	B1	N1	83.53(16)	C12	C11	B1	C1	-95.04(14)
C24	C11	B1	N1	-100.08(15)	C24	C11	B1	C1	81.36(15)	C11	C12	C13	C14	178.39(12)
C17	C12	C13	C14	-2.03(18)	C11	C12	C17	C16	-178.74(12)	C11	C12	C17	C18	0.83(19)
C13	C12	C17	C16	1.68(18)	C13	C12	C17	C18	-178.75(12)	C12	C13	C14	C15	0.7(2)
C13	C14	C15	C16	1.2(2)	C14	C15	C16	C17	-1.5(2)	C15	C16	C17	C12	0.0(2)
C15	C16	C17	C18	-179.53(14)	C12	C17	C18	C19	-2.1(2)	C16	C17	C18	C19	177.49(13)
C17	C18	C19	C20	-178.58(13)	C17	C18	C19	C24	1.0(2)	C18	C19	C20	C21	179.64(14)
C24	C19	C20	C21	0.1(2)	C18	C19	C24	C11	1.38(19)	C18	C19	C24	C23	179.94(14)
C20	C19	C24	C11	-179.04(12)	C20	C19	C24	C23	-0.48(19)	C19	C20	C21	C22	0.1(2)

```
 C20    C21    C22    C23          0.2(2)    C21    C22    C23    C24         -0.6(2)    C22    C23    C24    C11       179.33(13)
 C22    C23    C24    C19         0.77(19)

 N1     Si1    C5     H5A             -55    N1     Si1    C5     H5B            -175    N1     Si1    C5     H5C              65
 C6     Si1    C5     H5A              63    C6     Si1    C5     H5B             -57    C6     Si1    C5     H5C            -177
```



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 C7     Si1    C5     H5A            -176    C7     Si1    C5     H5B              64    C7     Si1    C5     H5C            -56
 N1     Si1    C6     H6A             -59    N1     Si1    C6     H6B            -179    N1     Si1    C6     H6C             61
 C5     Si1    C6     H6A            -180    C5     Si1    C6     H6B              60    C5     Si1    C6     H6C            -60
 C7     Si1    C6     H6A              62    C7     Si1    C6     H6B             -58    C7     Si1    C6     H6C            -178
 Si1    N1     C4     H4A              22    Si1    N1     C4     H4B             -95    B1     N1     C4     H4A            -158
 B1     N1     C4     H4B              85    B1     C1     C2     H2              155    H1A    C1     C2     C3             -147
 H1A    C1     C2     H2               33    H1B    C1     C2     C3               96    H1B    C1     C2     H2              -84
 H1A    C1     B1     N1              141    H1A    C1     B1     C11             -40    H1B    C1     B1     N1             -101
 H1B    C1     B1     C11              77    C1     C2     C3     H3              179    H2     C2     C3     C4              179
 H2     C2     C3     H3               -1    C2     C3     C4     H4A             154    C2     C3     C4     H4B             -89
 H3     C3     C4     N1             -147    H3     C3     C4     H4A             -26    H3     C3     C4     H4B              91
 Si1    C7     C8     H8A             -55    Si1    C7     C8     H8B            -175    Si1    C7     C8     H8C              65
 C9     C7     C8     H8A             179    C9     C7     C8     H8B              59    C9     C7     C8     H8C             -61
 C10    C7     C8     H8A              63    C10    C7     C8     H8B             -57    C10    C7     C8     H8C            -177
 Si1    C7     C9     H9A             -67    Si1    C7     C9     H9B             173    Si1    C7     C9     H9C              53
 C8     C7     C9     H9A              57    C8     C7     C9     H9B             -63    C8     C7     C9     H9C             177
 C10    C7     C9     H9A             174    C10    C7     C9     H9B              54    C10    C7     C9     H9C             -66
 Si1    C7     C10    H10A            -57    Si1    C7     C10    H10B            -177    Si1    C7     C10    H10C             63
 C8     C7     C10    H10A            -176    C8     C7     C10    H10B             64    C8     C7     C10    H10C            -56
 C9     C7     C10    H10A             67    C9     C7     C10    H10B            -53    C9     C7     C10    H10C            -173
 C11    C12    C13    H13              -2    C17    C12    C13    H13             178    C12    C13    C14    H14             -179
 H13    C13    C14    C15             -179    H13    C13    C14    H14               1    C13    C14    C15    H15             -179
 H14    C14    C15    C16             -179    H14    C14    C15    H15               1    C14    C15    C16    H16              179
 H15    C15    C16    C17              179    H15    C15    C16    H16              -1    H16    C16    C17    C12             -180
 H16    C16    C17    C18                0    C12    C17    C18    H18             178    C16    C17    C18    H18              -3
 H18    C18    C19    C20                1    H18    C18    C19    C24            -179    C18    C19    C20    H20               0
 C24    C19    C20    H20             -180    C19    C20    C21    H21            -180    H20    C20    C21    C22             -180
 H20    C20    C21    H21                0    C20    C21    C22    H22            -180    H21    C21    C22    C23             -180
 H21    C21    C22    H22                0    C21    C22    C23    H23             179    H22    C22    C23    C24              179
 H22    C22    C23    H23               -1    H23    C23    C24    C11              -1    H23    C23    C24    C19             -179
```


Statistics of Bond Length per Bond Type (NOTE: A Indicates 10 Occurrences, B Indicates 11, Etc. and * more than 35)

Bond Type	Nr	B.P.	d(min)	d(max)	d(av)	Sumrad	Note	0.0 0.5 1.0 1.5 2.0 2.5 3.0 Angstrom
Si -- N	1	0.0012	1.7669	1.7669	1.7669	1.88		.....1.....
Si -- C4	3	0.0014	1.8606	1.9150	1.8804	1.88		.....21.....
N3 -- C4	1	0.0016	1.4962	1.4962	1.4962	1.36		.....1.....
N -- B	1	0.0018	1.4053	1.4053	1.4053	1.51		.....1.....
C4 -- C3	1	0.0019	1.4946	1.4946	1.4946	1.36		.....1.....
C -- B	2	0.0020	1.5860	1.5946	1.5903	1.51		.....2.....
C3 -- C3	17	0.0019	1.3280	1.4395	1.4014	1.36		.....566.....
C3 -- C4	1	0.0019	1.4989	1.4989	1.4989	1.36		.....1.....
C4 -- C4	3	0.0020	1.5350	1.5390	1.5373	1.36		.....3.....
C -- H	30		0.9500	0.9900	0.9703	1.03		.....BJ.....

Selected Bond Lengths (Angstrom) - see M.F.C. Ladd & R.A. Palmer, Structure Determination by X-ray Crystallography (1985)

Formal single bonds

```
C4-C4 1.54   C4-C3 1.52   C4-C2 1.46   C4-N3 1.47   C4-N2 1.47   C4-O2 1.43   C3-C3 1.46   C3-C2 1.45   C3-N3 1.40   C3-N2 1.40
C3-O2 1.36   C2-C2 1.38   C2-N3 1.33   C2-N2 1.33   C2-O2 1.36   N3-N3 1.45   N3-N2 1.45   N3-O2 1.36   N2-N2 1.45   N2-O2 1.41
```

Formal double bonds

```
C3-C3 1.34   C3-C2 1.31   C3-N2 1.32   C3-O1 1.22   C2-C2 1.28   C2-N2 1.32   C2-O1 1.16   N3-O1 1.24   N2-N2 1.25   N2-O1 1.21
```

Formal triple bonds

```
C2-C2 1.20   C2-N1 1.16   C3-C3 1.40
```

Aromatic bonds

```
C2-N2 1.34   N2-N2 1.35
```

The notation in the table indicates the connectivity of the atoms

For more detailed standard bond distance tabulations see: J. Chem. Soc. Perkin II, (1987), S1-S19;
J. Chem. Soc. Dalton Trans. (1989), S1 - S83 or International Tables C, (1992), 707-791.

Automatic Search for Rings (3 to 24-Membered) and Planes Determined by 4 or More Connected Atoms (with Deviation < 0.10 Ang.)

```
Least-Squares Planes - P*X+Q*Y+R*Z=S   ::  First Line Orthogonal(XO,YO,ZO), Second Line Fractional(X,Y,Z)
=====================================      Ring/Plan/Resd/Lspl N Indicates that the Ring/Plane/Residue Involves N Atoms
                                           Sigref - R.M.S-Error of the Contributing Atoms
  The Deviation D of an Atom with          Sigpln - Sqrt(Sum(j=1:N)(D(j)**2/(N-3))
                                           Chisq  - Chi-Squared = Sum(j=1:N)(D(j)**2)/Sigref**2
  Fractional Coordinates X,Y,Z may be      Pl.Hyp. - Result of the Chi.Sq. Test for Planarity (See Stout & Jensen, p424)

  Calculated via Substitution in
                                           **** - Atoms Deviating by More Than 1.5 Angstrom and Hydrogen Atoms are NOT Listed
  D = P*X + Q*Y + R*Z - S (2nd Line)       Note - Weights : UNIT
                                                - Deviations from planes are in Angstrom Units
                                                - The Plane determining Atoms have been Marked #
                                                - DISTANCES TO PLANES ROUNDED TO 3 DECIMALS !!(Use Graphical Interface for more)
```

Nr 1	P	Q	R	S	Sigref 0.001	Sigpln 0.233	Chisq 92121.4	Pl.Hyp.	P<5
Ring	0.7430(4)	-0.0819(6)	-0.6643(4)	-6.265(10)	#N1 -0.156(1)	#C1 0.206(1)	#C2 -0.125(1)	#C3	-0.110(1)
A 6	9.904(5)	-0.912(6)	-18.996(12)	-6.265(10)	#C4 0.253(1)	#B1 -0.068(1)	Si1 -0.700(1)	C5	-1.137(1)
					C6 0.706(2)	C11 -0.198(1)	C12 0.931(1)	C17	0.842(1)
					C18 -0.375(1)	C19 -1.499(1)	C24 -1.401(1)		

Nr 2	P	Q	R	S	Sigref 0.001	Sigpln 0.014	Chisq 375.0	Pl.Hyp.	P<5

```
Ring     0.4431(5)     0.2277(5)     0.8671(3)     19.111(2) #C11     0.013(1) #C12    -0.001(1) #C17    -0.011(1) #C18     0.012(1)
A  6      5.907(6)      2.536(6)     24.796(8)     19.111(2) #C19     0.001(1) #C24    -0.013(1)  N1      1.121(1)  C1     -1.436(1)
                                                            C2     -1.335(1)  C3     -0.244(1)  C4      0.917(1)  C13     0.002(1)
                                                            C14    -0.045(1)  C15    -0.085(1)  C16    -0.054(1)  C20    -0.006(1)
                                                            C21    -0.024(1)  C22    -0.035(1)  C23    -0.023(1)  B1     -0.025(1)
-------------------------------------------------------------------------------------------------------------------------------
Nr  3        P             Q             R             S     Sigref  0.001     Sigpln  0.012     Chisq     227.9    Pl.Hyp.    P<5
-------------------------------------------------------------------------------------------------------------------------------
Ring     0.4612(5)     0.2473(5)     0.8521(3)     19.183(2) #C12    -0.012(1) #C13     0.009(1) #C14     0.003(1) #C15    -0.010(1)
A  6      6.148(7)      2.754(6)     24.369(8)     19.183(2) #C16     0.006(1) #C17     0.005(1)  N1      1.026(1)  C2     -1.473(1)
                                                            C3     -0.389(1)  C4      0.800(1)  C11    -0.040(1)  C18     0.013(1)
                                                            C19    -0.041(1)  C20    -0.064(1)  C21    -0.123(1)  C22    -0.161(1)
                                                            C23    -0.135(1)  C24    -0.082(1)  B1     -0.109(1)
-------------------------------------------------------------------------------------------------------------------------------
Nr  4        P             Q             R             S     Sigref  0.001     Sigpln  0.003     Chisq      15.8    Pl.Hyp.    P<5
-------------------------------------------------------------------------------------------------------------------------------
Ring     0.4355(5)     0.2207(6)     0.8727(3)     19.098(3) #C19     0.001(1) #C20     0.001(1) #C21    -0.001(1) #C22    -0.002(1)
A  6      5.805(7)      2.457(6)     24.958(8)     19.098(3) #C23     0.004(1) #C24    -0.003(1)  N1      1.139(1)  C1     -1.416(1)
                                                            C2     -1.301(1)  C3     -0.208(1)  C4      0.941(1)  C11     0.017(1)
                                                            C12    -0.015(1)  C13    -0.019(1)  C14    -0.082(1)  C15    -0.132(1)
                                                            C16    -0.094(1)  C17    -0.034(1)  C18    -0.005(1)  B1     -0.011(1)

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===============================================================================================================================
-------------------------------------------------------------------------------------------------------------------------------
Nr  5        P             Q             R             S     Sigref  0.001     Sigpln  0.023     Chisq    2070.9    Pl.Hyp.    P<5
-------------------------------------------------------------------------------------------------------------------------------
Ring     0.4529(2)     0.2377(4)     0.8593(1)     19.1331(17) #C11     0.002(1) #C12     0.010(1) #C13     0.023(1) #C14    -0.003(1)
A 10      6.037(3)      2.647(4)     24.574(4)     19.1331(17) #C15    -0.029(1) #C16    -0.006(1) #C17     0.014(1) #C18     0.028(1)
                                                            #C19    -0.005(1) #C24    -0.033(1)  N1      1.089(1)  C1     -1.471(1)
                                                            C2     -1.390(1)  C3     -0.302(1)  C4      0.873(1)  C20    -0.021(1)
                                                            C21    -0.061(1)  C22    -0.085(1)  C23    -0.065(1)  B1     -0.052(1)
-------------------------------------------------------------------------------------------------------------------------------
Nr  6        P             Q             R             S     Sigref  0.001     Sigpln  0.012     Chisq     574.9    Pl.Hyp.    P<5
-------------------------------------------------------------------------------------------------------------------------------
Ring     0.4381(2)     0.2248(4)     0.8704(1)     19.1042(19) #C11     0.019(1) #C12    -0.005(1) #C17    -0.019(1) #C18     0.009(1)
A 10      5.840(3)      2.503(4)     24.890(4)     19.1042(19) #C19     0.008(1) #C20     0.006(1) #C21    -0.003(1) #C22    -0.009(1)
                                                            #C23    -0.003(1) #C24    -0.002(1)  N1      1.132(1)  C1     -1.423(1)
                                                            C2     -1.316(1)  C3     -0.225(1)  C4      0.930(1)  C13    -0.008(1)
                                                            C14    -0.064(1)  C15    -0.108(1)  C16    -0.071(1)  B1     -0.016(1)
-------------------------------------------------------------------------------------------------------------------------------
Nr  7        P             Q             R             S     Sigref  0.001     Sigpln  0.028     Chisq    4577.7    Pl.Hyp.    P<5
-------------------------------------------------------------------------------------------------------------------------------
Ring     0.4457(1)     0.2327(3)     0.8644(1)     19.1084(15) #C11     0.026(1) #C12     0.019(1) #C13     0.024(1) #C14    -0.015(1)
A 14     5.9408(19)     2.591(4)     24.720(3)     19.1084(15) #C15    -0.049(1) #C16    -0.018(1) #C17     0.016(1) #C18     0.038(1)
                                                            #C19     0.019(1) #C20     0.011(1) #C21    -0.015(1) #C22    -0.033(1)
                                                            #C23    -0.020(1) #C24    -0.002(1)  N1      1.122(1)  C1     -1.436(1)
                                                            C2     -1.344(1)  C3     -0.255(1)  C4      0.911(1)  B1     -0.021(1)
-------------------------------------------------------------------------------------------------------------------------------
Nr  8        P             Q             R             S     Sigref  0.001     Sigpln  1.516     Chisq  999999.9    Pl.Hyp.
-------------------------------------------------------------------------------------------------------------------------------
Resd     0.4489(4)     0.6193(2)     0.6442(2)     18.8114(17) #Si1     1.201(1) #N1     -0.512(1) #C1     -2.814(1) #C2     -3.379(1)
A 27      5.983(5)     6.8973(19)     18.421(6)     18.8114(17) #C3     -2.662(1) #C4     -1.275(1) #C5      2.156(1) #C6      1.920(2)
                                                            #C7      1.392(1) #C8      0.347(2) #C9      1.287(2) #C10     2.791(2)
                                                            #C11    -0.526(1) #C12    -0.084(1) #C13    -0.201(1) #C14     0.198(1)
                                                            #C15     0.759(1) #C16     0.922(1) #C17     0.513(1) #C18     0.671(1)
                                                            #C19     0.221(1) #C20     0.350(1) #C21    -0.098(1) #C22    -0.707(1)
                                                            #C23    -0.843(1) #C24    -0.396(1) #B1     -1.230(1)
-------------------------------------------------------------------------------------------------------------------------------
Nr  9        P             Q             R             S     Sigref  0.001     Sigpln  0.028     Chisq    1136.0    Pl.Hyp.    P<5
-------------------------------------------------------------------------------------------------------------------------------
Plan     0.8373(3)     0.2046(5)    -0.5070(5)    -1.376(10) #Si1    -0.028(1) #N1     -0.002(1) #C4      0.018(1) #C5      0.021(1)
A  5     11.161(5)      2.279(6)   -14.499(13)    -1.376(10) #B1     -0.009(1)  C1     -0.250(1)  C2     -0.905(1)  C3     -0.785(1)
                                                            C11     0.247(1)  C18     0.743(1)  C19    -0.574(1)  C24    -0.819(1)
-------------------------------------------------------------------------------------------------------------------------------
Nr 10        P             Q             R             S     Sigref  0.001     Sigpln  0.005     Chisq      13.5    Pl.Hyp.    P<5
-------------------------------------------------------------------------------------------------------------------------------
Plan     0.6317(6)    -0.3292(10)    -0.7019(4)    -8.524(12) #C1     -0.001(1) #C2      0.003(1) #C3     -0.003(1) #C4      0.002(1)
A  4      8.420(8)     -3.666(11)   -20.071(13)    -8.524(12)  N1     -0.728(1)  C6     -0.357(2)  C11    -1.120(1)  C12    -0.257(1)
                                                            C13     1.032(1)  C15     1.478(1)  C16     0.251(1)  C17    -0.659(1)
                                                            B1     -0.639(1)

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===============================================================================================================================
-------------------------------------------------------------------------------------------------------------------------------
Nr 11        P             Q             R             S     Sigref  0.001     Sigpln  0.027     Chisq    4703.5    Pl.Hyp.    P<5
-------------------------------------------------------------------------------------------------------------------------------
Plan     0.4461(1)     0.2303(3)     0.8649(1)     19.0969(12) #C11     0.030(1) #C12     0.022(1) #C13     0.028(1) #C14    -0.013(1)
A 15     5.9455(19)     2.565(3)     24.733(3)     19.0969(12) #C15    -0.050(1) #C16    -0.021(1) #C17     0.015(1) #C18     0.035(1)
                                                            #C19     0.018(1) #C20     0.008(1) #C21    -0.016(1) #C22    -0.030(1)
                                                            #C23    -0.016(1) #C24     0.001(1) #B1     -0.013(1)  N1      1.133(1)
                                                            C1     -1.426(1)  C2     -1.330(1)  C3     -0.240(1)  C4      0.925(1)
-------------------------------------------------------------------------------------------------------------------------------
Nr 12        P             Q             R             S     Sigref  0.001     Sigpln  0.009     Chisq      55.3    Pl.Hyp.    P<5
-------------------------------------------------------------------------------------------------------------------------------
Plan     0.8198(4)     0.0342(6)    -0.5716(5)    -3.555(13) #N1      0.003(1) #C1      0.003(1) #C11     0.003(1) #B1     -0.008(1)
A  4     10.928(5)      0.381(7)   -16.346(16)    -3.555(13)  Si1    -0.265(1)  C2     -0.449(1)  C3     -0.332(1)  C4      0.267(1)
                                                            C5     -0.520(1)  C6      1.263(1)  C12     1.227(1)  C17     1.259(1)
                                                            C18     0.067(1)  C19    -1.153(1)  C24    -1.180(1)
```

(Acute) Angles (Degrees) Between Planes (Numbers I,J from List Above)

```
-------------------------------------------------------------------------------------------------------------------------------
 1, 2=   74.61(6)   1, 3=   75.90(6)   1, 4=   74.09(6)   1, 5=   75.30(5)   1, 6=   74.27(5)   1, 7=   74.81(5)   1, 8=   81.66(5)
 1, 9=   19.58(6)   1,10=   15.74(8)   1,11=   74.82(5)   1,12=    9.59(7)   2, 3=    1.75(6)   2, 4=    0.68(6)   2, 5=    0.92(5)
 2, 6=    0.38(5)   2, 7=    0.36(5)   2, 8=   26.05(5)   2, 9=   88.74(6)   2,10=   66.20(8)   2,11=    0.26(5)   2,12=   82.85(7)
 3, 4=    2.43(6)   3, 5=    0.84(5)   3, 6=    2.12(5)   3, 7=    1.41(5)   3, 8=   24.62(5)   3, 9=   89.73(6)   3,10=   67.16(8)
 3,11=    1.49(5)   3,12=   84.23(7)   4, 5=    1.59(5)   4, 6=    0.31(5)   4, 7=    1.02(5)   4, 8=   26.58(5)   4, 9=   88.13(6)
 4,10=   65.79(9)   4,11=    0.94(5)   4,12=   82.28(7)   5, 6=    1.29(4)   5, 7=    0.58(3)   5, 8=   25.31(4)   5, 9=   89.55(5)
 5,10=   66.72(8)   5,11=    0.66(3)   5,12=   83.58(6)   6, 7=    0.72(3)   6, 8=   26.30(4)   6, 9=   88.37(5)   6,10=   65.91(8)
 6,11=    0.64(3)   6,12=   82.49(6)   7, 8=   25.71(3)   7, 9=   89.00(5)   7,10=   66.31(7)   7,11=    0.14(3)   7,12=   83.07(6)
 8, 9=   79.86(5)   8,10=   68.14(8)   8,11=   25.85(3)   8,12=   88.80(6)   9,10=   35.17(8)   9,11=   88.98(5)   9,12=   10.51(7)
10,11=   66.36(7)  10,12=   24.80(9)  11,12=   83.06(6)
```

(Acute) Angles (Degrees) Between Axes, Lines, and Bonds with L.S.-Planes

```
-------------------------------------------------------------------------------------------------------------------------------
 Bond  /  Plane NM --> M      1          2          3          4          5          6          7          8          9          10
-------------------------------------------------------------------------------------------------------------------------------
Axes O --->a  / 0M =    47.99(5),  26.30(4),  27.47(4),  25.82(5),  26.93(3),  25.98(3),  26.47(2),  26.67(3),  56.86(4),  39.18(7),
                1M =    26.49(2),  55.07(5),
           b  / 0M =     4.70(5),  13.16(4),  14.32(4),  12.75(5),  13.75(3),  12.99(3),  13.46(2),  38.27(3),  11.81(4),  19.22(7),
                1M =    13.32(2),   1.96(5),
           c  / 0M =    41.63(5),  60.12(4),  58.45(4),  60.78(5),  59.24(3),  60.50(3),  59.82(2),  40.10(3),  30.47(4),  44.58(7),
                1M =    59.87(2),  34.86(5),
           a* / 0M =    47.99(5),  26.30(4),  27.47(4),  25.82(5),  26.93(3),  25.98(3),  26.47(2),  26.67(3),  56.86(4),  39.18(7),
                1M =    26.49(2),  55.07(5),
           b* / 0M =     4.70(5),  13.16(4),  14.32(4),  12.75(5),  13.75(3),  12.99(3),  13.46(2),  38.27(3),  11.81(4),  19.22(7),
```

```
                1M =    13.32(2),   1.96(5),
           c* / 0M =    41.63(5),  60.12(4),  58.45(4),  60.78(5),  59.24(3),  60.50(3),  59.82(2),  40.10(3),  30.47(4),  44.58(7),
                1M =    59.87(2),  34.86(5),
Si1   -N1     / 0M =    17.93(6),  75.50(6),  76.31(6),  75.18(6),  75.92(5),  75.39(5),  75.75(4),  75.83(5),   0.83(6),  29.49(8),
```



```
                1M =    75.61(4),   8.71(7),
      -C5     / 0M =    13.59(6),   7.57(6),   8.46(6),   7.26(6),   8.02(5),   7.46(5),   7.82(5),  30.89(5),   1.48(6),  26.99(8),
                1M =     7.68(5),   7.89(7),
      -C6     / 0M =    48.89(6),  24.38(6),  25.41(6),  23.94(6),  24.94(5),  24.08(5),  24.51(5),  22.65(5),  55.09(6),  41.70(8),
                1M =    24.55(5),  54.95(7),
      -C7     / 0M =    53.92(6),  26.39(6),  24.65(6),  27.07(6),  25.48(5),  26.77(5),  26.06(5),   5.71(5),  56.40(6),  43.97(8),
                1M =    26.13(5),  54.07(7),
N1    -C4     / 0M =    15.86(8),   7.87(7),   8.70(8),   7.59(8),   8.28(7),   7.78(7),   8.11(6),  30.68(7),   0.79(8),  29.19(9),
                1M =     7.97(6),  10.17(8),
      -B1     / 0M =     3.59(9),  54.68(8),  53.87(9),  54.94(9),  54.28(8),  54.76(8),  54.45(8),  30.70(8),   0.29(9),   3.64(10),
                1M =    54.58(8),   0.45(9),
C1    -C2     / 0M =    12.82(9),   3.86(8),   2.43(9),   4.39(9),   3.13(8),   4.11(8),   3.53(8),  22.18(8),  26.01(9),   0.18(10),
                1M =     3.66(8),  17.59(9),
      -B1     / 0M =     9.95(9),  62.77(8),  64.11(8),  62.27(9),  63.47(8),  62.55(8),  63.10(8),  87.66(8),   8.72(8),  23.70(10),
                1M =    62.96(7),   0.39(9),
C2    -C3     / 0M =   0.67(10),  55.29(10),  54.72(10),  55.45(10),  55.02(9),  55.31(9),  55.10(9),  32.70(9),   5.20(10),   0.27(11),
                1M =    55.23(9),   5.07(10),
C3    -C4     / 0M =    14.00(9),  50.73(8),  52.48(9),  50.05(9),  51.64(8),  50.36(8),  51.07(8),  67.65(8),  32.40(8),   0.18(10),
                1M =    50.99(7),  23.56(9),
C7    -C8     / 0M =    35.73(9),  38.32(9),  39.76(9),  37.74(9),  39.09(8),  37.96(8),  38.56(8),  42.90(8),  50.10(9),  24.41(10),
                1M =    38.55(8),  44.42(9),
      -C9     / 0M =    11.61(9),  18.73(9),  18.00(9),  18.97(9),  18.37(8),  18.79(8),  18.51(8),   3.89(8),   3.89(9),  19.57(10),
                1M =    18.64(8),  10.11(9),
      -C10    / 0M =    30.94(9),  53.75(9),  54.04(9),  53.66(9),  53.89(8),  53.77(8),  53.90(8),  65.47(8),  11.58(9),  45.56(10),
                1M =    53.78(8),  21.38(9),
C11   -C12    / 0M =    52.96(8),   0.60(8),   1.13(8),   1.27(8),   0.31(7),   0.98(7),   0.27(7),  18.21(7),  69.33(8),  37.58(10),
                1M =     0.34(7),  59.97(9),
      -C24    / 0M =    58.56(8),   1.08(8),   1.68(8),   0.80(8),   1.42(7),   0.86(7),   1.12(7),   5.28(7),  49.09(8),  62.11(10),
                1M =     1.19(7),  56.91(9),
      -B1     / 0M =     4.67(8),   1.39(8),   2.47(8),   1.01(8),   1.94(7),   1.24(7),   1.67(7),  26.17(7),   9.25(8),  17.55(10),
                1M =     1.53(7),   0.39(9),
C12   -C13    / 0M =    61.90(9),   0.14(8),   0.84(8),   0.18(9),   0.52(8),   0.10(8),   0.19(8),   4.67(8),  52.53(8),  64.32(10),
                1M =     0.26(7),  60.43(9),
      -C17    / 0M =     3.55(8),   0.39(8),   0.71(8),   0.78(9),   0.17(8),   0.55(8),   0.10(7),  24.51(8),   9.96(8),  16.20(10),
                1M =     0.24(7),   1.27(9),
C13   -C14    / 0M =    53.33(9),   1.97(9),   0.24(9),   2.65(9),   1.06(8),   2.35(8),   1.64(8),  16.97(8),  69.12(9),  38.08(11),
                1M =     1.71(8),  60.06(10),
C14   -C15    / 0M =     3.70(9),   1.62(9),   0.53(9),   2.01(9),   1.07(8),   1.78(9),   1.34(8),  23.22(9),   9.49(9),  16.12(11),
                1M =     1.48(8),   0.93(10),
C15   -C16    / 0M =   60.85(10),   1.33(9),   0.69(10),  1.62(10),   0.98(9),   1.56(9),   1.29(9),   6.94(9),  50.38(10),  64.81(11),
                1M =     1.22(9),  58.65(10),
C16   -C17    / 0M =    54.89(9),   1.70(9),   0.02(9),   2.37(9),   0.80(8),   2.08(8),   1.38(8),  16.65(8),  70.95(9),  39.53(10),
                1M =     1.44(8),  61.79(9),
C17   -C18    / 0M =    60.82(9),   0.94(9),   0.29(9),   1.23(9),   0.58(8),   1.16(8),   0.89(8),   6.49(8),  50.58(9),  64.54(11),
                1M =     0.82(8),  58.76(9),
C18   -C19    / 0M =    53.62(9),   0.45(9),   2.18(9),   0.22(9),   1.36(8),   0.07(8),   0.78(8),  18.80(8),  70.52(9),  38.12(11),
                1M =     0.71(8),  60.92(9),
C19   -C20    / 0M =    60.54(9),   0.28(9),   0.94(9),   0.01(9),   0.65(8),   0.06(8),   0.33(8),   5.20(8),  50.98(9),  63.61(11),
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                1M =     0.40(8),  58.90(10),
      -C24    / 0M =     3.89(9),   0.55(8),   1.65(8),   0.16(9),   1.11(8),   0.40(8),   0.84(7),  25.43(8),   9.85(8),  16.67(10),
                1M =     0.70(7),   1.06(9),
C20   -C21    / 0M =   52.94(10),   0.76(9),  2.49(10),  0.08(10),   1.67(9),   0.38(9),   1.09(9),  19.29(9),  69.89(10),  37.45(11),
                1M =     1.02(9),  60.26(10),
C21   -C22    / 0M =     3.47(9),   0.43(9),   1.53(9),   0.04(9),   0.99(8),   0.27(9),   0.71(8),  25.36(9),  10.25(9),  16.25(11),
                1M =     0.57(8),   1.48(10),
C22   -C23    / 0M =    58.94(9),   0.51(9),   1.11(9),   0.23(9),   0.84(8),   0.29(8),   0.54(8),   5.76(8),  49.22(9),  62.67(11),
                1M =     0.61(8),  57.15(10),
C23   -C24    / 0M =    55.14(9),   0.39(8),   2.11(8),   0.28(9),   1.30(8),   0.01(8),   0.72(8),  18.20(8),  72.20(8),  39.59(10),
                1M =     0.65(7),  62.56(9),
```


Ring Puckering Analysis (Cremer & Pople) - (e.s.d. following Norrestam, Acta Cryst. (1981), A37, 764-765)

	Symmetrical Forms	References
6-Membered Rings :	C : Chair - Th = 0.0	J.C.A. Boeyens, J.Cryst.Mol.Struct. 8,(1978),317-320
	H : Half-Chair- Th = 50.8; Phi = k X 60 + 30	
	E : Envelope - Th = 54.7; Phi = k X 60	
	S : Screw-Boat- Th = 67.5; Phi = k X 60 + 30	
	B : Boat - Th = 90.0; Phi = k X 60	
	T : Twist-Boat- Th = 90.0; Phi = k X 60 + 30	

Definitions (All Values Rounded on Esd)

Dev	- Deviation of Atom I from Cremer&Pople Plane (Defined Differently from Least-Squares Plane)
Cs(I),C2(I)	- Mirror Plane and 2-Axis Asym. Par. for Atom I (See Duax et al., Topics in Stereochemistry,V-9, (1976) pp.271-383)
Cs(I-J),C2(I-J)	- Asymmetry Parameters for Bond I-J
Tors(I-J)	- Torsion Angle for Bond I-J

Descriptors for Torsion Angles

Torsion Angle Range	Full Descriptor	Short Descriptor
0 TO 30 Deg	+ Syn-Periplanar	+sp
30 to 90	+ Syn-Clinal	+sc
90 to 150	+ Anti-Clinal	+ac
150 to 180	+ Anti-Periplanar	+ap
0 to -30	- Syn-Periplanar	-sp
-30 to -90	- Syn-Clinal	-sc
-90 to -150	- Anti-Clinal	-ac
-150 to -180	- Anti-Periplanar	-ap

Descriptors for Ring Substituents (J.Appl.Cryst.,1983,16,431)

Angle Range of Subst.	Full Descriptor	Short Descriptor
0 TO 30 Deg.	Axial	ax
30 to 60	Bisectional	bi
60 to 90	Equatorial	eq

*** NOTE *** - For Ring Puckering Comparisons: Make Sure that the Absolute Configuration, Pivot Atom and Cyclic Sense Agree.
- The "RING AT1 AT2 AT3 ... ATn" Instruction Gives the User Explicit Choice of Pivot Atom (AT1) and Sense (AT2).
- Use TRNS Instructions to Obtain the Required Absolute Configuration.
- The Values of Theta and Phi [= Phi(2)] Depend on the Abs. Conf. and the Choice of the First and Second Ring Atom.
- Alternatively, Appropriate Phase Shifts may be Applied to the Same Effect (see Below)
- C&P Analysis is with reference to the Cremer-Pople plane, not to be confused with the associated LS-plane.
  See H.Essen & D.Cremer (1984) Acta Cryst. B40, 418-420.

For Correct Usage of C&P Puckering Parameters see also: D. Cremer (1984) Acta Cryst. B40, 498-500.

6-Membered Ring (1) N1 --> C4 --> C3 --> C2 --> C1 --> B1 -->

	sp2	sp3	sp2	sp2	sp3	
Dev (A) from CPplane	0.1605(12)	-0.2494(14)	0.1087(15)	0.1209(15)	-0.2099(15)	0.0692(15)
Cs(I)-Asym-Par (Deg)	37.18(15)	6.80(15)	43.94(14)	37.18(15)	6.80(15)	43.94(14)
C2(I)-Asym-Par (Deg)	31.49(14)	48.25(14)	21.06(16)	31.49(14)	48.25(14)	21.06(16)
Ring Bond Angle(Deg)	117.44(11)	113.90(11)	121.63(12)	120.61(12)	113.29(12)	118.97(12)

Tors(I-J) (Deg)	-36.39(16)	32.76(19)	-0.7(2)	-25.45(18)	20.11(17)	10.54(17)
Cs(I-J)-Asym-Par (Deg)	33.55(18)	28.27(18)	12.62(17)	33.55(18)	28.27(18)	12.62(17)
C2(I-J)-Asym-Par (Deg)	21.53(18)	35.84(18)	57.36(18)	21.53(18)	35.84(18)	57.36(18)
Ring Bond Distance (Ang)	1.4962(16)	1.4989(19)	1.328(2)	1.4946(19)	1.586(2)	1.4053(18)

Weighted Average Ring Bond Distance = 1.4692(8,344) Ang. - NOTE: 1st esd. Internal, 2nd esd External.
Weighted Average Abs. Torsion Angl. = 21.86(7,537) Deg. see: e.g. Domenicano et al., Acta Cryst.(1975), B31, 221-234.

Cremer & Pople Puckering Parameters [D. Cremer & J.A. Pople, J.Amer.Chem.Soc., 97, (1975), 1354-1358]

Q(2) = 0.4011(14) Ang., Phi(2) = 52.6(2) Deg
Q(3) = 0.0484(14) Ang.

Puckering Amplitude (Q) = 0.4040(14) Ang, Theta = 83.1(2) Deg, Phi = 52.6(2) Deg

* NOTE * - A Change of the Absolute Configuration Transforms Theta into 180 - Theta and Phi into 180 + Phi.
- A Cyclic Forward Shift of the Pivot Atom from At1 to At2 Transforms Theta into 180 - Theta and Phi into Phi + 120.
- A Change of the Sense Transforms Theta into 180 - Theta and Phi into 180 - Phi, and Vice Versa.

Conformational Analysis (G.G. Evans & J.A. Boeyens, Acta Cryst. (1989), B45, 581-590)

Coefficients of Primitive and Normalised Forms

M	Primitive	Coefficient	Angular Value
CosForm 2	0.308	0.670	4.0
SinForm	0.103	0.225	2.0
3		0.105	1.0

6-Membered Ring (2) C11 --> C12 --> C17 --> C18 --> C19 --> C24 -->

	sp2	sp2	sp2	sp2	sp2	sp2
Dev (A) from CPplane	-0.0135(13)	0.0013(13)	0.0112(15)	-0.0116(15)	-0.0006(15)	0.0131(13)
Cs(I)-Asym-Par (Deg)	1.56(15)	3.30(15)	1.74(15)	1.56(15)	3.30(15)	1.74(15)
C2(I)-Asym-Par (Deg)	2.95(15)	0.50(15)	2.85(15)	2.95(15)	0.50(15)	2.85(15)
Ring Bond Angle(Deg)	118.47(11)	120.62(11)	119.46(12)	121.15(12)	119.28(12)	120.97(11)

Tors(I-J) (Deg)	1.46(17)	0.83(19)	-2.1(2)	1.0(2)	1.38(19)	-2.56(17)
Cs(I-J)-Asym-Par (Deg)	1.33(18)	1.19(19)	2.39(18)	1.33(18)	1.19(19)	2.39(18)
C2(I-J)-Asym-Par (Deg)	3.44(19)	3.56(19)	0.13(19)	3.44(19)	3.56(19)	0.13(19)
Ring Bond Distance (Ang)	1.4145(17)	1.4395(18)	1.3940(19)	1.3961(19)	1.4369(18)	1.4109(17)

Weighted Average Ring Bond Distance = 1.4159(7, 77) Ang. - NOTE: 1st esd. Internal, 2nd esd External.
Weighted Average Abs. Torsion Angl. = 1.59(8, 27) Deg. see: e.g. Domenicano et al., Acta Cryst.(1975), B31, 221-234.

No C & P - Puckering Analysis since <Tau> = 1.6 < 5.0 Deg.

Centroid Cg2 : x ,y ,z 0.50568(4) 0.77262(5) 0.571257(18)
XO,YO,ZO 6.7403(5) 8.6043(5) 16.3364(5)

6-Membered Ring (3) C12 --> C13 --> C14 --> C15 --> C16 --> C17 -->

	sp2	sp2	sp2	sp2	sp2	sp2
Dev (A) from CPplane	0.0126(13)	-0.0084(14)	-0.0030(15)	0.0102(15)	-0.0061(15)	-0.0053(15)
Cs(I)-Asym-Par (Deg)	0.48(16)	2.03(16)	2.51(16)	0.48(16)	2.03(16)	2.51(16)
C2(I)-Asym-Par (Deg)	2.68(15)	1.82(16)	1.06(16)	2.68(15)	1.82(16)	1.06(16)
Ring Bond Angle(Deg)	117.50(11)	121.65(12)	120.36(13)	120.11(13)	121.34(13)	119.00(12)

Tors(I-J) (Deg)	-2.03(18)	0.7(2)	1.2(2)	-1.5(2)	0.0(2)	1.68(18)
Cs(I-J)-Asym-Par (Deg)	1.89(19)	0.60(19)	1.54(19)	1.89(19)	0.60(19)	1.54(19)
C2(I-J)-Asym-Par (Deg)	1.1(2)	3.21(19)	2.1(2)	1.1(2)	3.21(19)	2.1(2)
Ring Bond Distance (Ang)	1.4300(18)	1.3647(19)	1.422(2)	1.357(2)	1.4285(19)	1.4395(18)

Weighted Average Ring Bond Distance = 1.4086(8,146) Ang. - NOTE: 1st esd. Internal, 2nd esd External.
Weighted Average Abs. Torsion Angl. = 1.23(8, 30) Deg. see: e.g. Domenicano et al., Acta Cryst.(1975), B31, 221-234.

No C & P - Puckering Analysis since <Tau> = 1.2 < 5.0 Deg.

Centroid Cg3 : x ,y ,z 0.66678(4) 0.78298(5) 0.530518(19)
XO,YO,ZO 8.8876(5) 8.7197(5) 15.1714(5)

6-Membered Ring (4) C19 --> C20 --> C21 --> C22 --> C23 --> C24 -->

	sp2	sp2	sp2	sp2	sp2	sp2
Dev (A) from CPplane	-0.0009(15)	-0.0012(16)	0.0008(16)	0.0017(16)	-0.0037(15)	0.0033(13)
Cs(I)-Asym-Par (Deg)	0.60(16)	0.22(16)	0.38(16)	0.60(16)	0.22(16)	0.38(16)
C2(I)-Asym-Par (Deg)	0.69(16)	0.88(16)	0.83(16)	0.69(16)	0.88(16)	0.83(16)
Ring Bond Angle(Deg)	119.13(12)	120.99(13)	120.28(13)	120.48(13)	121.53(13)	117.59(11)

Tors(I-J) (Deg)	0.1(2)	0.1(2)	0.2(2)	-0.6(2)	0.77(19)	-0.48(19)
Cs(I-J)-Asym-Par (Deg)	0.7(2)	0.8(2)	0.7(2)	0.7(2)	0.8(2)	0.7(2)
C2(I-J)-Asym-Par (Deg)	0.6(2)	0.1(2)	0.7(2)	0.6(2)	0.1(2)	0.7(2)
Ring Bond Distance (Ang)	1.430(2)	1.358(2)	1.421(2)	1.3614(19)	1.4317(18)	1.4369(18)

Weighted Average Ring Bond Distance = 1.4077(8,149) Ang. - NOTE: 1st esd. Internal, 2nd esd External.
Weighted Average Abs. Torsion Angl. = 0.38(8, 12) Deg. see: e.g. Domenicano et al., Acta Cryst.(1975), B31, 221-234.

No C & P - Puckering Analysis since <Tau> = 0.4 < 5.0 Deg.

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Centroid Cg4   : x ,y ,z       0.34257(4)      0.76480(5)      0.61023(2)
                 XO,YO,ZO        4.5661(6)       8.5172(6)      17.4509(6)
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 10-Membered Ring ( 5)   C11    -->   C12    -->   C13    -->   C14    -->   C15    -->   C16    -->   C17    -->   C18    -->
-------------------------------------------------------------------------------------------------------------------------------
                         sp2           sp2           sp2           sp2           sp2           sp2           sp2           sp2
Dev (A) from CPplane  -0.0023(13)  -0.0099(13)  -0.0233(13)   0.0020(14)   0.0291(15)   0.0063(14)  -0.0136(14)  -0.0272(14)
Cs(I)-Asym-Par (Deg)   161.23(10)     1.73(11)   159.56(10)    195.16(9)    195.09(9)   161.23(10)     1.73(11)   159.56(10)
C2(I)-Asym-Par (Deg)   158.26(10)    225.92(8)   159.95(10)   113.82(10)   113.93(11)   158.26(10)    225.92(8)   159.95(10)
Ring Bond Angle(Deg)   118.47(11)   121.88(11)   121.65(12)   120.36(13)   120.11(13)   121.34(13)   121.54(12)   121.15(12)

Tors(I-J) (Deg)           -178.98(11)   178.39(12)       0.7(2)       1.2(2)      -1.5(2)  -179.53(14)   177.49(13)       1.0(2)
Cs(I-J)-Asym-Par   (Deg)    124.40(11)   126.15(12)   180.26(11)     1.28(11)   178.38(12)   124.40(11)   126.15(12)   180.26(11)
C2(I-J)-Asym-Par   (Deg)    127.26(11)   127.38(12)   176.94(11)    252.58(9)   178.83(12)   127.26(11)   127.38(12)   176.94(11)
Ring Bond Distance (Ang)    1.4145(17)   1.4300(18)   1.3647(19)     1.422(2)     1.357(2)   1.4285(19)   1.3940(19)   1.3961(19)
-------------------------------------------------------------------------------------------------------------------------------
     (Continued)         C19    -->   C24    -->
-------------------------------------------------------------------------------------------------------------------------------
                         sp2           sp2
Dev (A) from CPplane   0.0058(14)   0.0331(13)
Cs(I)-Asym-Par (Deg)    195.16(9)    195.09(9)
C2(I)-Asym-Par (Deg)   113.82(10)   113.93(11)
Ring Bond Angle(Deg)   119.28(12)   120.97(11)

Tors(I-J) (Deg)           1.38(19)    -2.56(17)
Cs(I-J)-Asym-Par   (Deg)    1.28(11)   178.38(12)
C2(I-J)-Asym-Par   (Deg)  252.58(9)   178.83(12)
Ring Bond Distance (Ang)    1.4369(18)   1.4109(17)

Weighted Average Ring Bond Distance = 1.4067(  6, 84) Ang. - NOTE: 1st esd. Internal, 2nd esd External.
Weighted Average Abs. Torsion Angl. =   1.43(  5, 23) Deg.   see: e.g. Domenicano et al., Acta Cryst.(1975), B31, 221-234.


No C & P - Puckering Analysis since <Tau> =  1.4 <    5.0 Deg.


Centroid Cg5   : x ,y ,z       0.58626(3)      0.77786(4)    0.550795(15)
                 XO,YO,ZO        7.8144(4)       8.6626(4)      15.7513(4)
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 10-Membered Ring ( 6)   C11    -->   C12    -->   C17    -->   C18    -->   C19    -->   C20    -->   C21    -->   C22    -->
-------------------------------------------------------------------------------------------------------------------------------
                         sp2           sp2           sp2           sp2           sp2           sp2           sp2           sp2
Dev (A) from CPplane  -0.0200(13)   0.0052(13)   0.0204(14)  -0.0075(14)  -0.0068(14)  -0.0050(15)   0.0030(15)   0.0081(15)
Cs(I)-Asym-Par (Deg)   160.71(10)   112.54(11)    196.03(9)   160.78(11)    160.22(8)   160.71(10)   112.54(11)    196.03(9)
C2(I)-Asym-Par (Deg)   159.72(10)    196.65(9)   113.62(10)   159.65(11)    160.21(9)   159.72(10)    196.65(9)   113.62(10)
Ring Bond Angle(Deg)   118.47(11)   120.62(11)   119.46(12)   121.15(12)   121.59(12)   120.99(13)   120.28(13)   120.48(13)

Tors(I-J) (Deg)           1.46(17)     0.83(19)      -2.1(2)  -178.58(13)   179.64(14)       0.1(2)       0.2(2)      -0.6(2)
Cs(I-J)-Asym-Par   (Deg)  179.01(12)   179.49(10)   179.36(11)   125.82(12)   127.03(11)   179.01(12)   179.49(10)   179.36(11)
C2(I-J)-Asym-Par   (Deg)  179.24(12)    178.76(9)   178.89(11)   127.73(12)   126.07(11)   179.24(12)    178.76(9)   178.89(11)
Ring Bond Distance (Ang)    1.4145(17)   1.4395(18)   1.3940(19)   1.3961(19)     1.430(2)     1.358(2)     1.421(2)   1.3614(19)
-------------------------------------------------------------------------------------------------------------------------------
     (Continued)         C23    -->   C24    -->
-------------------------------------------------------------------------------------------------------------------------------
                         sp2           sp2
Dev (A) from CPplane   0.0009(14)   0.0017(13)
Cs(I)-Asym-Par (Deg)   160.78(11)    160.22(8)
C2(I)-Asym-Par (Deg)   159.65(11)    160.21(9)
Ring Bond Angle(Deg)   121.53(13)   121.43(11)

Tors(I-J) (Deg)         179.33(13)   178.93(11)
Cs(I-J)-Asym-Par   (Deg)  125.82(12)   127.03(11)
C2(I-J)-Asym-Par   (Deg)  127.73(12)   126.07(11)
Ring Bond Distance (Ang)    1.4317(18)   1.4109(17)

Weighted Average Ring Bond Distance = 1.4068(  6, 87) Ang. - NOTE: 1st esd. Internal, 2nd esd External.
Weighted Average Abs. Torsion Angl. =   0.91(  5, 17) Deg.   see: e.g. Domenicano et al., Acta Cryst.(1975), B31, 221-234.


No C & P - Puckering Analysis since <Tau> =  0.9 <    5.0 Deg.


Centroid Cg6   : x ,y ,z       0.42399(3)      0.76874(4)    0.590753(15)
                 XO,YO,ZO        5.6515(4)       8.5611(4)      16.8939(4)
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 14-Membered Ring ( 7)   C11    -->   C12    -->   C13    -->   C14    -->   C15    -->   C16    -->   C17    -->   C18    -->
-------------------------------------------------------------------------------------------------------------------------------
                         sp2           sp2           sp2           sp2           sp2           sp2           sp2           sp2
Dev (A) from CPplane  -0.0283(12)  -0.0201(12)  -0.0260(13)   0.0146(14)   0.0506(15)   0.0212(14)  -0.0147(14)  -0.0352(14)
Cs(I)-Asym-Par (Deg)    135.21(7)    135.52(9)    165.00(9)    213.45(7)    252.77(7)    214.00(8)    191.85(8)    135.21(7)
C2(I)-Asym-Par (Deg)    234.18(7)    234.00(8)    214.24(8)    166.03(8)     96.08(9)    165.32(9)    190.58(8)    234.18(7)
Ring Bond Angle(Deg)   118.47(11)   121.88(11)   121.65(12)   120.36(13)   120.11(13)   121.34(13)   121.54(12)   121.15(12)

Tors(I-J) (Deg)           -178.98(11)   178.39(12)       0.7(2)       1.2(2)      -1.5(2)  -179.53(14)   177.49(13)  -178.58(13)
Cs(I-J)-Asym-Par   (Deg)    230.88(8)   178.76(10)    206.80(9)    146.55(8)   145.97(10)   178.22(10)    178.69(8)    230.88(8)
C2(I-J)-Asym-Par   (Deg)    103.43(10)   178.86(10)    206.26(9)    252.65(7)    252.99(8)   179.12(10)    179.46(8)    103.43(10)
Ring Bond Distance (Ang)    1.4145(17)   1.4300(18)   1.3647(19)     1.422(2)     1.357(2)   1.4285(19)   1.3940(19)   1.3961(19)
-------------------------------------------------------------------------------------------------------------------------------
     (Continued)         C19    -->   C20    -->   C21    -->   C22    -->   C23    -->   C24    -->
-------------------------------------------------------------------------------------------------------------------------------
                         sp2           sp2           sp2           sp2           sp2           sp2
Dev (A) from CPplane  -0.0178(14)  -0.0083(15)   0.0159(15)   0.0309(15)   0.0168(14)   0.0004(12)
Cs(I)-Asym-Par (Deg)    135.52(9)    165.00(9)    213.45(7)    252.77(7)    214.00(8)    191.85(8)
C2(I)-Asym-Par (Deg)    234.00(8)    214.24(8)    166.03(8)     96.08(9)    165.32(9)    190.58(8)
Ring Bond Angle(Deg)   121.59(12)   120.99(13)   120.28(13)   120.48(13)   121.53(13)   121.43(11)

Tors(I-J) (Deg)         179.64(14)       0.1(2)       0.2(2)      -0.6(2)   179.33(13)   178.93(11)
Cs(I-J)-Asym-Par   (Deg)  178.76(10)    206.80(9)    146.55(8)   145.97(10)   178.22(10)    178.69(8)
C2(I-J)-Asym-Par   (Deg)  178.86(10)    206.26(9)    252.65(7)    252.99(8)   179.12(10)    179.46(8)
Ring Bond Distance (Ang)      1.430(2)     1.358(2)     1.421(2)   1.3614(19)   1.4317(18)   1.4109(17)

Weighted Average Ring Bond Distance = 1.4024(  5, 77) Ang. - NOTE: 1st esd. Internal, 2nd esd External.
Weighted Average Abs. Torsion Angl. =   1.06(  4, 17) Deg.   see: e.g. Domenicano et al., Acta Cryst.(1975), B31, 221-234.


No C & P - Puckering Analysis since <Tau> =  1.1 <    5.0 Deg.
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Centroid Cg7   : x ,y ,z       0.50489(3)      0.77359(3)    0.570567(13)
                 XO,YO,ZO        6.7298(4)       8.6151(4)      16.3167(4)
```


Analysis of Short Ring-Interactions with Cg-Cg Distances < 6.0 Ang., Alpha < 20.000 Deg. and Beta < 60.0 Deg.

- Cg(I)   = Plane number I (= ring number in () above)
- Alpha   = Dihedral Angle between Planes I and J (Deg)
- Beta   = Angle Cg(I)-->Cg(J) or Cg(I)-->Me vector and normal to plane I (Deg)
- Gamma   = Angle Cg(I)-->Cg(J) vector and normal to plane J (Deg)
- Cg-Cg   = Distance between ring Centroids (Ang.)
- CgI_Perp = Perpendicular distance of Cg(I) on ring J (Ang.)
- CgJ_Perp = Perpendicular distance of Cg(J) on ring I (Ang.)
- Slippage = Distance between Cg(I) and Perpendicular Projection of Cg(J) on Ring I (Ang).
- P,Q,R,S = J-Plane Parameters for Carth. Coord. (Xo, Yo, Zo)

Cg(I)	Res(I)	Cg(J)	[ARU(J)]	Cg-Cg	Transformed J-Plane P, Q, R, S	Alpha	Beta	Gamma	CgI_Perp	CgJ_Perp	Slippage
Cg2	[1]	-> Cg3	[3466.01]	5.4092(8)	0.4612-0.2473-0.8521 -12.3897	53.79(6)	30.4	84.2	0.5497(5)	4.6663(5)	
Cg3	[1]	-> Cg4	[3566.01]	4.6877(8)	0.4355-0.2207-0.8727 -6.6434	53.32(6)	58.0	7.2	4.6506(5)	2.4807(6)	
Cg4	[1]	-> Cg3	[3466.01]	4.6876(8)	0.4612-0.2473-0.8521 -12.3897	53.32(6)	7.2	58.0	2.4807(6)	4.6505(5)	
Cg4	[1]	-> Cg5	[3466.01]	5.7534(7)	0.4529-0.2377-0.8593 -12.4294	52.76(5)	12.8	64.0	2.5226(6)	5.6114(4)	
Cg6	[1]	-> Cg3	[3466.01]	4.9105(7)	0.4612-0.2473-0.8521 -12.3897	53.48(5)	18.7	72.0	1.5163(4)	4.6500(5)	
Cg7	[1]	-> Cg3	[3466.01]	5.3911(7)	0.4612-0.2473-0.8521 -12.3897	53.95(5)	30.3	84.2	0.5405(4)	4.6540(5)	
			Min or Max	4.688		52.8	7.2	84.2	-4.651	-5.611	

[3466] = -1/2+X,3/2-Y,1-Z
[3566] = 1/2+X,3/2-Y,1-Z

Analysis of X-H...Cg(Pi-Ring) Interactions (H..Cg < 3.0 Ang. - Gamma < 40.0 Deg)

- Cg(J)   = Center of gravity of ring J (Plane number above)
- H-Perp = Perpendicular distance of H to ring plane J
- Gamma   = Angle between Cg-H vector and ring J normal
- X-H..Cg = X-H-Cg angle (degrees)
- X..Cg   = Distance of X to Cg (Angstrom)
- X-H, Pi = Angle of the X-H bond with the Pi-plane (i.e.' Perpendicular = 90 degrees, Parallel = 0 degrees)

X--H(I)		Res(I)	Cg(J)	[ARU(J)]	H..Cg	Transformed J-Plane P, Q, R, S	H-Perp	Gamma	X-H..Cg	X..Cg	X-H,Pi
C2	-H2	[1]	-> Cg3	[5666.01]	2.92	-0.4612-0.2473-0.8521 -14.0868	-2.88	9.73	133	3.6380(15)	51
C4	-H4B	[1]	-> Cg3	[7645.01]	2.97	-0.4612 0.2473 0.8521 8.5848	2.87	15.09	167	3.9373(15)	62
C5	-H5A	[1]	-> Cg2	[1555.01]	2.86	0.4431 0.2277 0.8671 19.1106	2.60	24.74	120	3.4529(15)	29
C5	-H5A	[1]	-> Cg5	[1555.01]	2.91	0.4529 0.2377 0.8593 19.1331	2.60	26.70	142	3.7305(15)	28
C5	-H5A	[1]	-> Cg7	[1555.01]	2.88	0.4457 0.2327 0.8644 19.1084	2.61	24.98	120	3.4772(15)	29
				Min or Max	2.860		-2.881	9.7	167.00	3.453	62.00

[5666] = 1-X,1-Y,1-Z
[7645] = 3/2-X,-1/2+Y,Z
[1555] = X,Y,Z

The Cg(I) refer to the Ring Centre-of-Gravity numbers given in () in the Ring-Analysis above

Cg(I)	x	y	z	Xo	Yo	Zo
Cg2	0.50568(4)	0.77262(5)	0.571257(18)	6.7403(5)	8.6043(5)	16.3364(5)
Cg3	0.66678(4)	0.78298(5)	0.530518(19)	8.8876(5)	8.7197(5)	15.1714(5)
Cg4	0.34257(4)	0.76480(5)	0.61023(2)	4.5661(6)	8.5172(6)	17.4509(6)
Cg5	0.58626(3)	0.77786(4)	0.550795(15)	7.8144(4)	8.6626(4)	15.7513(4)
Cg6	0.42399(3)	0.76874(4)	0.590753(15)	5.6515(4)	8.5611(4)	16.8939(4)
Cg7	0.50489(3)	0.77359(3)	0.570567(13)	6.7298(4)	8.6151(4)	16.3167(4)

:: SPF File spf on :GlieseP200207_0ma_pl.spf

Computationally Optimized Geometry

The data is provided in the .xyz format.

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57

C      1.2481957546  -0.5893021259 3.6919235361
C      2.3892740677  -0.9317315809 3.0939373824
C      2.4794810413  -1.3036730299 1.6389173446
N      1.3940644704  -0.7647445032 0.7665973256
B      0.1412199976  -0.4567134455 1.3502616010
C      -0.0470994723 -0.5470421472 2.9359003229
C      -1.1649180534 -0.0392960411 0.5422832744
C      -2.0471742278 -1.0349949009 0.0560116245
C      -3.2858125967 -0.6686711888 -0.5944438067
C      -3.6117819835 0.6841750732  -0.7310103257
C      -2.7753047010 1.6889240884  -0.2349951475
C      -1.5394677017 1.3201410789  0.4187534977
C      -1.7558690065 -2.4338452636 0.1791792150
C      -2.6100919459 -3.3930298439 -0.2999442853
C      -3.8256688878 -3.0216908252 -0.9430831452
C      -4.1490188879 -1.6988030124 -1.0842198990
C      -3.1141359819 3.0733905386  -0.3544233700
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H      3.5435547722  2.8278868445  -0.5764460623
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