PLATON(V-311206)-Run for: xray02 - SHELXL TIME: Mar 4 13:35:29 2010

Crystal Data

Input Cell (Lattice Type: C) - Temp = 200K

a =	30.333(18)	Angstrom	alpha =	90	Degree	a =	6.101	alpha =	105.01	V =	1741.5
b =	6.101(3)		beta =	105.313(11)		b =	15.470	beta =	90.00		
c =	19.513(11)		gamma =	90		c =	19.513	gamma =	101.37		

Reduced Cell (Acta Cryst.(1976),A32,297-298)

V =	3483(3)	Cubic-Angstrom	d(100) =	29.2561	Angstrom
			d(010) =	6.1010	
Lambda(MoKa) =	0.71073	Angstrom	d(001) =	18.8202	

Niggli Values

37.221	239.328	380.757
-78.157	0.000	-18.611

Orthogonalization Matrices

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

(XO)	(	30.33300	0	-5.15323)	(X)	,	(X)	(	0.03297	0	0.00903)	(XO)
(YO) =	(	0	6.10100	0)*(Y)	,	(Y) =	(	0	0.16391	0)*(YO)	
(ZO)	(	0	0	18.82024)	(Z)	,	(Z)	(	0	0	0.05313)	(ZO)

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 C2/c No: 15, Laue: 2/m [Hall: -C 2yc]

Lattice Type mC, Centric, Monoclinic, Order 8(2) [Schoenflies: C2h^6]

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

(Not-Rule Rounded) Coordinates of Unique Residue(s) Identified. Standard Deviations in the Last Digit are in Parentheses.

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          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	S
Cov.Rad(Ang):	0.68	0.35	1.04
Atom Volume :	13.87	5.08	25.20
Atom Number :	6	1	16
Atom Weight :	12.010	1.008	32.07
Scat.Fact.f0:	5.999	1.000	16.000
Scat.Fact.f':	0.003	0.000	0.125
Scat.Fact.f":	0.002	0.000	0.123
Mu/Rho(MoKa):	0.58	0.37	9.99
Elem. Type :	--	--	--

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Sources - Cov. Radii : Manual Cambridge Crystallographic Data Base
        - Atom Volume: D.W.M. Hofmann (2002). Acta Cryst. B58, 489-493
        - Atomic Wt. : SHELXL97                                                                                    NOMOVE
        - Scat. Fact.: SHELXL97 (International Tables)
        - mu/rho     : International Tables C, table 4.2.4.2, p193-199
```

Flags	Label	Fractional Coordinates (x,y,z)			Orthogonal Coordinates (XO,YO,ZO)			Site	SSN	*SSOF = S.O.F	Move	Type
-	S(501)	0.33589	0.03489	0.13729	9.4809	0.2129	2.5838	1	1	1	-	D/A
-	S(502)	0.09445	0.04914	0.11878	2.2528	0.2998	2.2355	1	1	1	-	D/A
-	C(501)	0.18942	0.32181	0.19330	4.7496	1.9634	3.6379	1	1	1	-	-
-	C(502)	0.18542	0.11637	0.16082	4.7956	0.7099	3.0267	1	1	1	-	-
-	C(503)	0.25119	0.20852	0.11822	7.0101	1.2722	2.2249	1	1	1	-	-
-	C(504)	0.21726	0.06609	0.12240	5.9595	0.4032	2.3036	1	1	1	-	-
-	C(505)	0.22398	0.46665	0.18802	5.8250	2.8470	3.5387	1	1	1	-	-
-	C(506)	0.25480	0.41361	0.15225	6.9441	2.5235	2.8654	1	1	1	-	-
-	C(507)	0.37103	-0.05456	0.08141	10.8348	-0.3329	1.5321	1	1	1	-	-
-	C(508)	0.14998	-0.04501	0.16840	3.6814	-0.2746	3.1694	1	1	1	-	-
-	C(509)	0.28501	0.14715	0.07404	8.2638	0.8977	1.3934	1	1	1	-	-
-	C(510)	0.05383	-0.12568	0.14236	0.8992	-0.7668	2.6792	1	1	1	-	-
-	C(511)	0.00731	-0.04581	0.10878	-0.3389	-0.2795	2.0473	1	1	1	-	-
-	C(512)	0.38261	0.13846	0.04031	11.3979	0.8447	0.7586	1	1	1	-	-
-	C(513)	0.34563	-0.24123	0.03254	10.3164	-1.4718	0.6124	1	1	1	-	-
-	C(514)	0.41322	-0.14448	0.12508	11.8896	-0.8815	2.3540	1	1	1	-	-
-	C(515)	0.05058	-0.33417	0.08632	1.0894	-2.0388	1.6247	1	1	1	-	-
-	C(516)	0.06904	-0.38377	0.15390	1.3012	-2.3414	2.8965	1	1	1	-	-
-	C(517)	0.05828	-0.11638	0.22562	0.6051	-0.7101	4.2463	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	S
1	1	0.208	0.027	0.128	268.31	1	8	17	-	2
				Unit Cell Weight =	2146.48		136	0	16	

Calculated Analysis (Percent) = 76.1 0.0 23.9

Moiety_Formula = C17 S2

Sum_Formula = C17 S2

Formula_Weight = 268.31 [Note: Based on SHELXL97 Atomic Weights]

Formula_Z = 8

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

Calculated Density = 1.0234(9) g cm-3 [= Mg m-3]

F(000) = 1072.0 [1074.33]

mu(MoKa) = 2.89 cm-1 = 0.289 mm-1

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

Resonant Scattering = 0.73 Percent - (Girard,E. et al. (2003). Acta Cryst. D59, 1914-1922)

Predicted Volume = 2289.5[2268.2] Ang**3, 298[200]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"

(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	S501	0.07664						0.07664				
2	S502	0.08103						0.08103				
3	C501	0.05520						0.05520				
4	C502	0.04868						0.04868				
5	C503	0.05200						0.05200				
6	C504	0.05310						0.05310				
7	C505	0.05468						0.05468				
8	C506	0.05960						0.05960				
9	C507	0.06012						0.06012				
10	C508	0.07668						0.07668				
11	C509	0.07468						0.07468				
12	C510	0.06273						0.06273				
13	C511	0.12295						0.12295				
14	C512	0.11581						0.11581				
15	C513	0.16172						0.16172				
16	C514	0.15687						0.15687				
17	C515	0.21525						0.21525				
18	C516	0.21540						0.21540				
19	C517	0.24976						0.24976				

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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	S
Average	0.1049	0.1080	0.0000	0.0788

Minimum	0.0487	0.0487	0.0000	0.0766
Maximum	0.2498	0.2498	0.0000	0.0810
Ratio	5.1306	5.1306	0.0000	1.0573
Number	19	17	0	2

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
-	S(501)	- C(507) C(509)	1	103	103	103.5	1.799	1.835	2	14			
-	S(502)	- C(508) C(510)	1	106	106	106.4	1.780	1.801	2	15			
-	C(501)	- C(502) C(505)	1	121	121	120.8	1.395	1.395	2	3			?
-	C(502)	- C(501) C(504) C(508)	3	117	122	120.0	1.395	1.494	3	7	sp2		
-	C(503)	- C(504) C(506) C(509)	3	120	120	120.0	1.366	1.550	3	5	sp2		
-	C(504)	- C(502) C(503)	1	122	122	121.9	1.366	1.404	2	4			?
-	C(505)	- C(501) C(506)	1	122	122	121.6	1.345	1.395	2	1			?
-	C(506)	- C(503) C(505)	1	119	119	118.7	1.345	1.407	2	2			?
-	C(507)	- S(501) C(512) C(513) C(514)	6	108	113	109.5	1.445	1.799	4	10	sp3		
-	C(508)	- S(502) C(502)	1	109	109	109.4	1.494	1.801	2	13			?
-	C(509)	- S(501) C(503)	1	106	106	106.2	1.550	1.835	2	11			?
-	C(510)	- S(502) C(511) C(515) C(516) C(517)	10	47	132	102.9	1.473	1.780	5	12			A
-	C(511)	- C(510)	0	0	0	0.0	1.473	1.473	1	8			?
-	C(512)	- C(507)	0	0	0	0.0	1.517	1.517	1	6			?
-	C(513)	- C(507)	0	0	0	0.0	1.553	1.553	1	6			?
-	C(514)	- C(507)	0	0	0	0.0	1.445	1.445	1	6			?
-	C(515)	- C(510) C(516)	1	65	65	65.4	1.324	1.663	2	9			A
-	C(516)	- C(510) C(515)	1	67	67	67.3	1.324	1.640	2	9			A
-	C(517)	- C(510)	0	0	0	0.0	1.595	1.595	1	8			?

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. 0.0006 Ang. , Abs. Angle Error 0.011 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 ().

S(501)	C(507)	1.7992	S(501)	C(509)	1.8351	S(502)	C(508)	1.8009	S(502)	C(510)	1.7795
C(501)	C(502)	1.3952	C(501)	C(505)	1.3955	C(502)	C(504)	1.4041	C(502)	C(508)	1.4937
C(503)	C(504)	1.3657	C(503)	C(506)	1.4073	C(503)	C(509)	1.5503	C(505)	C(506)	1.3455
C(507)	C(512)	1.5173	C(507)	C(513)	1.5530	C(507)	C(514)	1.4453	C(510)	C(511)	1.4730
C(510)	C(515)	1.6632	C(510)	C(516)	1.6396	C(510)	C(517)	1.5954	C(515)	C(516)	1.3244

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

C(507)	S(501)	C(509)	103.48	C(508)	S(502)	C(510)	106.44	C(502)	C(501)	C(505)	120.82
C(501)	C(502)	C(504)	116.69	C(501)	C(502)	C(508)	121.71	C(504)	C(502)	C(508)	121.57
C(504)	C(503)	C(506)	120.23	C(504)	C(503)	C(509)	119.96	C(506)	C(503)	C(509)	119.79
C(502)	C(504)	C(503)	121.90	C(501)	C(505)	C(506)	121.62	C(503)	C(506)	C(505)	118.72
S(501)	C(507)	C(512)	109.99	S(501)	C(507)	C(513)	108.51	S(501)	C(507)	C(514)	109.39
C(512)	C(507)	C(513)	113.02	C(512)	C(507)	C(514)	108.28	C(513)	C(507)	C(514)	107.58
S(502)	C(508)	C(502)	109.39	S(501)	C(509)	C(503)	106.17	S(502)	C(510)	C(511)	109.52
S(502)	C(510)	C(515)	102.31	S(502)	C(510)	C(516)	114.97	S(502)	C(510)	C(517)	111.34
C(511)	C(510)	C(515)	94.42	C(511)	C(510)	C(516)	125.49	C(511)	C(510)	C(517)	104.76
C(515)	C(510)	C(516)	47.27	C(515)	C(510)	C(517)	132.15	C(516)	C(510)	C(517)	87.09
C(510)	C(515)	C(516)	65.43	C(510)	C(516)	C(515)	67.30				

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

C(505)	C(501)	C(502)	C(504)	-0.84	C(505)	C(501)	C(502)	C(508)	177.29	C(502)	C(501)	C(505)	C(506)	-0.60
C(501)	C(502)	C(504)	C(503)	1.48	C(508)	C(502)	C(504)	C(503)	-176.65	C(501)	C(502)	C(508)	S(502)	71.09
C(504)	C(502)	C(508)	S(502)	-110.87	C(506)	C(503)	C(504)	C(502)	-0.72	C(509)	C(503)	C(504)	C(502)	-178.94
C(504)	C(503)	C(506)	C(505)	-0.74	C(509)	C(503)	C(506)	C(505)	177.47	C(504)	C(503)	C(509)	S(501)	-96.65
C(506)	C(503)	C(509)	S(501)	85.13	C(501)	C(505)	C(506)	C(503)	1.39	C(512)	C(507)	S(501)	C(509)	60.22
C(513)	C(507)	S(501)	C(509)	-63.88	C(514)	C(507)	S(501)	C(509)	179.02	C(502)	C(508)	S(502)	C(510)	-170.50
C(503)	C(509)	S(501)	C(507)	175.01	C(511)	C(510)	S(502)	C(508)	174.78	C(515)	C(510)	S(502)	C(508)	-85.95
C(516)	C(510)	S(502)	C(508)	-37.59	C(517)	C(510)	S(502)	C(508)	59.40	S(502)	C(510)	C(515)	C(516)	112.74
C(511)	C(510)	C(515)	C(516)	-136.17	C(517)	C(510)	C(515)	C(516)	-21.68	S(502)	C(510)	C(516)	C(515)	-83.69
C(511)	C(510)	C(516)	C(515)	58.01	C(517)	C(510)	C(516)	C(515)	164.08					

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
S -- C	4		1.7795	1.8351	1.8037	1.72		.....31.....
C -- C	16		1.3244	1.6632	1.4730	1.36		.....12422212.....

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.
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