PLATON(V-311206)-Run for: joer04 - SHELXL TIME: Jun 9 13:21:22 2011

Crystal Data

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

a =	15.327(3)	Angstrom	alpha =	90	Degree	a =	15.163	alpha =	96.22
b =	15.163(3)		beta =	96.222(4)		b =	15.327	beta =	90.00
c =	16.209(3)		gamma =	90		c =	16.209	gamma =	90.00
V =	3744.8(13)	Cubic-Angstrom	d(100) =	15.2367	Angstrom				
			d(010) =	15.1630					
Lambda(MoKa) =	0.71073	Angstrom	d(001) =	16.1135					

Reduced Cell (Acta Cryst.(1976),A32,297-298): a = 15.163, b = 15.327, c = 16.209, alpha = 96.22, beta = 90.00, gamma = 90.00, V = 3744.8

Niggli Values: 229.917 234.917 262.732 -26.926 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)

$$\begin{pmatrix} XO \\ YO \\ ZO \end{pmatrix} = \begin{pmatrix} 15.32700 & 0 & -1.75675 \\ 0 & 15.16300 & 0 \\ 0 & 0 & 16.11352 \end{pmatrix} \begin{pmatrix} X \\ Y \\ Z \end{pmatrix}, \quad \begin{pmatrix} X \\ Y \\ Z \end{pmatrix} = \begin{pmatrix} 0.06524 & 0 & 0.00711 \\ 0 & 0.06595 & 0 \\ 0 & 0 & 0.06206 \end{pmatrix} \begin{pmatrix} XO \\ YO \\ ZO \end{pmatrix}$$

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 P21/c No: 14, Laue: 2/m [Hall: -P 2ybc]

Lattice Type mP, Centric, Monoclinic, Order 4(2) [Schoenflies: C2h^5]

Nr	***** Symmetry Operation(s) *****		
1	X ,	Y ,	Z
2	- X ,	1/2 + Y ,	1/2 - Z
3	- X ,	- Y ,	- Z
4	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
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Atom Types :	C	H	Br	N	Zn
Cov.Rad(Ang):	0.68	0.35	1.21	0.68	1.45
Atom Volume :	13.87	5.08	32.70	11.80	39.00
Atom Number :	6	1	35	7	30
Atom Weight :	12.010	1.008	79.90	14.01	65.39
Scat.Fact.f0:	5.999	1.000	34.993	6.995	29.985
Scat.Fact.f':	0.003	0.000	-0.290	0.006	0.284
Scat.Fact.f":	0.002	0.000	2.460	0.003	1.430
Mu/Rho(MoKa):	0.58	0.37	75.37	0.84	53.97
Elem. Type :	--	--	HL	--	TR

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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
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Flags	Label	Fractional Coordinates (x,y,z)			Orthogonal Coordinates (XO,YO,ZO)			Site	SSN	*SSOF = S.O.F	Move	Type
-	Br(51)	0.53700	0.17054	0.16725	7.9367	2.5859	2.6950	1	1	1	-	D/A
-	Br(52)	0.68762	0.35910	0.11714	10.3334	5.4450	1.8875	1	1	1	-	D/A
-	Br(53)	0.67609	0.24251	0.21931	9.9772	3.6772	3.5339	1	1	1	-	D/A
-	Br(54)	0.78782	0.13208	0.20226	11.7196	2.0027	3.2591	1	1	1	-	D/A

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	Br	N	Zn
1	1	0.672	0.226	0.176	319.60	1	4	-	-	4	-	-
				Unit Cell Weight =	1278.40			0	0	16	0	0
				Calculated Analysis (Percent) =				0.0	0.0	100.0	0.0	0.0

Moiety_Formula = Br4

Sum_Formula = Br4

Formula_Weight = 319.60 [Note: Based on SHELXL97 Atomic Weights]

Formula_Z = 4

SpaceGroup_Z = 4 ===> Z' = 4 / 4 = 1.000

Calculated Density = 0.5669(2) g cm-3 [= Mg m-3]

F(000) = 560.0 [556.64]

mu(MoKa) = 42.73 cm-1 = 4.273 mm-1

Resonant Scattering = 10.00 Percent - (Girard,E. et al. (2003). Acta Cryst. D59, 1914-1922)

Predicted Volume = 523.2[518.3] Ang**3, 298[200]K - (D.W.M. Hofmann (2002). Acta Cryst. B58, 489-493)

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

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	Br51	0.02760						0.02760				
2	Br52	0.03222						0.03222				
3	Br53	0.03435						0.03435				
4	Br54	0.03848						0.03848				

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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	Br	N	Zn
Average	0.0332	0.0000	0.0000	0.0332	0.0000	0.0000
Minimum	0.0276	0.0000	0.0000	0.0276	0.0000	0.0000
Maximum	0.0385	0.0000	0.0000	0.0385	0.0000	0.0000
Ratio	1.3942	0.0000	0.0000	1.3942	0.0000	0.0000
Number	4	0	0	4	0	0

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
-	Br(51) - Br(53) ------- ------- ------- ------- ------- ------- ------- -------	0	0	0	0.0	2.461	2.461	1	2			
-	Br(52) - Br(53) ------- ------- ------- ------- ------- ------- ------- -------	0	0	0	0.0	2.442	2.442	1	2			
-	Br(53) - Br(51) Br(52) Br(54) ------- ------- ------- ------- ------- -------	3	102	109	105.1	2.432	2.461	3	1			
-	Br(54) - Br(53) ------- ------- ------- ------- ------- ------- ------- -------	0	0	0	0.0	2.432	2.432	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. 0.0002 Ang. , Abs. Angle Error 0.004 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 ().

Br(51) -	Br(53)	2.4613	Br(52) -	Br(53)	2.4419	Br(53) -	Br(54)	2.4321

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

Br(51) -	Br(53) -	Br(52)	102.25	Br(51) -	Br(53) -	Br(54)	104.49	Br(52) -	Br(53) -	Br(54)	108.53

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
Br -- Br	3		2.4321	2.4613	2.4451	2.42		.....3.....

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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