PLATON(V-311206)-Run for: joer009 in Cc TIME: Nov 11 10:56:23 2010

(C) 1980-2007 A.L.Spek

Crystal Data

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

						Reduced Cell					
a =	10.861(3)	Angstrom	alpha =	90	Degree	a =	10.248	alpha =	100.18	V =	1286.6
b =	17.383(4)		beta =	109.479(4)		b =	10.248	beta =	100.18		
c =	14.457(4)		gamma =	90		c =	14.457	gamma =	116.00		
V =	2573.2(12)	Cubic-Angstrom	d(100) =	10.2394	Angstrom						
			d(010) =	17.3827							
Lambda(MoKa) =	0.71073	Angstrom	d(001) =	13.6295							

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

Niggli Values: 105.030 105.030 209.005 / -26.180 -26.180 -46.049

Orthogonalization Matrices

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

$$\begin{pmatrix} XO \\ YO \\ ZO \end{pmatrix} = \begin{pmatrix} 10.86100 & 0 & -4.82085 \\ 0 & 17.38300 & 0 \\ 0 & 0 & 13.62954 \end{pmatrix} \begin{pmatrix} X \\ Y \\ Z \end{pmatrix} , \quad \begin{pmatrix} X \\ Y \\ Z \end{pmatrix} = \begin{pmatrix} 0.09207 & 0 & 0.03257 \\ 0 & 0.05753 & 0 \\ 0 & 0 & 0.07337 \end{pmatrix} \begin{pmatrix} XO \\ YO \\ ZO \end{pmatrix}$$

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 Cc No: 9, Laue: 2/m [Hall: C -2yc]

Lattice Type mC, Acentric, Monoclinic, Order 4(2) [Schoenflies: Cs^4]

ACHIRAL - See P.G. Jones, Acta Cryst. (1986), A42, 57.

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

ADDSYM - CHECK (cf. MISSYM (C): Le Page, Y., J. Appl. Cryst. (1987), 20, 264-269; J. Appl. Cryst. (1988), 21, 983-984)

- ADDSYM Search on ALL NON-H Chemical Types [Max NonFit 20 Perc]
- Number of Input Atoms Included in Search 31 (Unitcell 62)
- Density based on Input Atom Set = 1.682 g.cm-3 - Vol / Non-H atom = 20.8 Ang+3
- The Structure Implies the Following Symmetry Elements Subject to the Criteria:

Criteria: 1.00 Deg (Metric), 0.25 Ang (Rot.), 0.45 Ang (Inv), 0.45 Ang (Transl)

Symm. Elem	Input Cell_Row	Reduced Cell_Row	(Ang) d	Typ	Dot	(Deg) Angle	(%) Fit	(Ang) MaxDev.		Input Cell x	y	z
c	[0 1 0]	[1-1 0]	17.38	2	2	0.00	100	0	through	0	0	0
									Glide =	0	0	1/2

T.R.A.N.S.F.O.R.M.A.T.I.O.N M.A.T.R.I.X for CELL and HKL DATA

Reduced->Convent			Input->Reduced			T = Input->Convent:			a' = T a
(1	1	0)	(1/2	-1/2	0)	(1	0	0)	Det(T)
(-1	1	0) X	(1/2	1/2	0) =	(0	1	0)	=
(0	0	1)	(0	0	1)	(0	0	1)	1.000

Cell	Lattice	a	b	c	Alpha	Beta	Gamma	Volume	CrystalSystem	Laue
Input	mC	10.861	17.383	14.457	90.00	109.48	90.00	2573	Monoclinic	2/m
Reduced	P	10.248	10.248	14.457	100.18	100.18	116.00	1287		
Convent	mC	10.861	17.383	14.457	90.00	109.48	90.00	2573	Monoclinic	2/m

:: *** No Obvious Extra Crystallographic Symmetry was Detected ***

:: Note: Rerun in EQUAL Atom Type Mode for more Checks

(Not-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	Br	N	O	Pd
Cov.Rad(Ang):	0.68	0.35	1.21	0.68	0.68	1.50
Atom Volume :	13.87	5.08	32.70	11.80	11.39	35.00
Atom Number :	6	1	35	7	8	46
Atom Weight :	12.010	1.008	79.90	14.01	16.00	106.42
Scat.Fact.f0:	5.999	1.000	34.993	6.995	7.999	46.001
Scat.Fact.f':	0.003	0.000	-0.290	0.006	0.011	-0.999
Scat.Fact.f":	0.002	0.000	2.460	0.003	0.006	1.007
Mu/Rho(MoKa):	0.58	0.37	75.37	0.84	1.22	24.67
Elem. Type :	--	--	HL	--	--	TR

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

Residue = 1

Flags	Label	Fractional Coordinates (x,y,z)			Orthogonal Coordinates (XO,YO,ZO)			Site	SSN*SSOF =	S.O.F	Move	Type
-	NI	0.69639	0.24419	0.42708	5.5047	4.2448	5.8208	1	1	1	3.545	Met
-	Br1	0.84437	0.12979	0.47333	6.8889	2.2561	6.4512	1	1	1	3.545	D/A
-	Br2	0.62846	0.22842	0.57546	4.0516	3.9706	7.8432	1	1	1	3.545	D/A
-	N1	0.54564	0.39622	0.41371	3.9318	6.8876	5.6386	1	1	1	3.545	D/A
-	N2	0.48654	0.32644	0.28372	3.9165	5.6745	3.8670	1	1	1	3.545	D/A
-	N3	0.82911	0.25270	0.26817	7.7122	4.3927	3.6551	1	1	1	3.545	D/A
-	N4	0.62068	0.25649	0.21581	5.7008	4.4585	2.9414	1	1	1	3.545	D/A
-	C1	0.56696	0.32865	0.37376	4.3560	5.7129	5.0942	1	1	1	3.545	-
-	C2	0.44460	0.43585	0.34199	3.1801	7.5764	4.6611	1	1	1	3.545	-
-	C3	0.40744	0.39059	0.26090	3.1675	6.7897	3.5559	1	1	1	3.545	-
-	C4	0.67684	0.50622	0.50337	4.9244	8.7997	6.8607	1	1	1	3.545	-
-	C5	0.75944	0.53258	0.60599	5.3268	9.2578	8.2594	1	1	1	3.545	-
-	C6	0.67612	0.53835	0.67134	4.1069	9.3582	9.1500	1	1	1	3.545	-
-	C7	0.61134	0.45984	0.67708	3.3757	7.9933	9.2282	1	1	1	3.545	-

-	C8	0.53110	0.43139	0.57479	2.9973	7.4988	7.8341	1	1	1	3.545 -
-	C9	0.61532	0.42673	0.51063	4.2213	7.4179	6.9597	1	1	1	3.545 -
-	C10	0.48460	0.26381	0.21621	4.2209	4.5858	2.9469	1	1	1	3.545 -
-	C11	0.71826	0.25143	0.29663	6.3711	4.3705	4.0429	1	1	1	3.545 -
-	C12	0.79153	0.25491	0.16562	7.7984	4.4311	2.2573	1	1	1	3.545 -
-	C13	0.65897	0.25686	0.13386	6.5118	4.4649	1.8245	1	1	1	3.545 -
-	C14	1.04235	0.18665	0.31609	9.7972	3.2445	4.3081	1	1	1	3.545 -
-	C15	1.18496	0.19053	0.38522	11.0127	3.3120	5.2504	1	1	1	3.545 -
-	C16	1.24850	0.26561	0.37503	11.7520	4.6171	5.1114	1	1	1	3.545 -
-	C17	1.17348	0.33439	0.38974	10.8663	5.8126	5.3120	1	1	1	3.545 -
-	C18	1.03207	0.33245	0.31480	9.6917	5.7790	4.2906	1	1	1	3.545 -
-	C19	0.96372	0.25674	0.33205	8.8662	4.4630	4.5257	1	1	1	3.545 -
-	H2A	0.40951	0.48468	0.34913	2.7646	8.4251	4.7585	1	1	1	3.545 -
-	H3A	0.34034	0.40102	0.20047	2.7300	6.9708	2.7323	1	1	1	3.545 -
-	H4A	0.60704	0.54427	0.47353	4.3102	9.4611	6.4540	1	1	1	3.545 -
-	H4B	0.73209	0.50209	0.46123	5.7277	8.7278	6.2864	1	1	1	3.545 -
-	H5A	0.83126	0.49547	0.63451	5.9695	8.6128	8.6480	1	1	1	3.545 -
-	H5B	0.79859	0.58336	0.60197	5.7715	10.1406	8.2046	1	1	1	3.545 -
-	H6A	0.60762	0.57781	0.64495	3.4901	10.0441	8.7904	1	1	1	3.545 -
-	H6B	0.73109	0.55449	0.73800	4.3825	9.6386	10.0586	1	1	1	3.545 -
-	H7A	0.67977	0.42158	0.70918	3.9641	7.3283	9.6658	1	1	1	3.545 -
-	H7B	0.55394	0.46529	0.71741	2.5579	8.0882	9.7780	1	1	1	3.545 -
-	H8A	0.49462	0.37996	0.57972	2.5773	6.6048	7.9013	1	1	1	3.545 -
-	H8B	0.45738	0.46703	0.54506	2.3399	8.1183	7.4289	1	1	1	3.545 -
-	H9A	0.68860	0.39052	0.54295	4.8614	6.7883	7.4001	1	1	1	3.545 -
-	H10A	0.42425	0.27583	0.14958	3.8867	4.7947	2.0387	1	1	1	3.545 -
-	H10B	0.45591	0.21536	0.23874	3.8007	3.7436	3.2539	1	1	1	3.545 -
-	H12A	0.84683	0.25503	0.12671	8.5865	4.4332	1.7269	1	1	1	3.545 -
-	H13A	0.60292	0.25822	0.06748	6.2230	4.4886	0.9197	1	1	1	3.545 -
-	H14A	1.00150	0.13860	0.32855	9.2934	2.4094	4.4779	1	1	1	3.545 -
-	H14B	1.04037	0.18581	0.24713	10.1080	3.2299	3.3683	1	1	1	3.545 -
-	H15A	1.18731	0.18450	0.45389	10.7073	3.2072	6.1863	1	1	1	3.545 -
-	H15B	1.23490	0.14751	0.37013	11.6279	2.5641	5.0447	1	1	1	3.545 -
-	H16A	1.33770	0.26718	0.42372	12.4861	4.6444	5.7751	1	1	1	3.545 -
-	H16B	1.25647	0.26829	0.30885	12.1576	4.6637	4.2096	1	1	1	3.545 -
-	H17A	1.21788	0.38210	0.38065	11.3924	6.6420	5.1880	1	1	1	3.545 -
-	H17B	1.17038	0.33424	0.45741	10.5064	5.8101	6.2343	1	1	1	3.545 -
-	H18A	0.98267	0.37798	0.32405	9.1105	6.5705	4.4166	1	1	1	3.545 -
-	H18B	1.03460	0.33343	0.24699	10.0461	5.7960	3.3664	1	1	1	3.545 -
-	H19A	0.96536	0.25620	0.40162	8.5487	4.4535	5.4739	1	1	1	3.545 -

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********** Residue = 2 **********
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Flags	Label	Fractional Coordinates (x,y,z)			Orthogonal Coordinates (XO,YO,ZO)			Site	SSN*SSOF =	S.O.F	Move Type
-	O1	0.44511	0.13761	0.07116	4.4914	2.3920	0.9698	1	1	1	2.564 D/A
-	N5	0.52650	0.02920	0.01787	5.6322	0.5076	0.2436	1	1	1	2.564 D/A
-	C20	0.44385	0.09309	0.00753	4.7843	1.6181	0.1027	1	1	1	2.564 -
-	C21	0.50887	-0.02502	-0.05847	5.8087	-0.4349	-0.7969	1	1	1	2.564 -
-	C22	0.63538	0.02135	0.10889	6.3760	0.3712	1.4841	1	1	1	2.564 -
-	H20A	0.38133	0.10180	-0.05554	4.4094	1.7696	-0.7570	1	1	1	2.564 -
-	H21A	0.43141	-0.01126	-0.11409	5.2355	-0.1957	-1.5550	1	1	1	2.564 -
-	H21B	0.58586	-0.02496	-0.07946	6.7460	-0.4339	-1.0830	1	1	1	2.564 -
-	H21C	0.49714	-0.07638	-0.03473	5.5668	-1.3278	-0.4734	1	1	1	2.564 -
-	H22A	0.63330	0.06355	0.15329	6.1393	1.1047	2.0893	1	1	1	2.564 -
-	H22B	0.62864	-0.02790	0.13983	6.1535	-0.4850	1.9059	1	1	1	2.564 -
-	H22C	0.71766	0.02311	0.09493	7.3369	0.4018	1.2939	1	1	1	2.564 -

NOTE: A # in the Atom Label Indicates a Label that was Modified to Conform with the Label Convention (A4)

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	O	Pd
1	1	0.734	0.280	0.427	578.67	1	4	19	28	2	4	-	1
2	1	0.513	0.051	0.030	73.10	1	4	3	7	-	1	1	-
				Unit Cell Weight =	2607.08			88	140	8	20	4	4

Calculated Analysis (Percent) = 40.5 5.4 24.5 10.7 2.5 16.3

Moiety_Formula = C19 H28 Br2 N4 Pd, C3 H7 N O

Sum_Formula = C22 H35 Br2 N5 O Pd

Formula_Weight = 651.77 [Note: Based on SHELXL97 Atomic Weights]

Formula_Z = 4

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

Calculated Density = 1.6824(8) g cm-3 [= Mg m-3]

F(000) = 1304.0 [1298.12]

mu(MoKa) = 38.50 cm-1 = 3.850 mm-1

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

Resonant Scattering = 6.85 Percent - (Girard,E. et al. (2003). Acta Cryst. D59, 1914-1922)

Predicted Volume = 2614.9[2590.6] 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]

Residue = 1

Atom	Label	U11 or Uiso	U22	U33	U23	U13	U12	Ueq(sUeq)	U1	U2	U3	U3/U1
1	NI	0.01934						0.01934				
2	Br1	0.03098						0.03098				
3	Br2	0.02922						0.02922				
4	N1	0.02527						0.02527				
5	N2	0.02643						0.02643				
6	N3	0.01908						0.01908				
7	N4	0.02619						0.02619				
8	C1	0.02593						0.02593				
9	C2	0.03308						0.03308				
10	C3	0.03120						0.03120				
11	C4	0.03275						0.03275				
12	C5	0.03659						0.03659				
13	C6	0.04360						0.04360				
14	C7	0.03801						0.03801				
15	C8	0.03430						0.03430				
16	C9	0.02199						0.02199				
17	C10	0.02437						0.02437				
18	C11	0.02417						0.02417				
19	C12	0.03040						0.03040				
20	C13	0.02877						0.02877				
21	C14	0.03041						0.03041				
22	C15	0.03359						0.03359				
23	C16	0.03972						0.03972				
24	C17	0.04067						0.04067				
25	C18	0.02861						0.02861				
26	C19	0.02116						0.02116				
27	H2A	0.03970						0.03970				
28	H3A	0.03744						0.03744				
29	H4A	0.03930						0.03930				
30	H4B	0.03930						0.03930				
31	H5A	0.04391						0.04391				
32	H5B	0.04391						0.04391				
33	H6A	0.05232						0.05232				
34	H6B	0.05232						0.05232				
35	H7A	0.04561						0.04561				
36	H7B	0.04561						0.04561				

37	H8A	0.04116						0.04116				
38	H8B	0.04116						0.04116				
39	H9A	0.02639						0.02639				
40	H10A	0.02924						0.02924				
41	H10B	0.02924						0.02924				
42	H12A	0.03648						0.03648				
43	H13A	0.03452						0.03452				
44	H14A	0.03649						0.03649				
45	H14B	0.03649						0.03649				
46	H15A	0.04031						0.04031				
47	H15B	0.04031						0.04031				
48	H16A	0.04766						0.04766				
49	H16B	0.04766						0.04766				
50	H17A	0.04880						0.04880				
51	H17B	0.04880						0.04880				
52	H18A	0.03433						0.03433				
53	H18B	0.03433						0.03433				
54	H19A	0.02539						0.02539				

********** Residue = 2 **********

Atom	Label	U11 or Uiso	U22	U33	U23	U13	U12	Ueq(sUeq)	U1	U2	U3	U3/U1
1	O1	0.06884						0.06884				
2	N5	0.09115						0.09115				
3	C20	0.05130						0.05130				
4	C21	0.10975						0.10975				
5	C22	0.13911						0.13911				
6	H20A	0.06156						0.06156				
7	H21A	0.16463						0.16463				
8	H21B	0.16463						0.16463				
9	H21C	0.16463						0.16463				
10	H22A	0.20866						0.20866				
11	H22B	0.20866						0.20866				
12	H22C	0.20866						0.20866				

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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	O	Pd
Average	0.0399	0.0409	0.0657	0.0301	0.0376	0.0688	0.0193
Minimum	0.0191	0.0212	0.0254	0.0292	0.0191	0.0688	0.0193
Maximum	0.1391	0.1391	0.2087	0.0310	0.0912	0.0688	0.0193
Ratio	7.2909	6.5742	8.2177	1.0602	4.7773	1.0000	1.0000
Number	31	22	35	2	5	1	1

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

Residue = 1

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
-	NI	- Br1	Br2	C1	C11	-------	-------	-------	-------	-------	6	83	173	116.9	1.982	2.505	4	31			
-	Br1	- NI	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	2.504	2.504	1	30			
-	Br2	- NI	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	2.505	2.505	1	30			
-	N1	- C1	C2	C9	-------	-------	-------	-------	-------	-------	3	108	128	120.0	1.362	1.453	3	26			
-	N2	- C1	C3	C10	-------	-------	-------	-------	-------	-------	3	112	125	120.0	1.304	1.457	3	27	sp2		
-	N3	- C11	C12	C19	-------	-------	-------	-------	-------	-------	3	110	127	120.0	1.396	1.447	3	26			
-	N4	- C10	C11	C13	-------	-------	-------	-------	-------	-------	3	113	126	120.0	1.292	1.485	3	27	sp2		
-	C1	- NI	N1	N2	-------	-------	-------	-------	-------	-------	3	107	132	120.0	1.304	2.001	3	22	sp2		
-	C2	- N1	C3	H2A	-------	-------	-------	-------	-------	-------	3	107	127	120.0	0.950	1.412	3	16	sp2		
-	C3	- N2	C2	H3A	-------	-------	-------	-------	-------	-------	3	106	127	120.0	0.950	1.379	3	18	sp2		
-	C4	- C5	C9	H4A	H4B	-------	-------	-------	-------	-------	6	108	110	109.5	0.990	1.554	4	12	sp3		
-	C5	- C4	C6	H5A	H5B	-------	-------	-------	-------	-------	6	108	110	109.5	0.990	1.526	4	11	sp3		
-	C6	- C5	C7	H6A	H6B	-------	-------	-------	-------	-------	6	108	111	109.5	0.990	1.550	4	10	sp3		
-	C7	- C6	C8	H7A	H7B	-------	-------	-------	-------	-------	6	108	111	109.5	0.990	1.550	4	11	sp3		
-	C8	- C7	C9	H8A	H8B	-------	-------	-------	-------	-------	6	108	110	109.5	0.990	1.527	4	12	sp3		
-	C9	- N1	C4	C8	H9A	-------	-------	-------	-------	-------	6	107	113	109.4	1.000	1.554	4	15	sp3		
-	C10	- N2	N4	H10A	H10B	-------	-------	-------	-------	-------	6	106	111	109.5	0.990	1.485	4	19	sp3		
-	C11	- NI	N3	N4	-------	-------	-------	-------	-------	-------	3	105	132	120.0	1.292	1.982	3	22	sp2		
-	C12	- N3	C13	H12A	-------	-------	-------	-------	-------	-------	3	105	127	120.0	0.950	1.401	3	16	sp2		
-	C13	- N4	C12	H13A	-------	-------	-------	-------	-------	-------	3	107	126	120.0	0.950	1.380	3	18	sp2		
-	C14	- C15	C19	H14A	H14B	-------	-------	-------	-------	-------	6	108	111	109.5	0.990	1.549	4	12	sp3		
-	C15	- C14	C16	H15A	H15B	-------	-------	-------	-------	-------	6	108	112	109.5	0.990	1.540	4	11	sp3		
-	C16	- C15	C17	H16A	H16B	-------	-------	-------	-------	-------	6	108	113	109.5	0.990	1.506	4	10	sp3		
-	C17	- C16	C18	H17A	H17B	-------	-------	-------	-------	-------	6	108	110	109.5	0.990	1.557	4	11	sp3		
-	C18	- C17	C19	H18A	H18B	-------	-------	-------	-------	-------	6	108	110	109.5	0.990	1.571	4	12	sp3		
-	C19	- N3	C14	C18	H19A	-------	-------	-------	-------	-------	6	108	112	109.5	1.000	1.571	4	15	sp3		
-	H2A	- C2	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.950	0.950	1	6			
-	H3A	- C3	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.950	0.950	1	7			
-	H4A	- C4	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.990	0.990	1	3			
-	H4B	- C4	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.990	0.990	1	3			
-	H5A	- C5	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.990	0.990	1	2			
-	H5B	- C5	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.990	0.990	1	2			
-	H6A	- C6	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.990	0.990	1	1			
-	H6B	- C6	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.990	0.990	1	1			
-	H7A	- C7	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.990	0.990	1	2			
-	H7B	- C7	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.990	0.990	1	2			
-	H8A	- C8	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.990	0.990	1	3			
-	H8B	- C8	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.990	0.990	1	3			
-	H9A	- C9	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	1.000	1.000	1	5			

-	H10A	- C10	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.990	0.990	1	8	
-	H10B	- C10	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.990	0.990	1	8	
-	H12A	- C12	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.950	0.950	1	6	
-	H13A	- C13	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.950	0.950	1	7	
-	H14A	- C14	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.990	0.990	1	3	
-	H14B	- C14	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.990	0.990	1	3	
-	H15A	- C15	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.990	0.990	1	2	
-	H15B	- C15	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.990	0.990	1	2	
-	H16A	- C16	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.990	0.990	1	1	
-	H16B	- C16	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.990	0.990	1	1	
-	H17A	- C17	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.990	0.990	1	2	
-	H17B	- C17	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.990	0.990	1	2	
-	H18A	- C18	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.990	0.990	1	3	
-	H18B	- C18	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.990	0.990	1	3	
-	H19A	- C19	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	1.000	1.000	1	5	

Residue = 2

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
-	O1	- C20	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	1.199	1.199	1	29	sp2		
-	N5	- C20	C21	C22	-------	-------	-------	-------	-------	-------	3	118	122	120.0	1.404	1.453	3	24			
-	C20	- O1	N5	H20A	-------	-------	-------	-------	-------	-------	3	117	126	120.0	0.950	1.404	3	21	sp2		
-	C21	- N5	H21A	H21B	H21C	-------	-------	-------	-------	-------	6	109	109	109.5	0.980	1.415	4	14	sp3		
-	C22	- N5	H22A	H22B	H22C	-------	-------	-------	-------	-------	6	109	109	109.5	0.980	1.453	4	14	sp3		
-	H20A	- C20	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.950	0.950	1	9			
-	H21A	- C21	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.980	0.980	1	4			
-	H21B	- C21	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.980	0.980	1	4			
-	H21C	- C21	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.980	0.980	1	4			
-	H22A	- C22	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.980	0.980	1	4			
-	H22B	- C22	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.980	0.980	1	4			
-	H22C	- C22	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.980	0.980	1	4			

Page - Index

Page 1 --- GENERAL
Page 2 --- ADDSYM
Page 3 --- GEOMETRY
Page 7 --- ADP-Anal
Page 10 --- GEOMETRY
Page 14 --- SUMMARY

Summary and Remarks : N = NOTE, W = WARNING, E = ERROR

N: No S.U.'s (esd) on observed/calculated parameters.

N: Number of Isotropic Non-H Atoms 31
N: Number of moved primary input atoms: 66
N: Number of Ignored Lines on INPUT 4
of which blank in column 1 4
N: Number of modified (= #) ATOM labels 1

:: Input Xtal Data from File joer009.eld - Data Type SPF

:: NORMAL END of PLATON : 14 Pages on:
:: joer009.lis (ASCII, 132 Characters Wide)
:: joer009.lps (PostScript Version of .lis)
:: joer009.pdf (PDF Version of .lis)

PLATON(V-311206)-Run for: joer009 in Cc New: Cc TIME: Nov 11 10:56:23 2010

(C) 1980-2007 A.L.Spek

Crystal Data

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

a =	10.861(3)	Angstrom	alpha =	90	Degree	a = 10.249	alpha = 100.18	V =	1286.6
b =	17.383(4)		beta =	109.479(4)		b = 10.249	beta = 100.18		
c =	14.457(4)		gamma =	90		c = 14.457	gamma = 116.01		
V =	2573.2(12)	Cubic-Angstrom	d(100) =	10.2394	Angstrom	Niggli Values			
			d(010) =	17.3830		105.032	105.032	209.005	
Lambda(MoKa) =	0.71073	Angstrom	d(001) =	13.6295		-26.180	-26.180	-46.051	

Orthogonalization Matrices

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

$$\begin{pmatrix} XO \\ YO \\ ZO \end{pmatrix} = \begin{pmatrix} 10.86100 & 0 & -4.82085 \\ 0 & 17.38300 & 0 \\ 0 & 0 & 13.62954 \end{pmatrix} \begin{pmatrix} X \\ Y \\ Z \end{pmatrix} , \quad \begin{pmatrix} X \\ Y \\ Z \end{pmatrix} = \begin{pmatrix} 0.09207 & 0 & 0.03257 \\ 0 & 0.05753 & 0 \\ 0 & 0 & 0.07337 \end{pmatrix} \begin{pmatrix} XO \\ YO \\ ZO \end{pmatrix}$$

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 Cc No: 9, Laue: 2/m [Hall: C -2yc]

Lattice Type mC, Acentric, Monoclinic, Order 4(2) [Schoenflies: Cs^4]

ACHIRAL - See P.G. Jones, Acta Cryst. (1986), A42, 57.

Nr	***** Symmetry Operation(s) *****		
1	X ,	Y ,	Z
2	X ,	- Y ,	1/2 + Z
3	1/2 + X ,	1/2 + Y ,	Z
4	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.

```
         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	Br	N	O	Pd
Cov.Rad(Ang):	0.68	0.35	1.21	0.68	0.68	1.50
Atom Volume :	13.87	5.08	32.70	11.80	11.39	35.00
Atom Number :	6	1	35	7	8	46
Atom Weight :	12.010	1.008	79.90	14.01	16.00	106.42
Scat.Fact.f0:	5.999	1.000	34.993	6.995	7.999	46.001
Scat.Fact.f':	0.003	0.000	-0.290	0.006	0.011	-0.999
Scat.Fact.f":	0.002	0.000	2.460	0.003	0.006	1.007
Mu/Rho(MoKa):	0.58	0.37	75.37	0.84	1.22	24.67
Elem. Type :	--	--	HL	--	--	TR

```
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

                                                  =============
************************************************** Residue =   1 **************************************************
                                                  =============
```

Flags	Label	Fractional Coordinates (x,y,z)			Orthogonal Coordinates (XO,YO,ZO)			Site	SSN*SSOF =	S.O.F	Move	Type
-	Pd(1)	0.69639	0.24419	0.42708	5.5047	4.2448	5.8208	1	1	1	-	Met
-	Br(1)	0.84437	0.12979	0.47333	6.8889	2.2561	6.4512	1	1	1	-	D/A
-	Br(2)	0.62846	0.22842	0.57546	4.0516	3.9706	7.8432	1	1	1	-	D/A
-	N(1)	0.54564	0.39622	0.41371	3.9318	6.8876	5.6386	1	1	1	-	D/A
-	N(2)	0.48654	0.32644	0.28372	3.9165	5.6745	3.8670	1	1	1	-	D/A
-	N(3)	0.82911	0.25270	0.26817	7.7122	4.3927	3.6551	1	1	1	-	D/A
-	N(4)	0.62068	0.25649	0.21581	5.7008	4.4585	2.9414	1	1	1	-	D/A
-	C(1)	0.56696	0.32865	0.37376	4.3560	5.7129	5.0942	1	1	1	-	-
-	C(2)	0.44460	0.43585	0.34199	3.1801	7.5764	4.6611	1	1	1	-	-
-	C(3)	0.40744	0.39059	0.26090	3.1675	6.7897	3.5559	1	1	1	-	-
-	C(4)	0.67684	0.50622	0.50337	4.9244	8.7997	6.8607	1	1	1	-	-
-	C(5)	0.75944	0.53258	0.60599	5.3268	9.2578	8.2594	1	1	1	-	-
-	C(6)	0.67612	0.53835	0.67134	4.1069	9.3582	9.1500	1	1	1	-	-
-	C(7)	0.61134	0.45984	0.67708	3.3757	7.9933	9.2282	1	1	1	-	-

Flags	Label	Fractional Coordinates (x,y,z)			Orthogonal Coordinates (XO,YO,ZO)			Site	SSN*SSOF =	S.O.F	Move	Type
-	O(1)	0.44511	0.13760	0.07116	4.4914	2.3920	0.9698	1	1	1	-	D/A
-	N(5)	0.52650	0.02920	0.01788	5.6322	0.5076	0.2436	1	1	1	-	D/A
-	C(20)	0.44385	0.09309	0.00753	4.7843	1.6181	0.1027	1	1	1	-	-
-	C(21)	0.50887	-0.02502	-0.05847	5.8087	-0.4349	-0.7969	1	1	1	-	-
-	C(22)	0.63538	0.02135	0.10889	6.3760	0.3712	1.4841	1	1	1	-	-
-	H(20A)	0.38133	0.10180	-0.05554	4.4094	1.7696	-0.7570	1	1	1	-	-
-	H(21A)	0.43141	-0.01126	-0.11409	5.2355	-0.1957	-1.5550	1	1	1	-	-
-	H(21B)	0.58586	-0.02496	-0.07946	6.7460	-0.4339	-1.0830	1	1	1	-	-
-	H(21C)	0.49714	-0.07638	-0.03473	5.5668	-1.3278	-0.4734	1	1	1	-	-
-	H(22A)	0.63330	0.06355	0.15329	6.1393	1.1047	2.0893	1	1	1	-	-
-	H(22B)	0.62864	-0.02790	0.13983	6.1535	-0.4850	1.9059	1	1	1	-	-
-	H(22C)	0.71766	0.02311	0.09493	7.3369	0.4018	1.2939	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	Br	N	O	Pd
1	1	0.734	0.280	0.427	578.67	1	4	19	28	2	4	-	1
2	1	0.513	0.051	0.030	73.10	1	4	3	7	-	1	1	-
				Unit Cell Weight =	2607.08			88	140	8	20	4	4

Calculated Analysis (Percent) = 40.5 5.4 24.5 10.7 2.5 16.3

Moiety_Formula = C19 H28 Br2 N4 Pd, C3 H7 N O

Sum_Formula = C22 H35 Br2 N5 O Pd

Formula_Weight = 651.77 [Note: Based on SHELXL97 Atomic Weights]

Formula_Z = 4

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

Calculated Density = 1.6824(8) g cm-3 [= Mg m-3]

F(000) = 1304.0 [1298.12]

mu(MoKa) = 38.50 cm-1 = 3.850 mm-1

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

Resonant Scattering = 6.85 Percent - (Girard,E. et al. (2003). Acta Cryst. D59, 1914-1922)

Predicted Volume = 2614.9[2590.6] 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]

Residue = 1

Atom	Label	U11 or Uiso	U22	U33	U23	U13	U12	Ueq(sUeq)	U1	U2	U3	U3/U1
1	Pd1	0.01934						0.01934				
2	Br1	0.03098						0.03098				
3	Br2	0.02922						0.02922				
4	N1	0.02527						0.02527				
5	N2	0.02643						0.02643				
6	N3	0.01908						0.01908				
7	N4	0.02619						0.02619				
8	C1	0.02593						0.02593				
9	C2	0.03308						0.03308				
10	C3	0.03120						0.03120				
11	C4	0.03275						0.03275				
12	C5	0.03659						0.03659				
13	C6	0.04360						0.04360				
14	C7	0.03801						0.03801				
15	C8	0.03430						0.03430				
16	C9	0.02199						0.02199				
17	C10	0.02437						0.02437				
18	C11	0.02417						0.02417				
19	C12	0.03040						0.03040				
20	C13	0.02877						0.02877				
21	C14	0.03041						0.03041				
22	C15	0.03359						0.03359				
23	C16	0.03972						0.03972				
24	C17	0.04067						0.04067				
25	C18	0.02861						0.02861				
26	C19	0.02116						0.02116				

Residue = 2

Atom	Label	U11 or Uiso	U22	U33	U23	U13	U12	Ueq(sUeq)	U1	U2	U3	U3/U1

1	O1	0.06884										0.06884
2	N5	0.09115										0.09115
3	C20	0.05130										0.05130
4	C21	0.10975										0.10975
5	C22	0.13911										0.13911

==========

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	O	Pd
Average	0.0399	0.0409	0.0000	0.0301	0.0376	0.0688	0.0193
Minimum	0.0191	0.0212	0.0000	0.0292	0.0191	0.0688	0.0193
Maximum	0.1391	0.1391	0.0000	0.0310	0.0912	0.0688	0.0193
Ratio	7.2909	6.5742	0.0000	1.0602	4.7773	1.0000	1.0000
Number	31	22	0	2	5	1	1

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

Residue = 1

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
-	Pd(1)	- Br(1)	Br(2)	C(1)	C(11)	-------	-------	-------	-------	6	83	173	116.9	1.982	2.505	4	31			
-	Br(1)	- Pd(1)	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	2.504	2.504	1	30			
-	Br(2)	- Pd(1)	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	2.505	2.505	1	30			
-	N(1)	- C(1)	C(2)	C(9)	-------	-------	-------	-------	-------	3	108	128	120.0	1.362	1.453	3	26			
-	N(2)	- C(1)	C(3)	C(10)	-------	-------	-------	-------	-------	3	112	125	120.0	1.304	1.458	3	27	sp2		
-	N(3)	- C(11)	C(12)	C(19)	-------	-------	-------	-------	-------	3	110	127	120.0	1.396	1.447	3	26			
-	N(4)	- C(10)	C(11)	C(13)	-------	-------	-------	-------	-------	3	113	126	120.0	1.292	1.485	3	27	sp2		
-	C(1)	- Pd(1)	N(1)	N(2)	-------	-------	-------	-------	-------	3	107	132	120.0	1.304	2.001	3	22	sp2		
-	C(2)	- N(1)	C(3)	H(2A)	-------	-------	-------	-------	-------	3	107	127	120.0	0.950	1.412	3	16	sp2		
-	C(3)	- N(2)	C(2)	H(3A)	-------	-------	-------	-------	-------	3	106	127	120.0	0.950	1.379	3	18	sp2		
-	C(4)	- C(5)	C(9)	H(4A)	H(4B)	-------	-------	-------	-------	6	108	110	109.5	0.990	1.554	4	12	sp3		
-	C(5)	- C(4)	C(6)	H(5A)	H(5B)	-------	-------	-------	-------	6	108	110	109.5	0.990	1.526	4	11	sp3		
-	C(6)	- C(5)	C(7)	H(6A)	H(6B)	-------	-------	-------	-------	6	108	111	109.5	0.990	1.550	4	10	sp3		
-	C(7)	- C(6)	C(8)	H(7A)	H(7B)	-------	-------	-------	-------	6	108	111	109.5	0.990	1.550	4	11	sp3		
-	C(8)	- C(7)	C(9)	H(8A)	H(8B)	-------	-------	-------	-------	6	108	110	109.5	0.990	1.527	4	12	sp3		
-	C(9)	- N(1)	C(4)	C(8)	H(9A)	-------	-------	-------	-------	6	107	113	109.4	1.000	1.554	4	15	sp3		
-	C(10)	- N(2)	N(4)	H(10A)	H(10B)	-------	-------	-------	-------	6	106	111	109.5	0.990	1.485	4	19	sp3		
-	C(11)	- Pd(1)	N(3)	N(4)	-------	-------	-------	-------	-------	3	105	132	120.0	1.292	1.982	3	22	sp2		
-	C(12)	- N(3)	C(13)	H(12A)	-------	-------	-------	-------	-------	3	105	127	120.0	0.950	1.401	3	16	sp2		
-	C(13)	- N(4)	C(12)	H(13A)	-------	-------	-------	-------	-------	3	107	126	120.0	0.950	1.380	3	18	sp2		
-	C(14)	- C(15)	C(19)	H(14A)	H(14B)	-------	-------	-------	-------	6	108	111	109.5	0.990	1.549	4	12	sp3		
-	C(15)	- C(14)	C(16)	H(15A)	H(15B)	-------	-------	-------	-------	6	108	112	109.5	0.990	1.540	4	11	sp3		
-	C(16)	- C(15)	C(17)	H(16A)	H(16B)	-------	-------	-------	-------	6	108	113	109.5	0.990	1.506	4	10	sp3		
-	C(17)	- C(16)	C(18)	H(17A)	H(17B)	-------	-------	-------	-------	6	108	110	109.5	0.990	1.557	4	11	sp3		
-	C(18)	- C(17)	C(19)	H(18A)	H(18B)	-------	-------	-------	-------	6	108	110	109.5	0.990	1.571	4	12	sp3		
-	C(19)	- N(3)	C(14)	C(18)	H(19A)	-------	-------	-------	-------	6	108	112	109.5	1.000	1.571	4	15	sp3		
-	H(2A)	- C(2)	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.950	0.950	1	6			
-	H(3A)	- C(3)	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.950	0.950	1	7			
-	H(4A)	- C(4)	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.990	0.990	1	3			
-	H(4B)	- C(4)	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.990	0.990	1	3			
-	H(5A)	- C(5)	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.990	0.990	1	2			
-	H(5B)	- C(5)	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.990	0.990	1	2			
-	H(6A)	- C(6)	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.990	0.990	1	1			
-	H(6B)	- C(6)	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.990	0.990	1	1			
-	H(7A)	- C(7)	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.990	0.990	1	2			
-	H(7B)	- C(7)	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.990	0.990	1	2			
-	H(8A)	- C(8)	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.990	0.990	1	3			
-	H(8B)	- C(8)	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.990	0.990	1	3			
-	H(9A)	- C(9)	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	1.000	1.000	1	5			

-	H(10A) - C(10)	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.990	0.990	1	8	
-	H(10B) - C(10)	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.990	0.990	1	8	
-	H(12A) - C(12)	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.950	0.950	1	6	
-	H(13A) - C(13)	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.950	0.950	1	7	
-	H(14A) - C(14)	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.990	0.990	1	3	
-	H(14B) - C(14)	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.990	0.990	1	3	
-	H(15A) - C(15)	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.990	0.990	1	2	
-	H(15B) - C(15)	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.990	0.990	1	2	
-	H(16A) - C(16)	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.990	0.990	1	1	
-	H(16B) - C(16)	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.990	0.990	1	1	
-	H(17A) - C(17)	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.990	0.990	1	2	
-	H(17B) - C(17)	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.990	0.990	1	2	
-	H(18A) - C(18)	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.990	0.990	1	3	
-	H(18B) - C(18)	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.990	0.990	1	3	
-	H(19A) - C(19)	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	1.000	1.000	1	5	

Residue = 2

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
-	O(1)	- C(20)	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	1.199	1.199	1	29	sp2		
-	N(5)	- C(20)	C(21)	C(22)	-------	-------	-------	-------	-------	3	118	122	120.0	1.404	1.453	3	24			
-	C(20)	- O(1)	N(5)	H(20A)	-------	-------	-------	-------	-------	3	117	126	120.0	0.950	1.404	3	21	sp2		
-	C(21)	- N(5)	H(21A)	H(21B)	H(21C)	-------	-------	-------	-------	6	109	109	109.5	0.980	1.415	4	14	sp3		
-	C(22)	- N(5)	H(22A)	H(22B)	H(22C)	-------	-------	-------	-------	6	109	109	109.5	0.980	1.453	4	14	sp3		
-	H(20A)	- C(20)	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.950	0.950	1	9			
-	H(21A)	- C(21)	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.980	0.980	1	4			
-	H(21B)	- C(21)	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.980	0.980	1	4			
-	H(21C)	- C(21)	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.980	0.980	1	4			
-	H(22A)	- C(22)	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.980	0.980	1	4			
-	H(22B)	- C(22)	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.980	0.980	1	4			
-	H(22C)	- C(22)	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.980	0.980	1	4			

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********** N O T I C E **********

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- PLATON Reference : Spek, A.L. (2003), J.Appl.Cryst. 36, 7-13

- Output Values (Esd) may have been set to 99, 999 or 9999 to Avoid Format Overflow

- Derived Parameter SU's (= Esd's) may be Incorrect in Cases where Covariances in the Atom Parameters should have been taken into Account (e.g. Those Involving Atoms That were Refined with Constraints)

- ROUNDING, in particular of the Input Coordinate Data, may give deviating values for derived geometry parameters. However, differences should be within the associated esd-range.

- PLATON is NOT a Finished Program. The Implementation of Additional Options is Planned. Some of the More Advanced Features are Experimental and may Contain Loose Ends.

- The Communication of Glitches Encountered will be Appreciated: E-mail: a.l.spek@chem.uu.nl

- Recent versions of PLATON may be obtained by Anonymous FTP from xraysoft.chem.uu.nl

- More INFO can be found on http://www.cryst.chem.uu.nl/platon/

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Page 20 --- ADP-Anal
Page 22 --- GEOMETRY
Page 26 --- SUMMARY

Summary and Remarks : N = NOTE, W = WARNING, E = ERROR

W: NOMOVE option used.
:: >>> WARNING: 'CONNECTED INPUT SET' is assumed 'TRUE'
:: >>> Network Analysis may be INCORRECT when FALSE
N: No S.U.'s (esd) on observed/calculated parameters.

N: Number of Isotropic Non-H Atoms 31
N: Input Data following TRNS [e.g. (CELL/CESD)/SPGR/COORDS/UIJ)] have been
transformed according to the specified Cell Transformation Matrix:

1.00000	0.00000	0.00000
0.00000	1.00000	0.00000
0.00000	0.00000	1.00000

N: INPUT data (COORDINATES) have been transformed
according to additive coordinate shift vector:

0.00000	0.00000	0.00000

N: Number of Ignored Lines on INPUT 2
of which blank in column 1 0

:: Input Xtal Data from File joer009.eld - Data Type SPF

:: NORMAL END of PLATON : 27 Pages on:
:: joer009.lis (ASCII, 132 Characters Wide)
:: joer009.lps (PostScript Version of .lis)
:: joer009.pdf (PDF Version of .lis)

:: SHELXL Style Output on :joer009.res