SUPPLEMENTARY MATERIAL

Voronoi-Dirichlet polyhedron of an A point represents a convex polyhedron of minimum volume, containing this point, and bounded by perpendicular planes, which pass through middle points of segments, connecting this point with all other points $\{Y_i\}$. So each crystallographic sort of atoms in the crystal structure is associated with a VDP of definite shape and volume. VDP of an A atom in general has composition AX_nZ_m, where X are atoms, chemically bound with the A and n is the coordination number (**CN**) of A. VDP of Z atoms share faces with VDP of the A atom, but corresponding A…Z contacts are not chemical bonds. As the result the number of VDP faces ($\mathbf{N_f}$) is equal to n + m. There is no chemical bonding between Y_i and A atom if the center of the segment A-Y_i lies out of VDP surface, and Y_i atom is termed **indirect neighbor**. The contacts of this type are caused by steric effects and do not correspond to any chemical interaction. That is why all interactions of the A – #Y type, where #Y is an indirect neighbor of A atom are also stated to be non-valence ones. Additional descriptor of a contact A–Y_i is VDP face rank (**Rank**), it is the number of chemical bonds in the shortest chain connecting the A and Y atoms in the crystal structure. If a face of the VDP of the atom A is formed by the atom Y from another molecule (chain or layer), the rank of the A…Y contact is set to zero, because there is no chain of bonds connecting atoms A and Y in the structure of the compound. For all valence bonds Rank = 1, and for any pare of atoms in the structure of a unique molecule (chain, layer or framework) Rank > 1 (integer and positive). It should be stressed that information about faces Rank may be easily obtained within stereoatomic model of substances, has no need in any Van der Waals atom radii and helps one to objectively divide all non-valence contacts A…Z in the structure of a crystal with any composition and dimension onto intra- (with Rank > 1) and intermolecular (Rank = 0) ones.

The **solid angle** (Ω_{ij}, expressed in percents of 4π steradian) is equal to the segment area of the unit sphere which is cut by the pyramid formed by the VDP face in the base and a central atom at the vertex (fig. 1S).

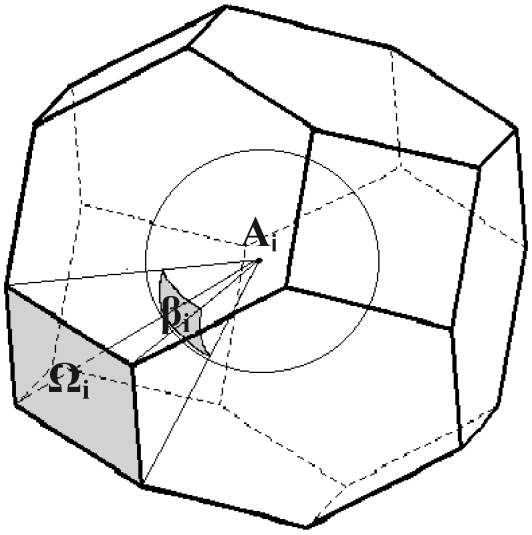


Figure 1S. The Voronoi-Dirichlet polyhedron of an A_i atom in the body-centred cubic lattice. The solid angle Ω_i is equal to the shaded β_i segment of the unit sphere cut off by the pyramid with the A_i atom at the vertex and the Voronoi-Dirichlet face in the base.

Table 1 Calculation of a Voronoi-Dirichlet polyhedron of the tin atom in the structure of (I).

Central atom	Atom of surrounding Y†	CP characteristics‡		Interatomic distance r(A-Y) (Å)	Solid angle of VDP face Ω(A-Y) (%)	Q_i §	Rank §
		CP type	CP path				
Sn1 Coordination polyhedron = O_3N Coordination number = 4	O2	(3, -1)	+	2.089	19.22	0.77	1
	O1	(3, -1)	+	2.118	16.25	0.65	1
	O1^{i}	(3, -1)	+	2.245	15.20	0.61	1
	N1	(3, -1)	+	2.472	11.64	0.47	1
	#H4B	(3, +1)		3.223	3.55	0.14	3
	#H2A	(3, +1)		3.244	0.09	0.00	3
	#H1A^{i}	-		3.251	3.23	0.13	3
	#C3	(3, -1)		3.318	0.00	0.00	2
	H8^{ii}	(3, -1)	+	3.330	9.17	0.37	0
	#H4C	(3, +1)		3.350	2.74	0.11	3
	#H4B	(3, +1)		3.387	0.01	0.00	3
	#H3A	-		3.399	2.50	0.10	3
	H3B^{iii}	(3, -1)	+	3.463	6.73	0.27	0
	H10^{i}	-		3.536	3.47	0.14	6
	C10^{i}	(3, -1)	+	3.633	2.04	0.08	5
	#H6	-		3.714	0.77	0.03	4
	#H9^{ii}	(3, +1)		3.721	0.16	0.01	0
	H6^{iv}	(3, +1)		4.018	2.71	0.11	0
	#C9^{i}	-		4.140	0.28	0.01	6
	#H9^{i}	-		4.370	0.09	0.00	7
	#H7^{iv}	(3, -1)		4.381	0.16	0.01	0

† Symmetry codes: (i) -x, 2-y, -z; (ii) -x+1/2, y-1/2, z; (iii) x, -y+3/2, z+1/2; (iv) x-1/2, -y+3/2, -z; atoms #Y are indirect neighbours in respect to Sn1; ‡ the search for CP for Sn1-Y contacts was carried out for experimental ρ (r) function, among all CPs (3, -1), those belonging to the shortest bond path were marked with + sign; § Q_i – the number of electrons corresponding to a bond, calculated by eq. (III); Rank – the number of chemical bonds in the shortest chain connecting the A and Y atoms in the crystal structure.

Table 2 Experimental and calculated topological parameters of the bonds involving the tin atom in (I).

Bond†	Experiment	AM05-PW	PBE0/6-311G(d,p)
ρ (r), e· Å^{-3}			
N1→Sn1	0.28	0.38	0.31
Sn1–O1	0.52	0.68	0.47
Sn1–O1^{i}	0.45	0.52	0.41
Sn1-O2	0.64	0.71	0.53
Sn1-C10^{i}	0.05	0.04	0.03
Sn1-H8^{ii}	0.03	0.05	
Sn1-H3B^{iii}	0.03		
$\nabla^2\rho$ (r), e· Å^{-5}			
N1→Sn1	2.63	2.89	2.60
Sn1–O1	7.00	8.48	7.03
Sn1–O1^{i}	3.93	6.75	5.50
Sn1-O2	6.54	8.93	8.23
Sn1-C10^{i}	0.38	0.33	0.23
Sn1-H8^{ii}	0.36	0.31	
Sn1-H3B^{iii}	0.28		
H^{e}(r), e· Å^{-3}			
N1→Sn1	-0.03	-0.10	-0.05
Sn1–O1	-0.11	-0.23	-0.07
Sn1–O1^{i}	-0.12	-0.11	-0.06
Sn1-O2	-0.23	-0.25	-0.08
Sn1-C10^{i}	<0.01	<0.01	<0.01
Sn1-H8^{ii}	0.01	<0.01	
Sn1-H3B^{iii}	<0.01		
V^{e}(r), a.u.			
N1→Sn1	-0.04	-0.06	-0.04
Sn1–O1	-0.11	-0.16	-0.09
Sn1–O1^{i}	-0.08	-0.10	-0.08
Sn1-O2	-0.14	-0.17	-0.11
Sn1-C10^{i}	-0.003	-0.002	-0.001
Sn1-H8^{ii}	-0.002	-0.003	
Sn1-H3B^{iii}	-0.002		

† Symmetry codes: (i) -x, 2-y, -z; (ii) -x+1/2, y-1/2, z; (iii) x, -y+3/2, z+1/2.

In accordance with the experimental ρ(r), the O2 atom is involved not only in chemical bonding with tin, nitrogen and carbon atoms, but also in three O…H contacts. They include the intramolecular O2… H3C interaction and two intermolecular O2…H9^{ii} and O2…H4A^{v} contacts (symmetry codes: (ii) –x+1/2, y-1/2, z; (v) x+1/2, y, -z+1/2). The energies of the O2…H interactions calculated using the correlation (1) are equal to 1.40, 0.76 and 0.66 kcal/mol. Similarly to the Si–O and Ge–O bonds in previously published monochelate complexes (Korlyukov, A. A., Lyssenko, K. A. & Antipin, M. Y. (2002). *Russ. Chem. Bull.* **51**, 1423-1432; Korlyukov, A. A., Komissarov, E. A., Antipin, M. Y., Alekseev, N. V., Pavlov, K. V., Krivolapova, O. V., Lahtin, V. G. & Chernyshev, E. A. (2008). *J. Mol. Struct.* **875**, 135-142.), the Sn–O and Sn-N bonds in (I) are characterized by a positive value of the Laplacian of ρ(r) and a negative value

of the local energy density $H^e(r)$ (Table 2S). Thus, these bonds formed by the Sn atom belong to interactions of intermediate type (Bader, R. F. W. & Essen, H. (1984). *J. Chem. Phys.* **80**, 1943.). At the same time, three other bonds (Sn-C and Sn-H) are characterized by $\nabla^2\rho(r) > 0$ and $H^e(r) > 0$ at CP (3, -1), thus are closed shell interactions. Three abovementioned O2…H interactions are also of the closed-shell type.

Table 3 Experimental and calculated AIM charges for atoms in 1.

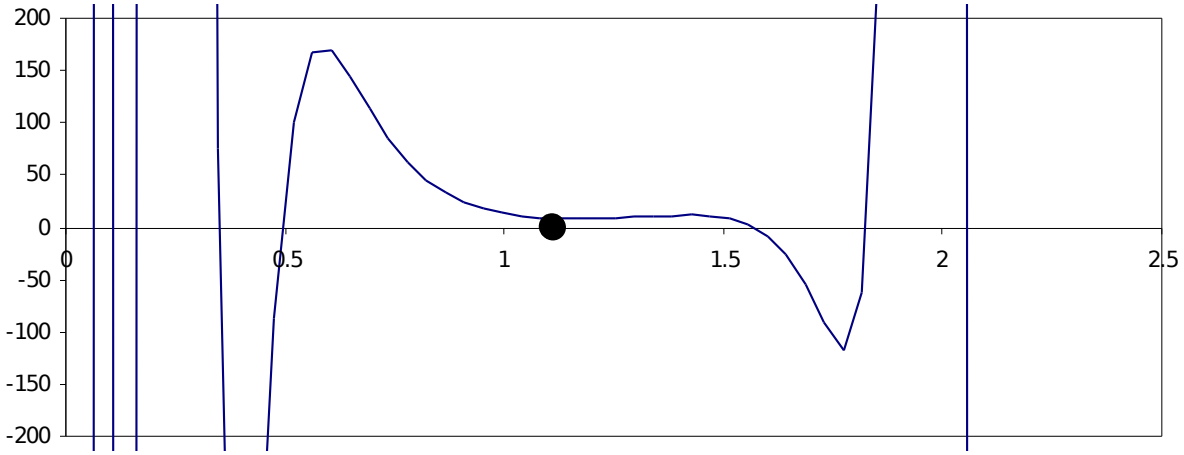
Atom	Experiment	PW-PBE	PBE0/6-311G(d,p)
Sn(1)	1.50	1.30	1.37
O(1)	-0.95	-1.09	-1.24
O(2)	-0.92	-1.14	-1.25
N(1)	-0.82	-1.02	-1.08
C(1)	0.43	0.50	0.53
C(2)	0.01	0.31	0.31
C(3)	0.14	0.32	0.29
C(4)	-0.13	0.30	0.29
C(5)	0.39	0.58	0.63
C(6)	-0.26	-0.06	-0.06
C(7)	-0.22	-0.04	-0.04
C(8)	-0.07	-0.06	-0.05
C(9)	-0.14	-0.05	-0.04
C(10)	-0.26	-0.07	-0.05
H(1B)	0.03	0.00	0.02
H(1A)	0.02	0.00	0.01
H(2A)	0.18	0.02	0.06
H(2B)	0.04	0.04	0.00
H(3C)	0.14	0.00	0.09
H(3B)	0.08	0.01	0.01
H(3A)	0.11	0.04	0.02
H(4C)	0.12	0.03	0.03
H(4B)	0.16	0.03	0.05
H(4A)	0.12	0.00	0.01
H(6)	0.06	0.01	0.02
H(7)	0.08	0.01	0.02
H(8)	0.14	0.01	0.02
H(9)	0.09	0.04	0.02
H(10)	-0.03	0.01	0.02

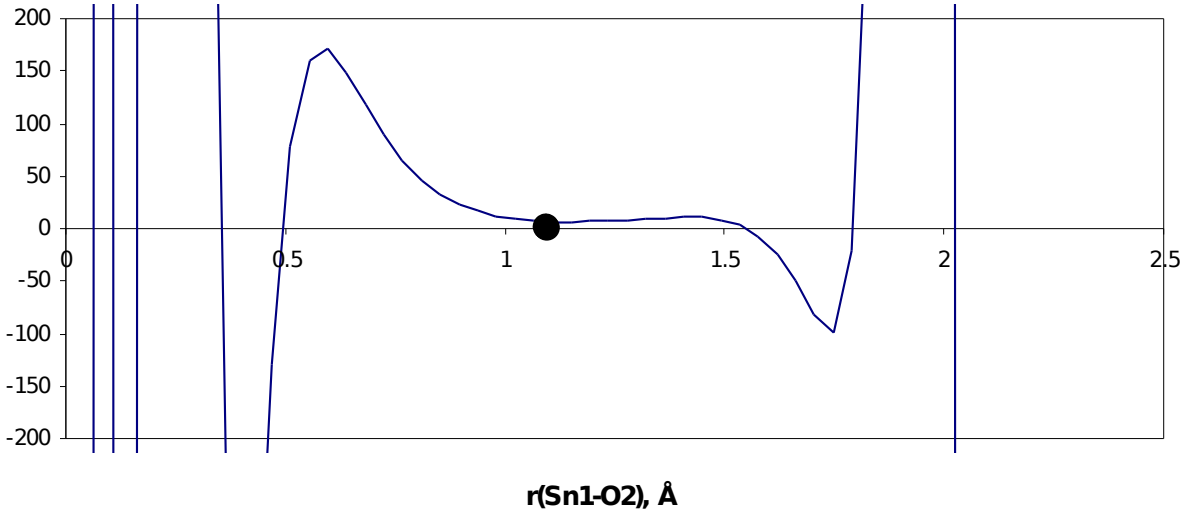
Table 4 Experimental and calculated atomic volumes in 1.

Atom	Experiment	V_{VDP}	PW-PBE	PBE0/6-311G(d,p)
Sn(1)	30.03	17.58	30.20	38.07
O(1)	12.17	11.50	12.12	13.25
O(2)	15.22	11.88	15.38	17.34
N(1)	8.45	6.54	8.82	8.99
C(1)	7.45	3.05	7.70	7.73
C(2)	8.77	3.08	7.84	8.06
C(3)	10.19	2.29	9.29	10.16
C(4)	12.45	2.17	10.03	10.09
C(5)	7.29	7.18	7.36	8.45
C(6)	12.79	5.94	11.76	13.74
C(7)	13.14	6.47	12.87	14.40
C(8)	13.38	5.92	12.90	14.98
C(9)	12.83	6.45	12.68	14.38
C(10)	11.67	6.60	12.00	13.59
H(1B)	7.41	12.03	7.75	8.32
H(1A)	8.05	12.71	8.30	10.12
H(2A)	6.51	11.14	8.03	7.86
H(2B)	6.00	11.08	5.98	10.11
H(3C)	7.47	11.69	8.60	7.59
H(3B)	7.87	13.33	8.30	10.25
H(3A)	8.14	12.13	8.19	9.68
H(4C)	7.78	12.64	7.22	9.54
H(4B)	6.74	13.14	7.42	8.02
H(4A)	6.48	10.90	9.10	10.12
H(6)	7.73	14.78	8.60	10.10
H(7)	9.64	14.81	9.22	10.13
H(8)	7.03	15.31	8.63	10.17
H(9)	7.34	13.21	7.50	10.16
H(10)	8.75	14.37	8.81	9.73

Figure 1S. $\nabla^2\rho$ (r) map in equatorial tin sections including Sn1, O1, O1' (top) and Sn1, N1, O2 (bottom) atoms.

Figure 2S. Map of electron localization function in equatorial tin sections including Sn1, O1, O1' (top) and Sn1, N1, O2 (bottom) atoms.





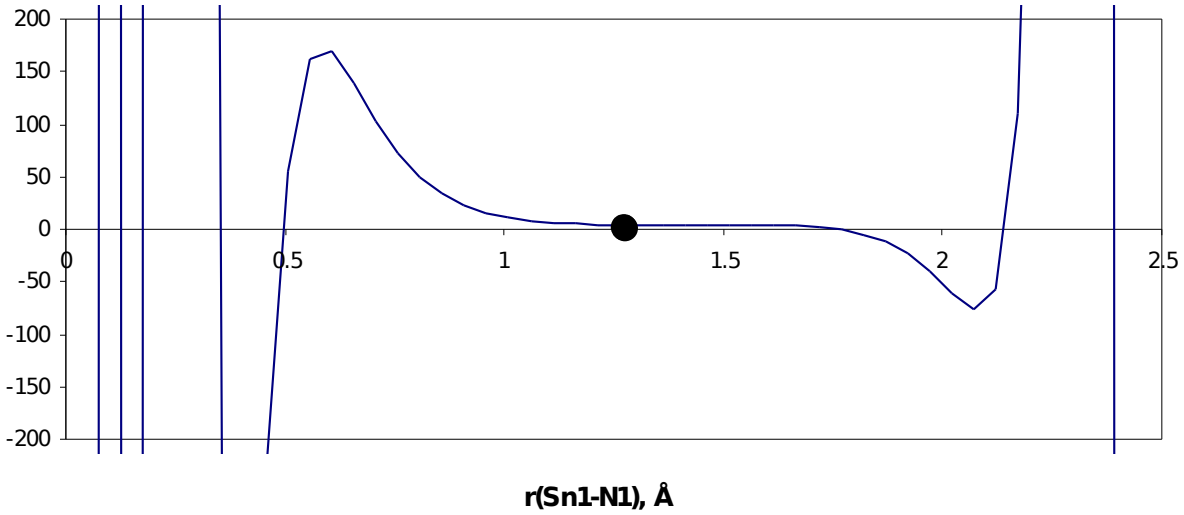


Figure 3S. $\nabla^2\rho$ (r) distribution along bond paths of tin bonds. Position of CP(3; -1) is depicted with black circle.

Optimized unit cell vectors and atomic positions (Å)

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Energy = -1330.023004 e.V.

The topological characteristics (a.u.) in the CP(3,-1) of all interatomic interactions in crystal of **1** according to AM05-PW calculation.

AtomNumber	Density	Laplacian	G(r)	V(r)	E(r)	Energy
ATOM	Sn1					
	0.00638		0.00294		0.00052	
C10	6	0.013891	6	-0.00242	7	-0.75825
	0.05703		0.04423			
N1	1	0.119847	6	-0.05851	-0.01427	-18.335
	0.10148		0.12203			
O1	4	0.351843	6	-0.15611	-0.03408	-48.9193
	0.07668		0.08640			
O1	5	0.27998	6	-0.10282	-0.01641	-32.2187
	0.00691		0.00287		0.00035	
H8	6	0.012945	8	-0.00252	8	-0.78982
	0.10555					
O2	7	0.370598	0.12946	-0.16627	-0.03681	-52.1028
ATOM	O1					
	0.26632		0.22459			
C1	3	-0.5516	8	-0.5871	-0.3625	-183.972
Sn1	0.10148	0.351843	0.12203	-0.15611	-0.03408	-48.9193

	4		6			
	0.07668		0.08640			
Sn1	5	0.27998	6	-0.10282	-0.01641	-32.2187
ATOM	O2					
	0.00836		0.00579		0.00141	
H2a	9	0.028816	3	-0.00438	1	-1.37328
	0.10555					
Sn1	7	0.370598	0.12946	-0.16627	-0.03681	-52.1028
	0.00988		0.00795		0.00201	
H3c	4	0.039882	4	-0.00594	6	-1.86065
	0.00743		0.00417		0.00086	
H9	1	0.020149	1	-0.0033	7	-1.03533
	0.32022		- 0.29704			
C5	6	0.799849	9	-0.79406	-0.49701	-248.827
	0.00660		0.00411		0.00105	
H4a	5	0.020691	6	-0.00306	7	-0.95872
ATOM	N1					
	0.26619		- 0.20817			
C4	5	0.648593	9	-0.57851	-0.37033	-181.281
	0.26351		- 0.20686			
C2	8	0.624791	3	-0.56992	-0.36306	-178.591
	0.26897		- 0.21122			
C3	3	0.663459	2	-0.58831	-0.37709	-184.352
	0.05703		0.04423			
Sn1	1	0.119847	6	-0.05851	-0.01427	-18.335
ATOM	C1					
			- 0.17914			
H1b	0.27501	0.928674	7	-0.59046	-0.41132	-185.027
	0.27369		- 0.17789			
H1a	9	0.920256	9	-0.58586	-0.40796	-183.586
	0.26632		0.22459			
O1	3	-0.5516	8	-0.5871	-0.3625	-183.972
	0.25603		- 0.18168			
C2	8	0.688423	4	-0.53547	-0.35379	-167.796
ATOM	C2					
	0.27233		- 0.17450			
H2b	3	0.924116	5	-0.58004	-0.40553	-181.761
	0.25603		- 0.18168			
C1	8	0.688423	4	-0.53547	-0.35379	-167.796
	0.26351		- 0.20686			
N1	8	0.624791	3	-0.56992	-0.36306	-178.591
	0.27558		- 0.17960			
H2a	8	0.932963	2	-0.59245	-0.41284	-185.649
ATOM	C3					
	0.26897		- 0.21122			
N1	3	0.663459	2	-0.58831	-0.37709	-184.352
	0.26971		- 0.17457			
H3b	2	0.892167	8	-0.5722	-0.39762	-179.304
	0.27301		- 0.17722			
H3a	7	0.916034	9	-0.58347	-0.40624	-182.835
	0.27652		- 0.17904			
H3c	6	0.947727	5	-0.59502	-0.41598	-186.456
ATOM	C4					
	0.27093		- 0.17510			
H4a	2	0.903625	9	-0.57612	-0.40102	-180.534
	0.27510		- 0.17936			
H4b	2	0.928503	1	-0.59085	-0.41149	-185.148
	0.27362		- 0.17813			
H4c	4	0.917924	7	-0.58576	-0.40762	-183.552
	0.26619		- 0.20817			
N1	5	0.648593	9	-0.57851	-0.37033	-181.281

ATOM	C5					
	0.32022		- 0.29704			
O2	6	0.799849	9	-0.79406	-0.49701	-248.827
	0.30695		- 0.25485			
C10	6	0.877158	4	-0.729	-0.47414	-228.439
	0.30721		- 0.25491			
C6	8	0.880202	7	-0.72989	-0.47497	-228.717
ATOM	C6					
	0.00737		0.00395		0.00077	
H1b	8	0.018901	3	-0.00318	2	-0.99671
	0.30721		- 0.25491			
C5	8	0.880202	7	-0.72989	-0.47497	-228.717
	0.27542		- 0.17903			
H6	9	0.934418	8	-0.59168	-0.41264	-185.409
	0.31213		- 0.26470			
C7	7	0.886119	5	-0.75094	-0.48624	-235.314
ATOM	C7					
	0.31213		- 0.26470			
C6	7	0.886119	5	-0.75094	-0.48624	-235.314
	0.31000					
C8	4	-0.88329	0.26049	-0.7418	-0.48131	-232.451
	0.27713		- 0.18072			
H7	5	0.945062	5	-0.59772	-0.41699	-187.3
ATOM	C8					
			0.00288		0.00077	
H4b	0.00517	0.014659	7	-0.00211	8	-0.66096
	0.31032		- 0.26146			
C9	5	0.881665	5	-0.74335	-0.48188	-232.935
	0.31000					
C7	4	-0.88329	0.26049	-0.7418	-0.48131	-232.451
	0.27627		- 0.17977			
H8	4	0.940278	4	-0.59462	-0.41484	-186.329
	0.00540		0.00330		0.00093	
H7	6	0.016941	2	-0.00237	4	-0.74202
ATOM	C9					
	0.31115		- 0.26340			
C10	5	0.880977	2	-0.74705	-0.48365	-234.095
	0.27748		- 0.17924			
H9	2	0.958169	8	-0.59804	-0.41879	-187.401
	0.31032		- 0.26146			
C8	5	0.881665	5	-0.74335	-0.48188	-232.935
ATOM	C10					
	0.00638		0.00294		0.00052	
Sn1	6	0.013891	6	-0.00242	7	-0.75825
	0.27557		- 0.17995			
H10	5	0.930687	5	-0.59258	-0.41263	-185.692
	0.30695		- 0.25485			
C5	6	0.877158	4	-0.729	-0.47414	-228.439
	0.31115		- 0.26340			
C9	5	0.880977	2	-0.74705	-0.48365	-234.095
	0.00807				0.00099	
H2b	7	0.023138	0.00479	-0.0038	5	-1.18933
ATOM	H1b					
	0.00737		0.00395		0.00077	
C6	8	0.018901	3	-0.00318	2	-0.99671
			- 0.17914			
C1	0.27501	0.928674	7	-0.59046	-0.41132	-185.027
ATOM	H1a					
	0.27369		- 0.17789			
C1	9	0.920256	9	-0.58586	-0.40796	-183.586
H3a	0.00813	0.023309	0.00482	-0.00383	0.00099	-1.20027

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ATOM	H2a					
	0.27558	-	0.17960			
C2	8	0.932963	2	-0.59245	-0.41284	-185.649
			0.00117		0.00046	
H7	0.00187	0.006559	5	-0.00071	5	-0.22236
	0.00836		0.00579		0.00141	
O2	9	0.028816	3	-0.00438	1	-1.37328
ATOM	H2b					
	0.00807				0.00099	
C10	7	0.023139	0.00479	-0.0038	5	-1.18933
	0.27233	-	0.17450			
C2	3	0.924116	5	-0.58004	-0.40553	-181.761
ATOM	H3c					
	0.27652	-	0.17904			
C3	6	0.947727	5	-0.59502	-0.41598	-186.456
	0.00988		0.00795		0.00201	
O2	4	0.039882	4	-0.00594	6	-1.86065
ATOM	H3b					
	0.26971	-	0.17457			
C3	2	0.892167	8	-0.5722	-0.39762	-179.304
	0.00532				0.00046	
Sn1	5	0.011186	0.00233	-0.00186	6	-0.58427
ATOM	H3a					
	0.00279				0.00068	
H10	1	0.010147	0.00185	-0.00116	7	-0.36454
	0.00088		0.00053			
H7	5	0.003043	1	-0.0003	0.00023	-0.09415
	0.27301	-	0.17722			
C3	7	0.916034	9	-0.58347	-0.40624	-182.835
	0.00813		0.00482		0.00099	
H1a	1	0.023309	9	-0.00383	9	-1.20027
ATOM	H4c					
	0.00431		0.00269		0.00085	
H6	1	0.014178	1	-0.00184	4	-0.5757
	0.27362	-	0.17813			
C4	4	0.917924	7	-0.58576	-0.40762	-183.552
ATOM	H4b					
			0.00288		0.00077	
C8	0.00517	0.014659	7	-0.00211	8	-0.66096
	0.27510	-	0.17936			
C4	2	0.928503	1	-0.59085	-0.41149	-185.148
ATOM	H4a					
	0.00660		0.00411		0.00105	
O2	5	0.020691	6	-0.00306	7	-0.95872
	0.00360		0.00242		0.00084	
H9	5	0.013095	6	-0.00158	8	-0.49449
	0.27093	-	0.17510			
C4	2	0.903625	9	-0.57612	-0.40102	-180.534
ATOM	H6					
	0.00389		0.00263		0.00089	
H9	8	0.01412	1	-0.00173	9	-0.54246
	0.27542	-	0.17903			
C6	9	0.934418	8	-0.59168	-0.41264	-185.409
	0.00431		0.00269		0.00085	
H4c	1	0.014178	1	-0.00184	4	-0.5757
	0.00204		0.00094		0.00032	
Sn1	3	0.005082	1	-0.00061	9	-0.1919
ATOM	H7					
	0.27713	-	0.18072			
C7	5	0.945062	5	-0.59772	-0.41699	-187.3

	0.00088		0.00053			
H3a	5	0.003043	1	-0.0003	0.00023	-0.09415
			0.00117		0.00046	
H2a	0.00187	0.006559	5	-0.00071	5	-0.22236
	0.00540		0.00330		0.00093	
C8	6	0.016941	2	-0.00237	4	-0.74202
ATOM	H8					
	0.27627	-	0.17977			
C8	4	0.940278	4	-0.59462	-0.41484	-186.329
	0.00691		0.00287		0.00035	
Sn1	6	0.012945	8	-0.00252	8	-0.78982
ATOM	H9					
	0.00389		0.00263		0.00089	
H6	8	0.01412	1	-0.00173	9	-0.54246
	0.00360		0.00242		0.00084	
H4a	5	0.013095	6	-0.00158	8	-0.49449
	0.27748	-	0.17924			
C9	2	0.958169	8	-0.59804	-0.41879	-187.401
	0.00743		0.00417		0.00086	
O2	1	0.020149	1	-0.0033	7	-1.03533
ATOM	H10					
	0.00279				0.00068	
H3a	1	0.010147	0.00185	-0.00116	7	-0.36454
	0.27557	-	0.17995			
C10	5	0.930687	5	-0.59258	-0.41263	-185.692

The optimized atomic positions in the isolated molecule of **1**

Sn	0.412832	1.444941	1.015374
O	-1.020207	0.615962	-0.379428
O	1.580643	2.212422	-0.566836
N	-1.051072	3.308147	0.209827
C	-1.977337	1.406871	-1.035879
C	-1.494291	2.845705	-1.107510
C	-0.280126	4.544995	0.108850
C	-2.156229	3.450916	1.155420
C	2.528773	1.516527	-1.199296
C	3.805638	1.348350	-0.642362
C	4.789864	0.639097	-1.318108
C	4.532525	0.078176	-2.565542
C	3.272124	0.247333	-3.131239
C	2.282548	0.953937	-2.460762
H	-2.943402	1.329679	-0.520381
H	-2.130311	1.041931	-2.061292
H	-0.621189	2.895563	-1.762387
H	-2.284053	3.499228	-1.511241
H	0.583810	4.369711	-0.533415
H	-0.891295	5.366812	-0.291770
H	0.077082	4.830013	1.101926
H	-1.760785	3.764131	2.124360
H	-2.669722	2.497317	1.295868
H	-2.881966	4.201552	0.810331
H	4.010724	1.797013	0.325138
H	5.772059	0.529172	-0.867314
H	5.305623	-0.468757	-3.094546
H	3.055253	-0.174774	-4.108390

H	1.301029	1.088555	-2.904128
Sn	-0.412832	-1.444941	-1.015374
O	1.020207	-0.615962	0.379428
O	-1.580643	-2.212422	0.566836
N	1.051072	-3.308147	-0.209827
C	1.977337	-1.406871	1.035879
C	1.494291	-2.845705	1.107510
C	0.280126	-4.544995	-0.108850
C	2.156229	-3.450916	-1.155420
C	-2.528773	-1.516527	1.199296
C	-3.805638	-1.348350	0.642362
C	-4.789864	-0.639097	1.318108
C	-4.532525	-0.078176	2.565542
C	-3.272124	-0.247333	3.131239
C	-2.282548	-0.953937	2.460762
H	2.943402	-1.329679	0.520381
H	2.130311	-1.041931	2.061292
H	0.621189	-2.895563	1.762387
H	2.284053	-3.499228	1.511241
H	-0.583810	-4.369711	0.533415
H	0.891295	-5.366812	0.291770
H	-0.077082	-4.830013	-1.101926
H	1.760785	-3.764131	-2.124360
H	2.669722	-2.497317	-1.295868
H	2.881966	-4.201552	-0.810331
H	-4.010724	-1.797013	-0.325138
H	-5.772059	-0.529172	0.867314
H	-5.305623	0.468757	3.094546
H	-3.055253	0.174774	4.108390
H	-1.301029	-1.088555	2.904128

Energy = -13238.3471437 a.u.

List of CP(3,-1) and CP(3,+1) and their topological characteristics

ID	Type	Atoms	ρ , e·Å^{-3}	Ve(r), a.e.	$\nabla^2\rho$ (r), e·Å^{-5}	E, kcal/mol
59	(3,-1)	Sn1 O2	0.47	-0.094	7.03	-29.61
60	(3,+1)	Sn1 O2 Sn30 O31	0.17	-0.025	2.90	NA
61	(3,-1)	Sn1 O3	0.53	-0.109	8.23	-34.30
62	(3,-1)	N4 Sn1	0.31	-0.042	2.60	-13.31
63	(3,+1)	Sn1 O2 C5 C6 N4	0.14	-0.018	2.18	NA
64	(3,+1)	Sn1 O3 H17 C6 N4	0.06	-0.007	0.92	NA
65	(3,+1)	Sn1 O3 H19 C7 N4	0.07	-0.008	1.10	NA
66	(3,-1)	H19 C7	1.90	-0.315	-23.51	-98.98
67	(3,-1)	O2 C5	1.75	-0.601	-9.39	-188.57
68	(3,-1)	C7 N4	1.77	-0.429	-16.65	-134.69
69	(3,-1)	C6 C5	1.71	-0.268	-14.74	-83.95
70	(3,-1)	N4 C6	1.76	-0.422	-16.47	-132.27
71	(3,-1)	H21 C7	1.87	-0.314	-22.66	-98.58
72	(3,-1)	H19 O3	0.08	-0.008	1.09	-2.64
73	(3,-1)	N4 C8	1.78	-0.421	-16.86	-132.09
74	(3,-1)	C9 O3	2.05	-0.797	-9.29	-250.08
75	(3,-1)	C10 C9	2.07	-0.410	-20.74	-128.66

76	(3,+1)	C9 C10 C11 C12 C13 C14	0.15	-0.025	3.91	NA
77	(3,-1)	C11 C10	2.09	-0.424	-20.83	-132.98
78	(3,+1)	Sn1 O3 C9 C14 Sn30 O31	0.03	-0.002	0.25	NA
79	(3,-1)	C11 C12	2.08	-0.420	-20.78	-131.76
80	(3,-1)	C9 C14	2.07	-0.410	-20.79	-128.69
81	(3,-1)	C12 C13	2.08	-0.420	-20.77	-131.70
82	(3,-1)	C13 C14	2.09	-0.424	-20.85	-133.07
83	(3,-1)	C5 H15	1.89	-0.314	-23.03	-98.41
84	(3,-1)	O2 Sn30	0.41	-0.076	5.50	-23.77
85	(3,-1)	C5 H16	1.87	-0.311	-22.65	-97.63
86	(3,-1)	O3 H17	0.06	-0.006	0.81	-2.02
87	(3,-1)	H17 C6	1.90	-0.317	-23.38	-99.44
88	(3,-1)	C6 H18	1.83	-0.305	-21.73	-95.74
89	(3,-1)	H20 C7	1.84	-0.307	-21.80	-96.27
90	(3,-1)	H22 C8	1.88	-0.315	-22.78	-98.73
91	(3,-1)	H24 C8	1.84	-0.306	-21.80	-96.13
92	(3,-1)	C8 H23	1.89	-0.314	-23.02	-98.61
93	(3,-1)	H25 C10	1.88	-0.317	-22.85	-99.39
94	(3,-1)	H26 C11	1.89	-0.318	-23.18	-99.92
95	(3,-1)	H27 C12	1.88	-0.320	-23.03	-100.33
96	(3,-1)	C13 H28	1.89	-0.318	-23.19	-99.88
97	(3,-1)	C14 H29	1.88	-0.317	-22.92	-99.57
98	(3,-1)	C14 Sn30	0.03	-0.001	0.23	-0.46
99	(3,-1)	Sn1 O31	0.41	-0.076	5.50	-23.77
100	(3,+1)	Sn1 O3 C9 C10 H44 C34 O31	0.03	-0.002	0.37	NA
101	(3,-1)	O31 Sn30	0.47	-0.094	7.03	-29.61
102	(3,+1)	O2 C5 H15 C39 C38 O32 Sn30	0.03	-0.002	0.37	NA
103	(3,-1)	H15 C39	0.03	-0.002	0.30	-0.70
104	(3,-1)	O32 Sn30	0.53	-0.109	8.23	-34.30
105	(3,-1)	Sn30 N33	0.31	-0.042	2.60	-13.31
106	(3,+1)	Sn30 O31 C34 C35 N33	0.14	-0.018	2.18	NA
107	(3,+1)	Sn30 O32 H46 C35 N33	0.06	-0.007	0.92	NA
108	(3,+1)	Sn30 O32 H48 C36 N33	0.07	-0.008	1.10	NA
109	(3,-1)	C36 H48	1.90	-0.315	-23.51	-98.98
110	(3,-1)	C10 H44	0.03	-0.002	0.30	-0.70
111	(3,+3)	Sn1 O3 C9 C10 C11 C12 C13 C14 Sn30 O31 N33 C34 C35 C37 H44 H52	0.01	-0.001	0.14	NA
112	(3,-1)	C34 O31	1.75	-0.601	-9.39	-188.57
113	(3,-1)	N33 C36	1.77	-0.429	-16.65	-134.69
114	(3,-1)	C34 C35	1.71	-0.268	-14.74	-83.95
115	(3,-1)	C35 N33	1.76	-0.422	-16.47	-132.27
116	(3,-1)	C36 H50	1.87	-0.314	-22.66	-98.58
117	(3,-1)	O32 H48	0.08	-0.008	1.09	-2.64
118	(3,-1)	C37 N33	1.78	-0.421	-16.86	-132.09
119	(3,+1)	Sn1 O2 Sn30 O32 C38 C43	0.03	-0.002	0.25	NA
120	(3,+3)	Sn1 O2 N4 C5 C6 C8 H15 H23 Sn30 O32 C38 C39 C40 C41 C42 C43	0.01	-0.001	0.14	NA
121	(3,-1)	O32 C38	2.05	-0.797	-9.29	-250.08
122	(3,+1)	N4 C6 C5 H15 C39 C40 C41 C42 H23 C8	0.01	-0.001	0.13	NA
123	(3,-1)	C38 C39	2.07	-0.410	-20.74	-128.66
124	(3,+1)	C38 C39 C40 C41 C42 C43	0.15	-0.025	3.91	NA
125	(3,-1)	C39 C40	2.09	-0.424	-20.83	-132.98
126	(3,-1)	C41 C40	2.08	-0.420	-20.78	-131.76

127	(3,+1)	Sn1 N4 C8 H23 C42 C43	0.01	-0.001	0.12	NA
128	(3,-1)	H23 C42	0.02	-0.001	0.16	-0.35
129	(3,-1)	C43 C38	2.07	-0.410	-20.79	-128.69
130	(3,-1)	C42 C41	2.08	-0.420	-20.77	-131.70
131	(3,-1)	Sn1 C43	0.03	-0.001	0.23	-0.46
132	(3,-1)	C43 C42	2.09	-0.424	-20.85	-133.07
133	(3,+1)	C10 C11 C12 C13 H52 C37 N33 C35 C34 H44	0.01	-0.001	0.13	NA
134	(3,-1)	H44 C34	1.89	-0.314	-23.03	-98.41
135	(3,-1)	H45 C34	1.87	-0.311	-22.65	-97.63
136	(3,-1)	H46 O32	0.06	-0.006	0.81	-2.02
137	(3,-1)	C35 H46	1.90	-0.317	-23.38	-99.44
138	(3,-1)	H47 C35	1.83	-0.305	-21.73	-95.74
139	(3,-1)	C36 H49	1.84	-0.307	-21.80	-96.27
140	(3,-1)	C37 H51	1.88	-0.315	-22.78	-98.73
141	(3,+1)	C13 C14 Sn30 N33 C37 H52	0.01	-0.001	0.12	NA
142	(3,-1)	C13 H52	0.02	-0.001	0.16	-0.35
143	(3,-1)	C37 H53	1.84	-0.306	-21.80	-96.13
144	(3,-1)	H52 C37	1.89	-0.314	-23.02	-98.61
145	(3,-1)	C39 H54	1.88	-0.317	-22.85	-99.39
146	(3,-1)	C40 H55	1.89	-0.318	-23.18	-99.92
147	(3,-1)	C41 H56	1.88	-0.320	-23.03	-100.33
148	(3,-1)	H57 C42	1.89	-0.318	-23.19	-99.88
149	(3,-1)	H58 C43	1.88	-0.317	-22.92	-99.57

```
#\#CIF_1.1

#  Archive CIF produced by XD routine XDCIF
#  Created on 13-Apr-04  at 16:37:07
#  Using CIFtbx version 2.6.2 16 Jun 1998

#  Dictionary name : cif_core.dic
#  Dictionary vers : 2.3
#  Request file    : c:/xd2006/lib/xd/xdcif.dat
#  CIF files read  : fft geo lsm


data_SN

_audit_creation_date          '13-Apr-04 T16:37:07-00:00'
_audit_creation_method        'XD routine XDCIF'
_audit_conform_dict_name      cif_core.dic
_audit_conform_dict_version   2.3
_audit_conform_dict_location  ftp://ftp.iucr.org/pub/cif_core.dic

#-----------------------------------------------------------------------#
#                CHEMICAL INFORMATION                                   #
#-----------------------------------------------------------------------#

_chemical_name_systematic            'bis(mu~2~-2-(dimethylamino)ethoxo-N,O,O)-
di(phenolyato-O)-di-tin(II)'
_chemical_name_common                ?
_chemical_formula_moiety             'C20 H30 N2 O4 Sn2'
_chemical_formula_analytical         'C20 H30 N2 O4 Sn2'
_chemical_formula_sum                'C20 H30 N2 O4 Sn2'
_chemical_formula_weight             599.84
_chemical_melting_point              ?

#-----------------------------------------------------------------------#
#                UNIT CELL INFORMATION                                  #
#-----------------------------------------------------------------------#

_symmetry_cell_setting           Orthorhombic
_symmetry_space_group_name_H-M   'P b c a'
_symmetry_space_group_name_Hall  '-P 2ac 2ab'

loop_
   _space_group_symop_id
   _space_group_symop_operation_xyz
1 +X,+Y,+Z
2 1/2-X,-Y,1/2+Z
3 -X,1/2+Y,1/2-Z
4 1/2+X,1/2-Y,-Z
5 -X,-Y,-Z
6 1/2+X,+Y,1/2-Z
7 +X,1/2-Y,1/2+Z
8 1/2-X,1/2+Y,+Z
```

```
_cell_length_a                    13.0745(2)
_cell_length_b                    12.9669(2)
_cell_length_c                    13.6824(3)
_cell_angle_alpha                  90
_cell_angle_beta                   90
_cell_angle_gamma                    90
_cell_volume                      2319.66(7)
_cell_formula_units_Z               4
_cell_measurement_temperature        100.0(2)
_cell_measurement_reflns_used        876
_cell_measurement_theta_min          3.48
_cell_measurement_theta_max          32.09
_cell_measurement_wavelength         0.71073

#------------------------------------------------------------------------------#
#                CRYSTAL INFORMATION                                           #
#------------------------------------------------------------------------------#

_exptl_crystal_description       prism
_exptl_crystal_colour            colorless
_exptl_crystal_size_max          0.19
_exptl_crystal_size_mid          0.12
_exptl_crystal_size_min          0.07
_exptl_crystal_density_meas      ?
_exptl_crystal_density_diffrn    1.718
_exptl_crystal_density_method    'not measured'
_exptl_crystal_F_000             1184
_exptl_special_details
;
?
;

#------------------------------------------------------------------------------#
#                ABSORPTION CORRECTION                                         #
#------------------------------------------------------------------------------#

_exptl_absorpt_coefficient_mu        2.179
_exptl_absorpt_correction_type       multi-scan
_exptl_absorpt_process_details       'SADABS (Sheldrick, 1998)'
_exptl_absorpt_correction_T_min      0.736
_exptl_absorpt_correction_T_max      0.860

#------------------------------------------------------------------------------#
#                DATA COLLECTION                                               #
#------------------------------------------------------------------------------#

_diffrn_source                   'fine-focus sealed tube'
_diffrn_ambient_temperature          100.0(2)
_diffrn_radiation_wavelength         0.71073
_diffrn_radiation_type               MoK\a
_diffrn_radiation_monochromator      graphite
```

```
_diffrn_radiation_probe              ?
_diffrn_detector                     ?
_diffrn_detector_dtime               ?
_diffrn_measurement_device           ?
_diffrn_measurement_device_type      'Bruker Apex II CCD area detector'
_diffrn_measurement_method           'omega scans'
_diffrn_standards_number             ?
_diffrn_standards_interval_count     ?
_diffrn_standards_interval_time      ?
_diffrn_standards_decay_%            ?
_diffrn_standards_decay_corr_max     ?
_diffrn_standards_decay_corr_min     ?
_diffrn_reflns_av_R_equivalents      0.0374
_diffrn_reflns_number                203973
_diffrn_reflns_limit_h_min           -28
_diffrn_reflns_limit_h_max           28
_diffrn_reflns_limit_k_min           -27
_diffrn_reflns_limit_k_max           27
_diffrn_reflns_limit_l_min           -29
_diffrn_reflns_limit_l_max           28
_diffrn_reflns_theta_min             3.14
_diffrn_reflns_theta_max             50.00
_diffrn_reflns_theta_full            50.00
_diffrn_measured_fraction_theta_full 1.00
_diffrn_measured_fraction_theta_max  1.00
_reflns_number_total                 12165
_reflns_number_gt                    7690
_reflns_threshold_expression         'I>2\s(I)'
_diffrn_reflns_reduction_process     ?

#-----------------------------------------------------------------------------#
#               COMPUTER PROGRAMS USED                                        #
#-----------------------------------------------------------------------------#

_computing_data_collection           'APEX2 (Bruker, 2005)'
_computing_cell_refinement           'APEX2 (Bruker, 2005)'
_computing_data_reduction            'APEX2 (Bruker, 2005)'
_computing_structure_solution        'SHELXTL ver. 5.1 (Sheldrick, 2008)'
_computing_structure_refinement      'SHELXTL ver. 5.1 (Sheldrick, 2008)'
_computing_molecular_graphics        'SHELXTL ver. 5.1 (Sheldrick, 2008)'
_computing_publication_material      'SHELXTL ver. 5.1 (Sheldrick, 2008)'

#-----------------------------------------------------------------------------#
#               REFINEMENT INFORMATION                                        #
#-----------------------------------------------------------------------------#

_refine_special_details
;
?
;
_refine_ls_structure_factor_coef     F
_refine_ls_matrix_type               full
```

```
_refine_ls_weighting_scheme           calc
_refine_ls_weighting_details
;
    calc w1 = Fo*sqrt(w2) + sqrt(Fo^2^w2^2^ + sqrt(w2^2^))
    where
    calc w2 = q/[s^2^(Fo^2^) + (0.02 P)^2^ + 1.30 P + 0.00 + 0.00 sin(th)]
    where P = (0.3333 Fo^2^ + 0.6667 Fc^2^)
        q = 1.0
;
_atom_sites_solution_primary          direct
_atom_sites_solution_secondary        difmap
_atom_sites_solution_hydrogens        difmap
_refine_ls_hydrogen_treatment         refall
_refine_ls_extinction_method          none
_refine_ls_extinction_expression      ?
_refine_ls_extinction_coef            ?
_refine_ls_number_reflns              5265
_refine_ls_number_parameters          199
_refine_ls_number_restraints          0
_refine_ls_R_factor_all               0.0226
_refine_ls_R_factor_gt                0.0162
_refine_ls_wR_factor_ref              0.0190
_refine_ls_wR_factor_gt               ?
_refine_ls_wR_factor_all              ?
_refine_ls_goodness_of_fit_gt         ?
_refine_ls_goodness_of_fit_all        ?
_refine_ls_goodness_of_fit_ref        1.5764
_refine_ls_restrained_S_all           ?
_refine_ls_restrained_S_gt            ?
_refine_ls_shift/su_max               0.0003
_refine_ls_shift/su_mean              0.00005
_refine_diff_density_max              0.373
_refine_diff_density_min              -0.346
_refine_diff_density_rms              0.034

#-------------------------------------------------------------------------#
#               ATOMIC TYPES, COORDINATES AND THERMAL PARAMETERS          #
#-------------------------------------------------------------------------#

loop_
   _atom_site_label
   _atom_site_fract_x
   _atom_site_fract_y
   _atom_site_fract_z
   _atom_site_U_iso_or_equiv
   _atom_site_occupancy
   _atom_site_symmetry_multiplicity
SN(1) -0.000279 0.866383 0.034599 0.013 1 8
O(1) -0.057579 1.014413 0.070971 0.014 1 8
O(2) 0.133302 0.887362 0.115958 0.019 1 8
N(1) -0.075611 0.853075 0.20011 0.018 1 8
C(1) -0.106927 1.034284 0.161051 0.017 1 8
```

C(2) -0.068375 0.959098 0.238187 0.018 1 8
C(3) -0.019492 0.780635 0.262022 0.03 1 8
C(4) -0.182842 0.818921 0.189695 0.024 1 8
C(5) 0.207774 0.951172 0.086084 0.016 1 8
C(6) 0.284295 0.916646 0.022104 0.019 1 8
C(7) 0.360939 0.982787 -0.009794 0.026 1 8
C(8) 0.363538 1.085182 0.022699 0.029 1 8
C(9) 0.289357 1.119852 0.08782 0.028 1 8
C(10) 0.212184 1.053539 0.119489 0.022 1 8
H(1B) -0.18863 1.02807 0.15127 0.024 1 8
H(1A) -0.0915 1.11166 0.18598 0.026 1 8
H(2A) 0.01171 0.97298 0.25161 0.025 1 8
H(2B) -0.11057 0.96873 0.30537 0.021 1 8
H(3C) 0.0585 0.80745 0.27212 0.045 1 8
H(3B) -0.05006 0.78073 0.33539 0.034 1 8
H(3A) -0.0205 0.70402 0.23132 0.027 1 8
H(4C) -0.18096 0.73963 0.16538 0.027 1 8
H(4B) -0.22286 0.86608 0.1374 0.027 1 8
H(4A) -0.22161 0.82159 0.25928 0.031 1 8
H(6) 0.27927 0.83744 -0.00159 0.029 1 8
H(7) 0.42016 0.95843 -0.05935 0.036 1 8
H(8) 0.42072 1.13623 -0.00734 0.031 1 8
H(9) 0.29396 1.19727 0.11484 0.034 1 8
H(10) 0.15504 1.08031 0.16977 0.037 1 8
DUM0 0 0 0 0 0 1

loop_
   _atom_site_aniso_label
   _atom_site_aniso_U_11
   _atom_site_aniso_U_22
   _atom_site_aniso_U_33
   _atom_site_aniso_U_23
   _atom_site_aniso_U_13
   _atom_site_aniso_U_12
SN(1) 0.014696 0.011491 0.013014 0.000168 0.000528 -0.000216
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O(2) 0.01406 0.022275 0.019594 0.005973 -0.001093 -0.000594
N(1) 0.017705 0.020367 0.014524 0.004539 0.001199 -0.000832
C(1) 0.018043 0.017742 0.013855 -0.001059 0.003522 0.000793
C(2) 0.01888 0.023799 0.011462 0.000238 0.000945 -0.002431
C(3) 0.03291 0.031838 0.024602 0.014233 -0.000538 0.004024
C(4) 0.021569 0.027195 0.023275 0.000682 0.003439 -0.006923
C(5) 0.013248 0.016899 0.017675 0.000918 -0.001582 0.000601
C(6) 0.015115 0.023083 0.02001 -0.002056 0.000464 -0.001235
C(7) 0.016977 0.037533 0.024734 0.004246 0.001396 -0.006046
C(8) 0.022715 0.030315 0.034452 0.010193 -0.006925 -0.010267
C(9) 0.027598 0.017098 0.040457 0.00311 -0.011422 -0.0022
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MULTIPOLE PARAMETERS

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_atom_rho_multipole_coeff_P3-2
_atom_rho_multipole_coeff_P33
_atom_rho_multipole_coeff_P3-3
_atom_rho_multipole_coeff_P40
_atom_rho_multipole_coeff_P41
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_atom_rho_multipole_coeff_P4-4
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_atom_rho_multipole_kappa_prime3
_atom_rho_multipole_kappa_prime4
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0.00(5) 0.07(4) 0.01(3) 0.04(4) 0.09(4) -0.04(4) 0.06(4) 0.01(4) 0.14(5)
-0.06(5) 0.15(4) -0.19(4) 0.17(5) 0.10(4) -0.06(5) 0.06(3) 0.19(5) 1.054067
1.085557 1.085557 1.085557 1.085557 1.085557 8 3.9443 8 3.9443 8 3.9443 8 3.9443
8 3.9443
O(1) 6.3947 0 -0.021(16) -0.025(16) -0.144(17) -0.118(18) -0.004(18) -0.007(17)

0.004(17) 0.040(17) 0.05(2) 0.02(2) -0.01(2) -0.07(2) 0.02(2) 0.04(2) -0.02(2) 0
0 0 0 0 0 0 0 0 0.998519 0.862591 0.862591 0.862591 0.862591 0.862591 2 4.466 2
4.466 2 4.466 3 4.466 4 4.466
O(2) 6.2536 0 0.007(18) -0.004(16) -0.062(18) -0.09(2) -0.01(2) 0.015(17)
0.039(18) -0.012(18) 0.04(3) -0.03(3) 0.01(2) 0.06(3) 0.00(2) -0.04(2) 0.01(2) 0
0 0 0 0 0 0 0 0 1.000397 0.870586 0.870586 0.870586 0.870586 0.870586 2 4.466 2
4.466 2 4.466 3 4.466 4 4.466
N(1) 5.2249 0 -0.14(2) -0.09(2) -0.01(2) -0.01(2) 0.05(2) 0.01(2) -0.03(2)
0.13(2) 0.18(3) 0.02(3) 0.06(3) 0.05(3) 0.03(3) 0.08(3) -0.11(3) 0 0 0 0 0 0 0 0
0 1.011377 0.895757 0.895757 0.895757 0.895757 0.895757 2 3.83936 2 3.83936 2
3.83936 3 3.83936 4 3.83936
C(1) 4.1037 0 -0.02(3) 0.00(3) -0.03(3) 0.00(3) -0.01(3) 0.07(3) -0.01(3)
-0.02(3) 0.29(4) 0.02(4) 0.00(4) -0.13(4) 0.10(4) -0.01(4) -0.34(4) 0 0 0 0 0 0
0 0 0 1.012921 0.827213 0.827213 0.827213 0.827213 0.827213 2 3.1762 2 3.1762 2
3.1762 3 3.1762 4 3.1762
C(2) 4.1227 0 -0.02(2) 0.03(2) -0.03(2) -0.05(2) 0.01(2) 0.03(2) 0.01(2)
-0.04(2) 0.21(3) 0.01(3) 0.05(3) -0.01(3) -0.03(3) 0.01(3) -0.18(3) 0 0 0 0 0 0
0 0 0 1.017614 1.002 1.002 1.002 1.002 1.002 2 3.1762 2 3.1762 2 3.1762 3 3.1762
4 3.1762
C(3) 4.0725 0 -0.08(3) 0.07(3) 0.09(3) 0.00(3) 0.07(3) -0.05(3) -0.01(3) 0.03(3)
0.22(4) -0.01(4) 0.02(4) 0.05(4) 0.10(4) 0.07(4) -0.20(4) 0 0 0 0 0 0 0 0 0
1.022047 0.949926 0.949926 0.949926 0.949926 0.949926 2 3.1762 2 3.1762 2 3.1762
3 3.1762 4 3.1762
C(4) 4.2139 0 -0.02(3) 0.00(3) -0.07(3) 0.10(3) 0.03(2) 0.00(2) -0.01(3)
-0.01(2) 0.12(4) 0.00(3) -0.05(3) -0.03(3) -0.11(3) 0.03(3) -0.15(3) 0 0 0 0 0 0
0 0 0 1.022047 0.949926 0.949926 0.949926 0.949926 0.949926 2 3.1762 2 3.1762 2
3.1762 3 3.1762 4 3.1762
C(5) 4.2341 0 -0.04(3) 0.05(3) 0 -0.24(3) 0 0 0.05(3) -0.02(3) 0 -0.12(3)
0.00(3) 0 0 0.39(3) 0.05(5) 0 0 0 0 0 0 0 0 0 1.010079 0.894752 0.894752
0.894752 0.894752 0.894752 2 3.1762 2 3.1762 2 3.1762 3 3.1762 4 3.1762
C(6) 4.2027 0 0.08(3) -0.05(3) 0 -0.12(2) 0 0 -0.05(3) -0.02(3) 0 0.04(3)
0.04(3) 0 0 0.18(3) 0.07(4) 0 0 0 0 0 0 0 0 0 1.016884 0.968231 0.968231
0.968231 0.968231 0.968231 2 3.1762 2 3.1762 2 3.1762 3 3.1762 4 3.1762
C(7) 4.2773 0 -0.04(3) 0.00(3) 0 -0.27(3) 0 0 -0.04(3) -0.04(3) 0 0.01(3)
-0.02(4) 0 0 0.37(4) 0.04(4) 0 0 0 0 0 0 0 0 0 1.016884 0.968231 0.968231
0.968231 0.968231 0.968231 2 3.1762 2 3.1762 2 3.1762 3 3.1762 4 3.1762
C(8) 4.0993 0 0.14(3) -0.11(4) 0 -0.11(3) 0 0 -0.04(4) -0.01(4) 0 0.04(3)
0.04(4) 0 0 0.18(4) 0.11(5) 0 0 0 0 0 0 0 0 0 1.016884 0.968231 0.968231
0.968231 0.968231 0.968231 2 3.1762 2 3.1762 2 3.1762 3 3.1762 4 3.1762
C(9) 4.144 0 -0.10(3) 0.23(3) 0 -0.12(3) 0 0 -0.01(3) -0.08(3) 0 0.00(3)
-0.06(4) 0 0 0.23(4) 0.03(5) 0 0 0 0 0 0 0 0 0 1.016884 0.968231 0.968231
0.968231 0.968231 0.968231 2 3.1762 2 3.1762 2 3.1762 3 3.1762 4 3.1762
C(10) 4.1483 0 -0.21(3) 0.08(3) 0 -0.17(3) 0 0 -0.13(3) 0.01(3) 0 0.04(3)
-0.05(3) 0 0 0.27(3) -0.01(4) 0 0 0 0 0 0 0 0 0 1.016884 0.968231 0.968231
0.968231 0.968231 0.968231 2 3.1762 2 3.1762 2 3.1762 3 3.1762 4 3.1762
H(1B) 0.9063 0 0 0 0.11(3) 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1.2 1.2 1.2
1.2 1.2 1.2 0 2 1 2 2 2 3 2 4 2
H(1A) 0.9157 0 0 0 0.12(3) 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1.2 1.2 1.2
1.2 1.2 1.2 0 2 1 2 2 2 3 2 4 2
H(2A) 0.8494 0 0 0 0.16(3) 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1.2 1.2 1.2
1.2 1.2 1.2 0 2 1 2 2 2 3 2 4 2
H(2B) 0.9149 0 0 0 0.04(3) 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1.2 1.2 1.2

1.2 1.2 1.2 0 2 1 2 2 2 3 2 4 2
H(3C) 0.8724 0 0 0 0.13(3) 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1.2 1.2 1.2
1.2 1.2 1.2 0 2 1 2 2 2 3 2 4 2
H(3B) 0.8808 0 0 0 0.07(3) 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1.2 1.2 1.2
1.2 1.2 1.2 0 2 1 2 2 2 3 2 4 2
H(3A) 0.8846 0 0 0 0.09(3) 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1.2 1.2 1.2
1.2 1.2 1.2 0 2 1 2 2 2 3 2 4 2
H(4C) 0.9127 0 0 0 0.13(3) 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1.2 1.2 1.2
1.2 1.2 1.2 0 2 1 2 2 2 3 2 4 2
H(4B) 0.8644 0 0 0 0.11(3) 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1.2 1.2 1.2
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H(4A) 0.9032 0 0 0 0.14(3) 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1.2 1.2 1.2
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H(6) 0.9599 0 0 0 0.13(3) 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1.2 1.2 1.2
1.2 1.2 1.2 0 2 1 2 2 2 3 2 4 2
H(7) 0.8737 0 0 0 0.08(3) 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1.2 1.2 1.2
1.2 1.2 1.2 0 2 1 2 2 2 3 2 4 2
H(8) 0.8916 0 0 0 0.14(3) 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1.2 1.2 1.2
1.2 1.2 1.2 0 2 1 2 2 2 3 2 4 2
H(9) 0.9003 0 0 0 0.13(3) 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1.2 1.2 1.2
1.2 1.2 1.2 0 2 1 2 2 2 3 2 4 2
H(10) 1.0077 0 0 0 0.20(3) 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1.2 1.2 1.2
1.2 1.2 1.2 0 2 1 2 2 2 3 2 4 2

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O(1) C(1) Z O(1) H(1B) Y
O(2) C(5) Z O(2) SN(1) Y
N(1) C(3) Z N(1) C(4) Y
C(1) H(1A) Z C(1) H(1B) Y
C(2) H(2A) Z C(2) H(2B) Y
C(3) H(3C) Z C(3) H(3B) Y
C(4) H(4B) Z C(4) H(4A) Y
C(5) O(2) X C(5) C(6) Y
C(6) H(6) X C(6) C(7) Y
C(7) H(7) X C(7) C(6) Y
C(8) H(8) X C(8) C(9) Y
C(9) H(9) X C(9) C(8) Y
C(10) H(10) X C(10) C(9) Y
H(1B) C(1) Z H(1B) H(1A) Y
H(1A) C(1) Z H(1A) H(1B) Y
H(2A) C(2) Z H(2A) H(2B) Y
H(2B) C(2) Z H(2B) H(2A) Y
H(3C) C(3) Z H(3C) H(3B) Y
H(3B) C(3) Z H(3B) H(3C) Y
H(3A) C(3) Z H(3A) H(3B) Y

H(4C) C(4) Z H(4C) H(4A) Y
H(4B) C(4) Z H(4B) H(4A) Y
H(4A) C(4) Z H(4A) H(4C) Y
H(6) C(6) Z H(6) C(5) Y
H(7) C(7) Z H(7) C(8) Y
H(8) C(8) Z H(8) C(7) Y
H(9) C(9) Z H(9) C(8) Y
H(10) C(10) Z H(10) C(5) Y

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MOLECULAR GEOMETRY
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C(1) C(2) 1.5226404800284 1_555 1_555 yes
C(1) H(1B) 1.0795872165543 1_555 1_555 yes
C(1) H(1A) 1.0787438914737 1_555 1_555 yes
C(2) H(2A) 1.0781886419505 1_555 1_555 yes
C(2) H(2B) 1.0793160434437 1_555 1_555 yes
C(3) H(3C) 1.0861815777331 1_555 1_555 yes
C(3) H(3B) 1.0804844671124 1_555 1_555 yes
C(3) H(3A) 1.0787023264992 1_555 1_555 yes
C(4) H(4C) 1.0809236347853 1_555 1_555 yes
C(4) H(4B) 1.0768773778595 1_555 1_555 yes
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C(7) C(8) 1.4006126841843 1_555 1_555 yes
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C(2) C(1) H(1B) 111.44981353786 1_555 1_555 1_555 yes
C(2) C(1) H(1A) 108.32849240317 1_555 1_555 1_555 yes
H(1B) C(1) H(1A) 107.07493699909 1_555 1_555 1_555 yes
C(1) C(2) H(2A) 109.42991177331 1_555 1_555 1_555 yes
C(1) C(2) H(2B) 110.3059115003 1_555 1_555 1_555 yes
H(2A) C(2) H(2B) 109.38974045215 1_555 1_555 1_555 yes
N(1) C(3) H(3C) 109.82295294121 1_555 1_555 1_555 yes
N(1) C(3) H(3B) 110.60256594946 1_555 1_555 1_555 yes
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H(3C) C(3) H(3B) 103.22104753666 1_555 1_555 1_555 yes
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O(2) C(5) C(10) 120.88650999497 1_555 1_555 1_555 yes
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C(5) C(6) C(7) 120.89430231687 1_555 1_555 1_555 yes
C(5) C(6) H(6) 116.60659610965 1_555 1_555 1_555 yes
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C(8) C(9) H(9) 118.97515716208 1_555 1_555 1_555 yes
C(10) C(9) H(9) 120.73475592579 1_555 1_555 1_555 yes
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C(9) C(10) H(10) 120.22028474333 1_555 1_555 1_555 yes

_publ_section_references
;
Bruker (2005). APEX2 softwarwe package, Bruker AXS Inc., 5465,
East Cheryl Parkway, Madison, WI 5317.

Sheldrick G.M. (1998). SADABS v.2.01, Bruker/Siemens Area Detector
Absorption Correction Program, Bruker AXS, Madison, Wisconsin, USA.

Sheldrick G.M. (2008).  G.M. Sheldrick, Acta Cryst. A64 (2008) 112.
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