PLATON(V-311206)-Run for: robs004 in P-1 TIME: Jul 7 14:44:47 2010

Crystal Data

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

a =	12.299(4)	Angstrom	alpha =	68.843(4)	Degree	a =	12.299	alpha =	68.84
b =	14.031(4)		beta =	85.869(5)		b =	14.031	beta =	85.87
c =	15.395(4)		gamma =	82.850(5)		c =	15.395	gamma =	82.85
V =	2457.2(12)	Cubic-Angstrom	d(100) =	12.1982	Angstrom				
			d(010) =	13.0114					
Lambda(MoKa) =	0.71073 Angstrom		d(001) =	14.3510					

Reduced Cell (Acta Cryst.(1976),A32,297-298) V = 2457.2

Niggli Values

151.268	196.861	237.003
77.960	13.639	21.479

Orthogonalization Matrices

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

$$(XO) = \begin{pmatrix} 12.29900 & 1.74640 & 1.10901 \\ 0 & 13.92189 & 5.46087 \\ 0 & 0 & 14.35114 \end{pmatrix} (X) \quad , \quad (X) = \begin{pmatrix} 0.08131 & -0.01020 & -0.00240 \\ 0 & 0.07183 & -0.02733 \\ 0 & 0 & 0.06968 \end{pmatrix} (XO)$$

$$(YO) = \begin{pmatrix} 0 & 13.92189 & 5.46087 \end{pmatrix} (Y) \quad , \quad (Y) = \begin{pmatrix} 0 & 0.07183 & -0.02733 \end{pmatrix} (YO)$$

$$(ZO) = \begin{pmatrix} 0 & 0 & 14.35114 \end{pmatrix} (Z) \quad , \quad (Z) = \begin{pmatrix} 0 & 0 & 0.06968 \end{pmatrix} (ZO)$$

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 P-1 No: 2, Laue: -1 [Hall: -P 1]

Lattice Type aP, Centric, Triclinic, Order 2(1) [Schoenflies: Ci^1]

Nr	***** Symmetry Operation(s) *****		
1	X ,	Y ,	Z
2	- X ,	- Y ,	- 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	B	Cl	N	Ni	O
Cov.Rad(Ang):	0.68	0.35	0.83	0.99	0.68	1.50	0.68
Atom Volume :	13.87	5.08	13.24	25.80	11.80	26.00	11.39
Atom Number :	6	1	5	17	7	28	8
Atom Weight :	12.010	1.008	10.81	35.45	14.01	58.69	16.00
Scat.Fact.f0:	5.999	1.000	4.999	17.001	6.995	27.988	7.999
Scat.Fact.f':	0.003	0.000	0.001	0.148	0.006	0.339	0.011
Scat.Fact.f":	0.002	0.000	0.001	0.159	0.003	1.112	0.006
Mu/Rho(MoKa):	0.58	0.37	0.37	11.52	0.84	46.89	1.22
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(1)	0.16046	0.38913	0.38193	3.0767	7.5030	5.4811	1	1	1	-	Met
-	O(1)	0.26308	0.50598	0.33196	4.4874	8.8570	4.7641	1	1	1	-	D/A
-	O(2)	0.13348	0.52444	0.43102	3.0356	9.6550	6.1857	1	1	1	-	D/A
-	N(1)	0.04879	0.28528	0.44555	1.5924	6.4047	6.3942	1	1	1	-	D/A
-	N(2)	0.20208	0.29688	0.30564	3.3428	5.8021	4.3862	1	1	1	-	D/A
-	N(3)	0.33169	0.39304	0.20438	4.9925	6.5880	2.9331	1	1	1	-	D/A
-	N(4)	0.26616	0.26359	0.16939	3.9217	4.5947	2.4310	1	1	1	-	D/A
-	N(5)	0.23904	0.30705	0.50771	4.0392	7.0472	7.2862	1	1	1	-	D/A
-	N(6)	0.41124	0.36365	0.47379	6.2184	7.6500	6.7995	1	1	1	-	D/A
-	N(7)	0.37926	0.23766	0.61493	5.7615	6.6667	8.8249	1	1	1	-	D/A
-	N(8)	0.02784	0.47102	0.29804	1.4955	8.1850	4.2772	1	1	1	-	D/A
-	C(1)	0.26351	0.31609	0.22974	4.0477	5.6552	3.2970	1	1	1	-	-
-	C(2)	0.32982	0.47284	0.11072	5.0051	7.1875	1.5890	1	1	1	-	-
-	C(3)	0.42743	0.53068	0.10051	6.2952	7.9369	1.4425	1	1	1	-	-

-	C(4)	0.22509	0.54473	0.09382	3.8238	8.0961	1.3464	1	1	1	-	-
-	C(5)	0.36857	0.23003	0.12683	5.0755	3.8950	1.8201	1	1	1	-	-
-	C(6)	0.42007	0.12781	0.19046	5.6009	2.8194	2.7333	1	1	1	-	-
-	C(7)	0.34046	0.22991	0.03301	4.6254	3.3810	0.4738	1	1	1	-	-
-	C(8)	0.13681	0.20869	0.33452	2.4181	4.7321	4.8007	1	1	1	-	-
-	C(9)	0.09366	0.18805	0.43235	1.9598	4.9790	6.2047	1	1	1	-	-
-	C(10)	0.33816	0.30198	0.53138	5.2758	7.1059	7.6259	1	1	1	-	-
-	C(11)	0.51990	0.32022	0.44985	7.4523	6.9147	6.4558	1	1	1	-	-
-	C(12)	0.58646	0.40960	0.39856	8.3702	7.8788	5.7197	1	1	1	-	-
-	C(13)	0.50968	0.25498	0.39082	7.1473	5.6841	5.6087	1	1	1	-	-
-	C(14)	0.45274	0.26454	0.67134	6.7747	7.3490	9.6345	1	1	1	-	-
-	C(15)	0.38914	0.30985	0.73680	6.1443	8.3372	10.5740	1	1	1	-	-
-	C(16)	0.52810	0.16991	0.72196	7.5925	6.3079	10.3609	1	1	1	-	-
-	C(17)	0.16133	0.25317	0.58019	3.0698	6.6929	8.3264	1	1	1	-	-
-	C(18)	0.04623	0.27735	0.54423	1.6566	6.8332	7.8103	1	1	1	-	-
-	C(19)	-0.06851	0.44214	0.36081	0.3297	8.1257	5.1780	1	1	1	-	-
-	C(20)	-0.05928	0.32580	0.40187	0.2856	6.7303	5.7672	1	1	1	-	-
-	C(21)	0.21363	0.55739	0.37974	4.0219	9.8336	5.4497	1	1	1	-	-
-	C(22)	0.25504	0.65563	0.37196	4.6943	11.1588	5.3380	1	1	1	-	-
-	H(2A)	0.33735	0.43850	0.06354	4.9854	6.4518	0.9119	1	1	1	-	-
-	H(3)	0.33486	0.41327	0.24513	5.1120	7.0921	3.5180	1	1	1	-	D-H
-	H(3A)	0.43102	0.58182	0.03735	6.3586	8.3040	0.5360	1	1	1	-	-
-	H(3B)	0.49434	0.48260	0.11161	7.0465	7.3282	1.6017	1	1	1	-	-
-	H(3C)	0.42073	0.56542	0.14591	6.3238	8.6685	2.0939	1	1	1	-	-
-	H(4)	0.22308	0.21148	0.19139	3.3252	3.9893	2.7466	1	1	1	-	D-H
-	H(4A)	0.16284	0.50582	0.09796	2.9947	7.5769	1.4059	1	1	1	-	-
-	H(4B)	0.22906	0.59777	0.03165	3.8962	8.4949	0.4542	1	1	1	-	-
-	H(4C)	0.21541	0.57728	0.14088	3.8137	8.8061	2.0218	1	1	1	-	-
-	H(5A)	0.42137	0.28209	0.11652	5.8043	4.5635	1.6722	1	1	1	-	-
-	H(6)	0.38471	0.39514	0.42917	5.8975	7.8448	6.1591	1	1	1	-	D-H
-	H(6A)	0.48832	0.10801	0.16134	6.3734	2.3847	2.3153	1	1	1	-	-
-	H(6B)	0.36938	0.07569	0.20158	4.8988	2.1546	2.8929	1	1	1	-	-
-	H(6C)	0.43604	0.13319	0.24987	5.8725	3.2188	3.5860	1	1	1	-	-
-	H(7)	0.34198	0.19400	0.64619	5.2615	6.2296	9.2736	1	1	1	-	D-H
-	H(7A)	0.31554	0.30010	-0.00732	4.3968	4.1380	-0.1051	1	1	1	-	-
-	H(7B)	0.28203	0.18563	0.04105	3.8384	2.8085	0.5891	1	1	1	-	-
-	H(7C)	0.40556	0.20390	0.00442	5.3490	2.8629	0.0634	1	1	1	-	-
-	H(8A)	0.18306	0.14719	0.33081	2.8754	3.8557	4.7474	1	1	1	-	-
-	H(8B)	0.07498	0.22379	0.29216	1.6370	4.7110	4.1928	1	1	1	-	-
-	H(9A)	0.03533	0.14155	0.44611	1.1765	4.4068	6.4021	1	1	1	-	-
-	H(9B)	0.15344	0.15346	0.47633	2.6834	4.7375	6.8358	1	1	1	-	-
-	H(11A)	0.55730	0.27615	0.50872	7.9006	6.6226	7.3007	1	1	1	-	-
-	H(12A)	0.65958	0.38311	0.38236	9.2053	7.4216	5.4873	1	1	1	-	-
-	H(12B)	0.59329	0.44898	0.43872	8.5675	8.6465	6.2961	1	1	1	-	-
-	H(12C)	0.54940	0.45427	0.34154	7.9292	8.1894	4.9015	1	1	1	-	-
-	H(13A)	0.45515	0.20669	0.41994	6.4246	5.1708	6.0266	1	1	1	-	-
-	H(13B)	0.58078	0.21661	0.38629	7.9497	5.1251	5.5437	1	1	1	-	-

Flags	Label	Fractional Coordinates (x,y,z)			Orthogonal Coordinates (XO,YO,ZO)			Site	SSN*SSOF =	S.O.F	Move	Type
-	H(13C)	0.48656	0.29972	0.32829	6.8716	5.9654	4.7113	1	1	1	-	-
-	H(14A)	0.49855	0.31731	0.62835	7.3826	7.8489	9.0176	1	1	1	-	-
-	H(15A)	0.33219	0.36278	0.70265	5.4984	8.8877	10.0838	1	1	1	-	-
-	H(15B)	0.43883	0.34067	0.76354	6.8389	8.9123	10.9576	1	1	1	-	-
-	H(15C)	0.35491	0.25564	0.78693	5.6842	7.8564	11.2933	1	1	1	-	-
-	H(16A)	0.56906	0.14407	0.67656	8.0008	5.7003	9.7094	1	1	1	-	-
-	H(16B)	0.48462	0.11682	0.76395	7.0115	5.7982	10.9635	1	1	1	-	-
-	H(16C)	0.57953	0.18741	0.75822	8.2958	6.7496	10.8813	1	1	1	-	-
-	H(17A)	0.16364	0.27421	0.63483	3.1955	7.2842	9.1105	1	1	1	-	-
-	H(17B)	0.18270	0.17815	0.60050	3.2241	5.7594	8.6179	1	1	1	-	-
-	H(18A)	0.00094	0.22246	0.58220	1.0457	6.2763	8.3552	1	1	1	-	-
-	H(18B)	0.01278	0.34301	0.54956	1.3656	7.7764	7.8868	1	1	1	-	-
-	H(19A)	-0.13683	0.46924	0.32572	-0.5022	8.3115	4.6745	1	1	1	-	-
-	H(19B)	-0.06989	0.47083	0.41099	0.4185	8.7991	5.8982	1	1	1	-	-
-	H(20A)	-0.11876	0.30346	0.44921	-0.4325	6.6778	6.4467	1	1	1	-	-
-	H(20B)	-0.06718	0.29811	0.35218	0.0849	6.0734	5.0542	1	1	1	-	-
-	H(22A)	0.30322	0.67818	0.31643	5.2646	11.1696	4.5411	1	1	1	-	-
-	H(22B)	0.29617	0.64506	0.42747	5.2432	11.3147	6.1347	1	1	1	-	-
-	H(22C)	0.19298	0.70825	0.36685	4.0172	11.8635	5.2647	1	1	1	-	-
-	H(81)	-0.00133	0.45564	0.24539	1.0515	7.6834	3.5216	1	1	1	-	D-H
-	H(82)	0.03152	0.53076	0.28337	1.6289	8.9366	4.0666	1	1	1	-	D-H

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

Flags	Label	Fractional Coordinates (x,y,z)			Orthogonal Coordinates (XO,YO,ZO)			Site	SSN*SSOF =	S.O.F	Move	Type
-	C(23)	0.73910	-0.00418	0.13883	9.2368	0.6999	1.9924	1	1	1	-	-
-	C(24)	0.67790	-0.02255	0.07451	8.3807	0.0929	1.0693	1	1	1	-	-
-	C(25)	0.63304	0.05599	0.00272	7.8866	0.7943	0.0390	1	1	1	-	-
-	C(26)	0.64890	0.15451	-0.00697	8.2429	2.1130	-0.1001	1	1	1	-	-
-	C(27)	0.70742	0.17327	0.05845	9.0679	2.7314	0.8388	1	1	1	-	-
-	C(28)	0.75635	0.09552	0.13203	9.6155	2.0508	1.8947	1	1	1	-	-
-	C(29)	0.76152	0.30340	0.19344	10.1103	5.2802	2.7761	1	1	1	-	-
-	C(30)	0.77229	0.40734	0.16785	10.3960	6.5876	2.4089	1	1	1	-	-
-	C(31)	0.86496	0.44691	0.12567	11.5580	6.9081	1.8036	1	1	1	-	-
-	C(32)	0.94985	0.38300	0.10909	12.4720	5.9278	1.5656	1	1	1	-	-
-	C(33)	0.94098	0.27855	0.13476	12.2091	4.6139	1.9339	1	1	1	-	-
-	C(34)	0.84653	0.23617	0.17730	11.0205	4.2561	2.5445	1	1	1	-	-
-	C(35)	0.99850	0.04644	0.12178	12.4967	1.3116	1.7477	1	1	1	-	-
-	C(36)	1.10558	0.00337	0.11148	13.7270	0.6557	1.5999	1	1	1	-	-
-	C(37)	1.16765	-0.04004	0.18783	14.4993	0.4683	2.6955	1	1	1	-	-
-	C(38)	1.12543	-0.04292	0.27459	14.0713	0.9020	3.9407	1	1	1	-	-
-	C(39)	1.02023	0.00170	0.28162	12.8632	1.5615	4.0415	1	1	1	-	-
-	C(40)	0.95282	0.04861	0.20554	12.0316	1.7992	2.9497	1	1	1	-	-
-	C(41)	0.81629	0.09695	0.38567	10.6365	3.4559	5.5348	1	1	1	-	-

-	C(42)	0.77358	0.06763	0.47512	10.1593	3.5361	6.8185	1	1	1	- -
-	C(43)	0.68316	0.01380	0.49871	8.9794	2.9155	7.1571	1	1	1	- -
-	C(44)	0.63643	-0.00947	0.43156	8.2895	2.2249	6.1934	1	1	1	- -
-	C(45)	0.68097	0.02061	0.34107	8.7895	2.1494	4.8948	1	1	1	- -
-	C(46)	0.77361	0.07509	0.31361	9.9936	2.7580	4.5006	1	1	1	- -
-	B(1)	0.83155	0.11124	0.20804	10.6522	2.6848	2.9857	1	1	1	- -
-	H(23A)	0.77019	-0.06115	0.18901	9.5753	0.1808	2.7125	1	1	1	- -
-	H(24A)	0.66802	-0.09111	0.08170	8.1475	-0.8223	1.1725	1	1	1	- -
-	H(25A)	0.59093	0.04366	-0.04078	7.2989	0.3851	-0.5852	1	1	1	- -
-	H(26A)	0.61967	0.21053	-0.05883	7.9238	2.6097	-0.8443	1	1	1	- -
-	H(27A)	0.71358	0.24240	0.05177	9.2571	3.6574	0.7430	1	1	1	- -
-	H(29A)	0.69500	0.27780	0.22244	9.2796	5.0822	3.1923	1	1	1	- -
-	H(30A)	0.71321	0.45153	0.18030	9.7603	7.2707	2.5874	1	1	1	- -
-	H(31A)	0.87090	0.51837	0.10779	11.7360	7.8053	1.5469	1	1	1	- -
-	H(32A)	1.01564	0.41001	0.07976	13.2959	6.1436	1.1446	1	1	1	- -
-	H(33A)	1.00127	0.23520	0.12279	12.8615	3.9450	1.7622	1	1	1	- -
-	H(35A)	0.95503	0.07575	0.06805	11.9537	1.4262	0.9766	1	1	1	- -
-	H(36A)	1.13401	0.00463	0.05209	14.0130	0.3489	0.7475	1	1	1	- -
-	H(37A)	1.24070	-0.06875	0.18191	15.3410	0.0362	2.6106	1	1	1	- -
-	H(38A)	1.16830	-0.07513	0.32843	14.6019	0.7475	4.7134	1	1	1	- -
-	H(39A)	0.99247	0.00035	0.34121	12.5854	1.8681	4.8967	1	1	1	- -
-	H(41A)	0.87854	0.13434	0.37165	11.4520	3.8998	5.3336	1	1	1	- -
-	H(42A)	0.80653	0.08454	0.52088	10.6448	4.0214	7.4752	1	1	1	- -
-	H(43A)	0.65350	-0.00697	0.56063	8.6470	2.9645	8.0457	1	1	1	- -
-	H(44A)	0.57361	-0.04614	0.44676	7.4697	1.7974	6.4115	1	1	1	- -
-	H(45A)	0.64716	0.00348	0.29586	8.2936	1.6642	4.2459	1	1	1	- -

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

Resd	Site	X(cen)	Y(cen)	Z(cen)	Mol.Wt	S.O.F	Z	C	H	B	Cl	N	Ni	O
1	1	0.262	0.351	0.374	516.38	1	2	22	49	-	-	8	1	2
2	1	0.835	0.116	0.206	319.21	1	2	24	20	1	-	-	-	-
				Unit Cell Weight =	1671.18			92	138	2	0	16	2	4
				Calculated Analysis (Percent) =				66.1	8.3	1.3	0.0	13.4	7.0	3.8

Moiety_Formula = C22 H49 N8 Ni O2, C24 H20 B

Sum_Formula = C46 H69 B N8 Ni O2

Formula_Weight = 835.59 [Note: Based on SHELXL97 Atomic Weights]

Formula_Z = 2

SpaceGroup_Z = 2 ===> Z' = 2 / 2 = 1.000

Calculated Density = 1.1294(6) g cm-3 [= Mg m-3]

F(000) = 900.0 [900.93]

mu(MoKa) = 4.37 cm-1 = 0.437 mm-1

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

Resonant Scattering = 2.84 Percent - (Girard,E. et al. (2003). Acta Cryst. D59, 1914-1922)

Predicted Volume = 2289.9[2268.6] 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"

Search for and Analysis of Solvent Accessible Voids in the Structure - Grid = 0.20 Ang., Probe Radius = 1.20 Ang., NStep = 6

van der Waals (or ion) Radii used in the Analysis

C	H	B	Cl	N	Ni	O
1.70	1.20	1.63	1.75	1.55	2.30	1.52

:: Grid: X-Axis Step = 0.0167 = Points 60, Angstrom Step = 0.20
:: Grid: Y-Axis Step = 0.0139 = Points 72, Angstrom Step = 0.19
:: Grid: Z-Axis Step = 0.0139 = Points 72, Angstrom Step = 0.21

:: Total Potential Solvent Area Vol 209.6 Ang^3
per Unit Cell Vol 2457.2 Ang^3 [8.5%]

Note: Expected volumes for solvent molecules are:
A hydrogen bonded H2O-molecule 40 Ang^3
Small molecules (e.g. Toluene) 100-300 Ang^3

Values below for gridpoints and volumes in []
refer to areas where atom centers may reside.

Area	#GridPoint	VolPerc.	Vol(A^3)	X(av)	Y(av)	Z(av)	Eigenvector(frac)			Sig(Ang)
1	13263[2044]	4	105[16.1]	0.020	0.257	0.856	1	1.000	0.172	0.240	1.62
							2	-0.604	0.156	1.000	1.33
							3	0.221	-1.000	0.465	1.09
2	13265[2044]	4	105[16.1]	-0.021	0.743	0.144	1	1.000	0.172	0.239	1.62
							2	-0.601	0.154	1.000	1.33
							3	0.222	-1.000	0.464	1.10

	x	y	z	Shortest Contacts within 4.5 Angstrom (Excl. H)
1	0.020	0.257	0.856	N8 3.70; C36 3.99; C4 4.07; C35 4.11; C35 4.18; C37 4.30; C23 4.30; C36 4.33; C19 4.42;
2	-0.021	0.743	0.144	N8 3.70; C36 3.99; C4 4.07; C35 4.11; C35 4.18; C37 4.30; C23 4.30; C36 4.33; C19 4.41;

:: Note: use CALC VOID (not CALC SOLV) for Packing Index.

Report the Distance from VOID-CG to Boundary in EV-Directions

Nr	MinEV1	MaxEV1	MinEV2	MaxEV2	MinEV3	MaxEV3	MaxDist (Ang)
1	-4.08	3.50	-3.12	3.12	-2.32	2.78	4.08
2	-3.54	4.06	-3.12	3.12	-2.78	2.32	4.06

(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	Ni1	0.03461	0.03237	0.03855	-0.01160	-0.00391	-0.00303	0.03536	0.0323	0.0334	0.0404	1.25
		[0.1595	0.3886	0.3832]	[0.1614	0.3897	0.3806]					
2	O1	0.04164	0.03563	0.04102	-0.01288	-0.00216	-0.00654	0.03937	0.0343	0.0403	0.0435	1.27
		[0.2648	0.5059	0.3312]	[0.2614	0.5061	0.3328]					
3	O2	0.03742	0.04283	0.05470	-0.02261	-0.00012	-0.00279	0.04371	0.0360	0.0397	0.0554	1.54
		[0.1338	0.5217	0.4338]	[0.1332	0.5272	0.4283]					
4	N1	0.02688	0.03301	0.03544	-0.00833	-0.00303	-0.00063	0.03297	0.0256	0.0328	0.0405	1.58
		[0.0483	0.2862	0.4478]	[0.0492	0.2843	0.4433]					
5	N2	0.03590	0.03940	0.04069	-0.01750	0.00283	-0.00211	0.03813	0.0311	0.0401	0.0432	1.39
		[0.2032	0.2951	0.3073]	[0.2010	0.2987	0.3040]					
6	N3	0.06486	0.03888	0.04618	-0.01622	-0.00240	-0.01991	0.04833	0.0284	0.0461	0.0704	2.48
		[0.3393	0.3904	0.2041]	[0.3241	0.3957	0.2046]					
7	N4	0.05121	0.04905	0.04769	-0.02879	0.00126	-0.00611	0.04616	0.0304	0.0507	0.0574	1.89
		[0.2682	0.2591	0.1722]	[0.2642	0.2681	0.1665]					
8	N5	0.02562	0.03541	0.03541	-0.01027	-0.00084	-0.00412	0.03272	0.0254	0.0337	0.0390	1.54
		[0.2383	0.3084	0.5095]	[0.2398	0.3057	0.5059]					
9	N6	0.03448	0.04017	0.03667	-0.00233	-0.00129	-0.00738	0.03994	0.0290	0.0346	0.0562	1.93
		[0.4094	0.3664	0.4765]	[0.4131	0.3609	0.4711]					
10	N7	0.03717	0.04156	0.04709	-0.00024	-0.01134	-0.01144	0.04508	0.0301	0.0326	0.0725	2.41
		[0.3745	0.2398	0.6193]	[0.3840	0.2355	0.6106]					
11	N8	0.04616	0.03262	0.04967	-0.01112	-0.01482	-0.00157	0.04333	0.0317	0.0363	0.0620	1.96
		[0.0236	0.4695	0.3015]	[0.0320	0.4725	0.2945]					
12	C1	0.05200	0.04692	0.03631	-0.01744	-0.01189	0.00047	0.04431	0.0293	0.0447	0.0589	2.01
		[0.2681	0.3189	0.2277]	[0.2589	0.3133	0.2318]					
13	C2	0.08756	0.04342	0.04351	-0.01486	0.00581	-0.02402	0.05719	0.0355	0.0441	0.0920	2.59
		[0.3389	0.4697	0.1116]	[0.3207	0.4760	0.1098]					
14	C3	0.07664	0.07424	0.09032	-0.01201	0.02399	-0.02242	0.08527	0.0468	0.0876	0.1214	2.60
		[0.4324	0.5293	0.1083]	[0.4224	0.5320	0.0928]					
15	C4	0.08279	0.06393	0.05645	0.01003	-0.01720	-0.02012	0.07457	0.0367	0.0682	0.1188	3.24
		[0.2160	0.5494	0.0989]	[0.2342	0.5401	0.0887]					
16	C5	0.04613	0.06393	0.05808	-0.03294	0.00388	-0.00155	0.05358	0.0378	0.0532	0.0697	1.85
		[0.3691	0.2249	0.1297]	[0.3681	0.2352	0.1239]					
17	C6	0.05479	0.06869	0.10747	-0.02063	-0.00127	0.00687	0.08123	0.0479	0.0770	0.1188	2.48
		[0.4211	0.1260	0.1990]	[0.4191	0.1296	0.1819]					
18	C7	0.08051	0.11603	0.07952	-0.06580	-0.01110	0.01372	0.08511	0.0443	0.0736	0.1374	3.10
		[0.3440	0.2412	0.0275]	[0.3370	0.2186	0.0385]					

19	C8	0.03947	0.03194	0.07011	-0.01920	-0.01186	-0.00055	0.04664	0.0301	0.0363	0.0735	2.44
		[0.1341	0.2047	0.3407]	[0.1395	0.2126	0.3283]					
20	C9	0.03028	0.03176	0.06039	-0.01151	-0.00159	-0.00255	0.04222	0.0300	0.0321	0.0645	2.15
		[0.0934	0.1858	0.4380]	[0.0940	0.1903	0.4267]					
21	C10	0.04179	0.02818	0.03786	-0.00818	-0.00307	-0.00396	0.03681	0.0279	0.0395	0.0431	1.55
		[0.3411	0.3022	0.5299]	[0.3352	0.3018	0.5328]					
22	C11	0.02981	0.05374	0.05307	-0.00264	-0.01246	0.00578	0.05043	0.0220	0.0502	0.0791	3.59
		[0.5181	0.3253	0.4557]	[0.5217	0.3151	0.4440]					
23	C12	0.04962	0.09861	0.08503	-0.01702	0.01881	-0.03031	0.08116	0.0327	0.0932	0.1175	3.59
		[0.5824	0.4180	0.4034]	[0.5905	0.4012	0.3937]					
24	C13	0.05987	0.05146	0.06511	-0.00874	0.00346	0.00828	0.06370	0.0420	0.0578	0.0913	2.17
		[0.5141	0.2568	0.3949]	[0.5053	0.2531	0.3868]					
25	C14	0.05895	0.06146	0.04582	0.00135	-0.01711	-0.02463	0.05864	0.0350	0.0399	0.1010	2.89
		[0.4447	0.2693	0.6748]	[0.4608	0.2598	0.6679]					
26	C15	0.15997	0.10033	0.08645	-0.05421	0.01061	-0.05031	0.10718	0.0531	0.0933	0.1752	3.30
		[0.4033	0.3029	0.7392]	[0.3750	0.3168	0.7344]					
27	C16	0.05917	0.07138	0.09077	0.01449	-0.03852	-0.01229	0.08346	0.0326	0.0600	0.1578	4.84
		[0.5180	0.1737	0.7326]	[0.5381	0.1661	0.7113]					
28	C17	0.03818	0.03291	0.04522	-0.00598	-0.00105	-0.00707	0.04068	0.0298	0.0388	0.0535	1.80
		[0.1602	0.2532	0.5839]	[0.1625	0.2531	0.5764]					
29	C18	0.03601	0.03859	0.03958	-0.00759	0.00506	-0.00855	0.03972	0.0282	0.0412	0.0497	1.76
		[0.0468	0.2783	0.5473]	[0.0457	0.2764	0.5412]					
30	C19	0.03088	0.04661	0.05629	-0.02399	-0.01067	0.00532	0.04337	0.0267	0.0417	0.0617	2.31
		[-0.0705	0.4369	0.3652]	[-0.0665	0.4473	0.3564]					
31	C20	0.02831	0.03593	0.05038	-0.01462	-0.00744	0.00226	0.03859	0.0253	0.0384	0.0521	2.06
		[-0.0609	0.3230	0.4064]	[-0.0577	0.3286	0.3973]					
32	C21	0.03805	0.03365	0.06167	-0.01836	-0.01270	0.00207	0.04401	0.0301	0.0360	0.0659	2.19
		[0.2108	0.5539	0.3848]	[0.2164	0.5609	0.3747]					
33	C22	0.05453	0.05257	0.10159	-0.03837	0.00651	-0.01574	0.06606	0.0380	0.0566	0.1036	2.73
		[0.2572	0.6488	0.3798]	[0.2529	0.6625	0.3641]					
34	H2A	0.06863						0.06863				
35	H3	0.05799						0.05799				
36	H3A	0.12791						0.12791				
37	H3B	0.12791						0.12791				
38	H3C	0.12791						0.12791				
39	H4	0.05539						0.05539				
40	H4A	0.11186						0.11186				
41	H4B	0.11186						0.11186				
42	H4C	0.11186						0.11186				
43	H5A	0.06430						0.06430				
44	H6	0.04793						0.04793				
45	H6A	0.12184						0.12184				
46	H6B	0.12184						0.12184				
47	H6C	0.12184						0.12184				
48	H7	0.05410						0.05410				
49	H7A	0.12766						0.12766				
50	H7B	0.12766						0.12766				
51	H7C	0.12766						0.12766				

52	H8A	0.05597						0.05597				
53	H8B	0.05597						0.05597				
54	H9A	0.05066						0.05066				
55	H9B	0.05066						0.05066				
56	H11A	0.06051						0.06051				
57	H12A	0.12174						0.12174				
58	H12B	0.12174						0.12174				
59	H12C	0.12174						0.12174				
60	H13A	0.09556						0.09556				
61	H13B	0.09556						0.09556				
62	H13C	0.09556						0.09556				
63	H14A	0.07037						0.07037				
64	H15A	0.16077						0.16077				
65	H15B	0.16077						0.16077				
66	H15C	0.16077						0.16077				
67	H16A	0.12519						0.12519				
68	H16B	0.12519						0.12519				
69	H16C	0.12519						0.12519				
70	H17A	0.04882						0.04882				
71	H17B	0.04882						0.04882				
72	H18A	0.04767						0.04767				
73	H18B	0.04767						0.04767				
74	H19A	0.05205						0.05205				
75	H19B	0.05205						0.05205				
76	H20A	0.04631						0.04631				
77	H20B	0.04631						0.04631				
78	H22A	0.09909						0.09909				
79	H22B	0.09909						0.09909				
80	H22C	0.09909						0.09909				
81	H81	0.05200						0.05200				
82	H82	0.05200						0.05200				
U(i,j)-Average		0.0506	0.0505	0.0574	-0.0155	-0.0035	-0.0074	0.0536	0.0483	0.0510	0.0616	1.28

Residue = 2

Atom	Label	U11 or Uiso	U22	U33	U23	U13	U12	Ueq(sUeq)	U1	U2	U3	U3/U1
1	C23	0.04815	0.04263	0.03564	-0.01297	0.00405	-0.01953	0.04135	0.0285	0.0366	0.0590	2.07
		[0.7442	-0.0077	0.1395]	[0.7340	-0.0006	0.1381]					
2	C24	0.06123	0.05626	0.04451	-0.02913	0.01730	-0.02045	0.05058	0.0297	0.0428	0.0792	2.67
		[0.6847	-0.0282	0.0778]	[0.6711	-0.0169	0.0712]					

3	C25	0.04812	0.08022	0.03925	-0.03556	0.00312	-0.02887	0.05012	0.0207	0.0397	0.0900	4.34
		[0.6259	0.0666	-0.0007]	[0.6402	0.0454	0.0062]					
4	C26	0.04587	0.07007	0.04632	-0.01328	-0.01166	-0.01227	0.05506	0.0340	0.0522	0.0790	2.32
		[0.6446	0.1602	-0.0058]	[0.6532	0.1488	-0.0081]					
5	C27	0.04422	0.04391	0.04707	-0.01581	-0.00736	-0.00377	0.04494	0.0391	0.0439	0.0518	1.32
		[0.7057	0.1725	0.0599]	[0.7091	0.1740	0.0569]					
6	C28	0.03077	0.03839	0.03833	-0.01443	0.00828	-0.01194	0.03535	0.0229	0.0372	0.0460	2.01
		[0.7595	0.0919	0.1346]	[0.7532	0.0992	0.1294]					
7	C29	0.05625	0.04266	0.05500	-0.01612	0.00254	-0.01324	0.05115	0.0380	0.0552	0.0603	1.59
		[0.7650	0.3013	0.1950]	[0.7581	0.3055	0.1919]					
8	C30	0.09809	0.04409	0.05827	-0.02053	-0.00335	-0.00860	0.06602	0.0417	0.0582	0.0981	2.35
		[0.7812	0.4069	0.1676]	[0.7634	0.4078	0.1681]					
9	C31	0.10779	0.03149	0.05688	-0.00246	-0.01720	-0.02954	0.06631	0.0228	0.0553	0.1208	5.29
		[0.8804	0.4444	0.1221]	[0.8495	0.4494	0.1293]					
10	C32	0.07129	0.06356	0.05173	0.00330	-0.01357	-0.03734	0.06548	0.0328	0.0464	0.1173	3.58
		[0.9394	0.3888	0.1128]	[0.9603	0.3772	0.1054]					
11	C33	0.05789	0.04699	0.03178	-0.00065	-0.00383	-0.02396	0.04748	0.0257	0.0395	0.0773	3.00
		[0.9329	0.2832	0.1363]	[0.9490	0.2739	0.1332]					
12	C34	0.05180	0.04504	0.02267	-0.00911	-0.00270	-0.01337	0.03983	0.0223	0.0391	0.0580	2.60
		[0.8532	0.2324	0.1772]	[0.8399	0.2399	0.1774]					
13	C35	0.04056	0.06501	0.03868	-0.01098	0.00690	-0.00604	0.05054	0.0316	0.0474	0.0726	2.29
		[0.9982	0.0526	0.1227]	[0.9988	0.0403	0.1209]					
14	C36	0.05579	0.06334	0.04120	-0.01262	-0.00312	-0.00488	0.05515	0.0408	0.0559	0.0687	1.68
		[1.1051	0.0076	0.1118]	[1.1060	-0.0008	0.1112]					
15	C37	0.03706	0.06293	0.06176	-0.02741	-0.00176	0.00469	0.05334	0.0340	0.0574	0.0687	2.02
		[1.1685	-0.0343	0.1850]	[1.1668	-0.0457	0.1907]					
16	C38	0.05715	0.05479	0.05024	-0.01696	-0.00798	0.00058	0.05479	0.0456	0.0553	0.0635	1.39
		[1.1277	-0.0411	0.2737]	[1.1232	-0.0447	0.2754]					
17	C39	0.05475	0.05118	0.03711	-0.01615	0.00000	-0.00178	0.04797	0.0363	0.0491	0.0585	1.61
		[1.0236	0.0036	0.2815]	[1.0169	-0.0002	0.2818]					
18	C40	0.04275	0.03869	0.02725	-0.01083	0.00269	-0.01732	0.03550	0.0254	0.0283	0.0528	2.08
		[0.9577	0.0452	0.2061]	[0.9480	0.0520	0.2050]					
19	C41	0.04621	0.04593	0.05165	-0.02174	-0.00933	-0.01113	0.04573	0.0292	0.0506	0.0574	1.97
		[0.8121	0.0955	0.3890]	[0.8204	0.0984	0.3824]					
20	C42	0.06000	0.04869	0.03300	-0.01522	-0.00192	0.00290	0.04779	0.0321	0.0449	0.0663	2.07
		[0.7790	0.0702	0.4747]	[0.7682	0.0650	0.4755]					
21	C43	0.05639	0.04151	0.03685	-0.00175	0.01359	0.00396	0.04991	0.0278	0.0394	0.0825	2.97
		[0.6904	0.0160	0.5023]	[0.6759	0.0116	0.4951]					
22	C44	0.05260	0.03594	0.04861	-0.00890	0.01531	-0.01250	0.04759	0.0276	0.0455	0.0697	2.53
		[0.6424	-0.0119	0.4360]	[0.6305	-0.0070	0.4271]					
23	C45	0.03868	0.02801	0.04208	-0.01370	0.00136	-0.00309	0.03608	0.0269	0.0375	0.0439	1.63
		[0.6830	0.0188	0.3437]	[0.6790	0.0224	0.3385]					
24	C46	0.04070	0.02354	0.03960	-0.00908	0.00170	-0.00291	0.03541	0.0235	0.0377	0.0450	1.91
		[0.7771	0.0738	0.3163]	[0.7701	0.0763	0.3109]					
25	B1	0.04140	0.03322	0.02845	-0.00823	-0.00188	-0.01428	0.03414	0.0250	0.0286	0.0489	1.96
		[0.8362	0.1089	0.2077]	[0.8269	0.1136	0.2084]					
26	H23A	0.04962						0.04962				
27	H24A	0.06069						0.06069				

28	H25A	0.06014						0.06014				
29	H26A	0.06608						0.06608				
30	H27A	0.05393						0.05393				
31	H29A	0.06137						0.06137				
32	H30A	0.07922						0.07922				
33	H31A	0.07957						0.07957				
34	H32A	0.07858						0.07858				
35	H33A	0.05698						0.05698				
36	H35A	0.06065						0.06065				
37	H36A	0.06618						0.06618				
38	H37A	0.06401						0.06401				
39	H38A	0.06575						0.06575				
40	H39A	0.05756						0.05756				
41	H41A	0.05488						0.05488				
42	H42A	0.05735						0.05735				
43	H43A	0.05989						0.05989				
44	H44A	0.05711						0.05711				
45	H45A	0.04330						0.04330				
U(i,j)-Average		0.0538	0.0479	0.0426	-0.0136	-0.0004	-0.0114	0.0483	0.0415	0.0460	0.0574	1.38

==========

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

where

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

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

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

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

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

Ueq [or U(iso)] Averages per Element

	Non-H	C	H	B	Cl	N	Ni	O
Average	0.0513	0.0543	0.0825	0.0341	0.0000	0.0408	0.0354	0.0415
Minimum	0.0327	0.0353	0.0433	0.0341	0.0000	0.0327	0.0354	0.0394
Maximum	0.1072	0.1072	0.1608	0.0341	0.0000	0.0483	0.0354	0.0437
Ratio	3.2761	3.0323	3.7129	1.0000	0.0000	1.4772	1.0000	1.1104
Number	58	46	69	1	0	8	1	2

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

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

N: Number of Ignored Lines on INPUT   4
          of which blank in column 1   4
N: Total Potential Solvent Accessible Void Vol ....   206.6 Ang^3
N: Electron Count / Cell =   34 - To be included in D(calc), F000 & Mol.Wght.

:: Input Xtal Data from File sg726.res - Data Type RES

:: NORMAL END of PLATON :   29 Pages on:
:: sg726.lis (ASCII, 132 Characters Wide)
:: sg726.lps (PostScript Version of .lis)
:: sg726.pdf (PDF   Version of .lis)

:: SQUEEZE xyz on :sg726.sqz
:: SQUEEZE CIF on :sg726.sqf