PLATON(V-311206)-Run for: i10466 in P2(1)2(1)2(1) TIME: Oct 14 11:18:27 2008

Crystal Data

Input Cell (Lattice Type: P) - Temp = 150K				Reduced Cell (Acta Cryst.(1976),A32,297-298)				
a = 7.9660(3)	Angstrom	alpha =	90 Degree	a = 7.966	alpha =	90.00	V =	2228.3
b = 12.1449(5)		beta =	90	b = 12.145	beta =	90.00		
c = 23.0321(9)		gamma =	90	c = 23.032	gamma =	90.00		
V = 2228.27(15)	Cubic-Angstrom	d(100) =	7.9660 Angstrom	Niggli Values				
		d(010) =	12.1449	63.457	147.499	530.478		
Lambda(MoKa) = 0.71073	Angstrom	d(001) =	23.0321	0.000	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)

$$\begin{pmatrix} XO \\ YO \\ ZO \end{pmatrix} = \begin{pmatrix} 7.96600 & 0 & 0 \\ 0 & 12.14490 & 0 \\ 0 & 0 & 23.03210 \end{pmatrix} \begin{pmatrix} X \\ Y \\ Z \end{pmatrix} \quad , \quad \begin{pmatrix} X \\ Y \\ Z \end{pmatrix} = \begin{pmatrix} 0.12553 & 0 & 0 \\ 0 & 0.08234 & 0 \\ 0 & 0 & 0.04342 \end{pmatrix} \begin{pmatrix} XO \\ YO \\ ZO \end{pmatrix}$$

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 P212121 No: 19, Laue: mmm [Hall: P 2ac 2ab]

Lattice Type oP, Acentric, Orthorhombic, Order 4(4) [Schoenflies: D2^4]

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

Nr	***** Symmetry Operation(s) *****		
1	X ,	Y ,	Z
2	1/2 - X ,	- Y ,	1/2 + Z
3	1/2 + X ,	1/2 - Y ,	- Z
4	- 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   27 (Unitcell 108)
- Density based on Input Atom Set = 1.244 g.cm-3 - Vol / Non-H atom = 20.6 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	(Deg) Dot	Angle	(%) Fit	(Ang) MaxDev.		Input Cell x	y	z
:: NonFits (i.e. Atoms with no symmetry related counterpart):												
	C16	C21										
c *	[1 0 0]	[1 0 0]	7.97	2	1	0.00	92	0.208	through	0.751	0	0
							C17	-C15	Glide =	0	0	1/2
:: NonFits (i.e. Atoms with no symmetry related counterpart):												
	C16	C21										
m *	[0 1 0]	[0-1 0]	12.14	2	1	0.00	92	0.208	through	0	1/2	0
							C17	-C15				
:: NonFits (i.e. Atoms with no symmetry related counterpart):												
	C16	C21										
n *	[0 0 1]	[0 0 1]	23.03	2	1	0.00	92	0.208	through	0	0	1/2
							C17	-C15	Glide =	1/2	1/2	0
-1 *	==========	==========					100	0.386	at	0.001	1/4	1/4
							C21	-C21				

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
(0 0 1)	(1 0 0)	(0 0 -1)	Det(T)
(0 1 0) X	(0 -1 0) =	(0 -1 0)	=
(-1 0 0)	(0 0 -1)	(-1 0 0)	1.000

Cell	Lattice	a	b	c	Alpha	Beta	Gamma	Volume	CrystalSystem	Laue
Input	oP	7.966	12.145	23.032	90.00	90.00	90.00	2228	Orthorhombic	mmm
Reduced	P	7.966	12.145	23.032	90.00	90.00	90.00	2228		
Convent	oP	23.032	12.145	7.966	90.00	90.00	90.00	2228	Orthorhombic	mmm

Conventional, New or Pseudo Symmetry

Space Group Pnma No: 62, Laue: mmm [Hall: -P 2ac 2n]

Lattice Type oP, Centric, Orthorhombic, Order 8(4) [Schoenflies: D2h^16]

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

:: Origin Shifted to:-0.2501,-0.2503,-0.0010 after Transformation

::   (0.0000 0.0000 -1.0000) (0.2501)
:: R/t for Coordinates (0.0000 -1.0000 0.0000) (0.2503)
::   (-1.0000 0.0000 0.0000) (0.0010)

:: * Symmetry Elements Preceded by an Asterisk are New and Indicate
::   Missed/Pseudosymmetry. Proposed Inversion or (Glide) Planes do NOT Apply
::   for Chiral Molecules.
:: Note: Glide Plane Codes are with Reference to the Input Cell !!

P! i10466 in P2(1)2(1)2(1)   oP=>oP 0.0 0 0 0.000 0.00 0.500   92% Pnma

:: An SPF-style file is written to be used for the cell transformation.

(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	Al	Cl	N	O
Cov.Rad(Ang):	0.68	0.35	1.35	0.99	0.68	0.68
Atom Volume :	13.87	5.08	39.60	25.80	11.80	11.39
Atom Number :	6	1	13	17	7	8
Atom Weight :	12.010	1.008	26.98	35.45	14.01	16.00
Scat.Fact.f0:	5.999	1.000	12.994	17.001	6.995	7.999
Scat.Fact.f':	0.003	0.000	0.064	0.148	0.006	0.011
Scat.Fact.f":	0.002	0.000	0.051	0.159	0.003	0.006
Mu/Rho(MoKa):	0.58	0.37	5.11	11.52	0.84	1.22
Elem. Type :	--	--	--	HL	--	--

```
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
```

Flags	Label	Fractional Coordinates (x,y,z)			Orthogonal Coordinates (XO,YO,ZO)			Site	SSN	*SSOF = S.O.F	Move	Type
-	Cl(1)	0.17758	0.35519	0.37400	1.4146	4.3137	8.6140	1	1	1	4.645	D/A
-	Cl(2)	0.17955	0.64532	0.37429	1.4303	7.8373	8.6207	1	1	1	4.645	D/A
-	Al	0.31567	0.50159	0.34796	2.5146	6.0918	8.0142	1	1	1	4.645	Met
-	N(1)	0.68652	0.50178	0.38022	5.4688	6.0941	8.7573	1	1	1	4.645	D/A
-	N(2)	0.53800	0.50053	0.45696	4.2857	6.0789	10.5247	1	1	1	4.645	D/A
-	C(1)	0.35914	0.49234	0.26345	2.8609	5.9794	6.0678	1	1	1	4.645	-
-	C(2)	0.53086	0.49685	0.39842	4.2288	6.0342	9.1764	1	1	1	4.645	-
-	C(3)	0.79863	0.50406	0.42701	6.3619	6.1218	9.8349	1	1	1	4.645	-
-	C(4)	0.70404	0.49559	0.47472	5.6084	6.0189	10.9338	1	1	1	4.645	-
-	C(5)	0.77495	0.60172	0.29265	6.1733	7.3078	6.7403	1	1	1	4.645	-
-	C(6)	0.84219	0.60097	0.23743	6.7089	7.2987	5.4685	1	1	1	4.645	-
-	C(7)	0.87690	0.50101	0.20979	6.9854	6.0847	4.8319	1	1	1	4.645	-
-	C(8)	0.84271	0.40525	0.23564	6.7130	4.9217	5.4273	1	1	1	4.645	-
-	C(9)	0.77994	0.40109	0.29467	6.2130	4.8712	6.7869	1	1	1	4.645	-
-	C(10)	0.74576	0.50315	0.32043	5.9407	6.1107	7.3802	1	1	1	4.645	-
-	C(11)	0.74023	0.70847	0.32214	5.8967	8.6043	7.4196	1	1	1	4.645	-
-	C(12)	0.95240	0.51573	0.14958	7.5868	6.2635	3.4451	1	1	1	4.645	-
-	C(13)	0.73876	0.29609	0.32292	5.8850	3.5960	7.4375	1	1	1	4.645	-
-	C(14)	0.33433	0.60100	0.51486	2.6633	7.2991	11.8583	1	1	1	4.645	-

-	C(15)	0.20140	0.58850	0.55392	1.6044	7.1473	12.7579	1	1	1	4.645 -
-	C(16)	0.13076	0.47648	0.57144	1.0416	5.7868	13.1615	1	1	1	4.645 -
-	C(17)	0.19990	0.37830	0.55130	1.5924	4.5944	12.6976	1	1	1	4.645 -
-	C(18)	0.33810	0.39862	0.51585	2.6933	4.8412	11.8811	1	1	1	4.645 -
-	C(19)	0.39757	0.49825	0.49660	3.1670	6.0512	11.4377	1	1	1	4.645 -
-	C(20)	0.42117	0.71106	0.49283	3.3550	8.6358	11.3509	1	1	1	4.645 -
-	C(21)	-0.02423	0.46846	0.61142	-0.1930	5.6894	14.0823	1	1	1	4.645 -
-	C(22)	0.41058	0.29612	0.50271	3.2707	3.5963	11.5785	1	1	1	4.645 -
-	H(1A)	0.42012	0.55638	0.25111	3.3467	6.7572	5.7836	1	1	1	4.645 -
-	H(1B)	0.42406	0.42756	0.25528	3.3781	5.1927	5.8796	1	1	1	4.645 -
-	H(1C)	0.25432	0.48857	0.24298	2.0259	5.9336	5.5963	1	1	1	4.645 -
-	H(3A)	0.91864	0.51040	0.42520	7.3179	6.1988	9.7932	1	1	1	4.645 -
-	H(4A)	0.74361	0.48759	0.51386	5.9236	5.9217	11.8353	1	1	1	4.645 -
-	H(6A)	0.86519	0.66920	0.21795	6.8921	8.1274	5.0198	1	1	1	4.645 -
-	H(8A)	0.86002	0.33782	0.21474	6.8509	4.1028	4.9459	1	1	1	4.645 -
-	H(11A)	0.69404	0.69471	0.35994	5.5287	8.4372	8.2902	1	1	1	4.645 -
-	H(11B)	0.84282	0.74931	0.32594	6.7139	9.1003	7.5071	1	1	1	4.645 -
-	H(11C)	0.66146	0.75018	0.29952	5.2692	9.1109	6.8986	1	1	1	4.645 -
-	H(12A)	0.97361	0.44481	0.13269	7.7558	5.4022	3.0561	1	1	1	4.645 -
-	H(12B)	0.87533	0.55581	0.12549	6.9729	6.7503	2.8903	1	1	1	4.645 -
-	H(12C)	1.05588	0.55584	0.15257	8.4111	6.7506	3.5140	1	1	1	4.645 -
-	H(13A)	0.69937	0.30985	0.36164	5.5712	3.7631	8.3293	1	1	1	4.645 -
-	H(13B)	0.65277	0.25919	0.30114	5.2000	3.1478	6.9359	1	1	1	4.645 -
-	H(13C)	0.83721	0.25060	0.32444	6.6692	3.0435	7.4725	1	1	1	4.645 -
-	H(15A)	0.15219	0.65343	0.57051	1.2123	7.9358	13.1400	1	1	1	4.645 -
-	H(17A)	0.15794	0.30633	0.56060	1.2581	3.7203	12.9118	1	1	1	4.645 -
-	H(20A)	0.36386	0.77346	0.50901	2.8985	9.3936	11.7236	1	1	1	4.645 -
-	H(20B)	0.53647	0.71195	0.50495	4.2735	8.6466	11.6301	1	1	1	4.645 -
-	H(20C)	0.41566	0.71429	0.45123	3.3111	8.6750	10.3928	1	1	1	4.645 -
-	H(21A)	-0.05129	0.39242	0.61792	-0.4086	4.7659	14.2320	1	1	1	4.645 -
-	H(21B)	-0.00003	0.50335	0.64787	-0.0002	6.1131	14.9218	1	1	1	4.645 -
-	H(21C)	-0.11779	0.50461	0.59334	-0.9383	6.1284	13.6659	1	1	1	4.645 -
-	H(22A)	0.50669	0.30690	0.47822	4.0363	3.7273	11.0144	1	1	1	4.645 -
-	H(22B)	0.44468	0.26048	0.53800	3.5423	3.1635	12.3913	1	1	1	4.645 -
-	H(22C)	0.32988	0.25094	0.48294	2.6278	3.0476	11.1231	1	1	1	4.645 -

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	Al	Cl	N	O
1	1	0.475	0.498	0.392	417.34	1	4	22	27	1	2	2	-
				Unit Cell Weight =	1669.34			88	108	4	8	8	0
				Calculated Analysis (Percent) =				63.3	6.5	6.5	17.0	6.7	0.0

Moiety_Formula = C22 H27 Al Cl2 N2

Sum_Formula = C22 H27 Al Cl2 N2

Formula_Weight = 417.34 [Note: Based on SHELXL97 Atomic Weights]

Formula_Z = 4

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

Calculated Density = 1.2440(1) g cm-3 [= Mg m-3]

F(000) = 880.0 [881.65]

mu(MoKa) = 3.40 cm-1 = 0.340 mm-1

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

Resonant Scattering = 0.79 Percent - (Girard,E. et al. (2003). Acta Cryst. D59, 1914-1922)

Predicted Volume = 2228.4[2197.1] Ang**3, 298[150]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	Cl1	0.03547						0.03547				
2	Cl2	0.03430						0.03430				
3	Al	0.02254						0.02254				
4	N1	0.02171						0.02171				
5	N2	0.02001						0.02001				
6	C1	0.02257						0.02257				
7	C2	0.01817						0.01817				
8	C3	0.02207						0.02207				
9	C4	0.02055						0.02055				
10	C5	0.02618						0.02618				
11	C6	0.02299						0.02299				
12	C7	0.02934						0.02934				
13	C8	0.04510						0.04510				
14	C9	0.02117						0.02117				
15	C10	0.01783						0.01783				
16	C11	0.02895						0.02895				
17	C12	0.04158						0.04158				
18	C13	0.05834						0.05834				
19	C14	0.02252						0.02252				
20	C15	0.03162						0.03162				
21	C16	0.04094						0.04094				
22	C17	0.05000						0.05000				
23	C18	0.04642						0.04642				
24	C19	0.02068						0.02068				
25	C20	0.04834						0.04834				
26	C21	0.04667						0.04667				
27	C22	0.03957						0.03957				
28	H1A	0.03385						0.03385				
29	H1B	0.03385						0.03385				
30	H1C	0.03385						0.03385				
31	H3A	0.02648						0.02648				
32	H4A	0.02466						0.02466				
33	H6A	0.02759						0.02759				
34	H8A	0.05412						0.05412				
35	H11A	0.04343						0.04343				
36	H11B	0.04343						0.04343				
37	H11C	0.04343						0.04343				
38	H12A	0.06237						0.06237				
39	H12B	0.06237						0.06237				
40	H12C	0.06237						0.06237				
41	H13A	0.08751						0.08751				

42	H13B	0.08751	0.08751
43	H13C	0.08751	0.08751
44	H15A	0.03794	0.03794
45	H17A	0.06000	0.06000
46	H20A	0.07251	0.07251
47	H20B	0.07251	0.07251
48	H20C	0.07251	0.07251
49	H21A	0.07000	0.07000
50	H21B	0.07000	0.07000
51	H21C	0.07000	0.07000
52	H22A	0.05935	0.05935
53	H22B	0.05935	0.05935
54	H22C	0.05935	0.05935

==========

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	Al	Cl	N	O
Average	0.0317	0.0328	0.0562	0.0225	0.0349	0.0209	0.0000
Minimum	0.0178	0.0178	0.0247	0.0225	0.0343	0.0200	0.0000
Maximum	0.0583	0.0583	0.0875	0.0225	0.0355	0.0217	0.0000
Ratio	3.2720	3.2720	3.5487	1.0000	1.0341	1.0850	0.0000
Number	27	22	27	1	2	2	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
-	Cl(1)	- Al	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	2.175	2.175	1	41			
-	Cl(2)	- Al	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	2.143	2.143	1	41			
-	Al	- Cl(1)	Cl(2)	C(1)	C(2)	-------	-------	-------	-------	6	104	114	109.4	1.980	2.175	4	40			
-	N(1)	- C(2)	C(3)	C(10)	-------	-------	-------	-------	-------	3	111	128	120.0	1.310	1.456	3	39	sp2		
-	N(2)	- C(2)	C(4)	C(19)	-------	-------	-------	-------	-------	3	109	127	119.9	1.350	1.444	3	38			
-	C(1)	- Al	H(1A)	H(1B)	H(1C)	-------	-------	-------	-------	6	109	109	109.5	0.960	1.980	4	33	sp3		
-	C(2)	- Al	N(1)	N(2)	-------	-------	-------	-------	-------	3	106	127	119.9	1.310	2.072	3	34	sp2		
-	C(3)	- N(1)	C(4)	H(3A)	-------	-------	-------	-------	-------	3	106	127	120.0	0.960	1.400	3	31	sp2		
-	C(4)	- N(2)	C(3)	H(4A)	-------	-------	-------	-------	-------	3	107	127	120.0	0.960	1.386	3	29	sp2		
-	C(5)	- C(6)	C(10)	C(11)	-------	-------	-------	-------	-------	3	119	121	120.0	1.377	1.490	3	27	sp2		
-	C(6)	- C(5)	C(7)	H(6A)	-------	-------	-------	-------	-------	3	120	120	120.0	0.960	1.398	3	23	sp2		
-	C(7)	- C(6)	C(8)	C(12)	-------	-------	-------	-------	-------	3	113	126	120.0	1.335	1.522	3	17	sp2		
-	C(8)	- C(7)	C(9)	H(8A)	-------	-------	-------	-------	-------	3	119	121	120.0	0.960	1.449	3	23	sp2		
-	C(9)	- C(8)	C(10)	C(13)	-------	-------	-------	-------	-------	3	116	122	119.9	1.401	1.469	3	27	sp2		
-	C(10)	- N(1)	C(5)	C(9)	-------	-------	-------	-------	-------	3	117	123	120.0	1.377	1.456	3	32	sp2		
-	C(11)	- C(5)	H(11A)	H(11B)	H(11C)	-------	-------	-------	-------	6	109	109	109.5	0.960	1.490	4	22	sp3		
-	C(12)	- C(7)	H(12A)	H(12B)	H(12C)	-------	-------	-------	-------	6	109	109	109.5	0.960	1.522	4	13	sp3		
-	C(13)	- C(9)	H(13A)	H(13B)	H(13C)	-------	-------	-------	-------	6	109	109	109.5	0.960	1.469	4	22	sp3		
-	C(14)	- C(15)	C(19)	C(20)	-------	-------	-------	-------	-------	3	112	129	120.0	1.398	1.588	3	25	sp2		
-	C(15)	- C(14)	C(16)	H(15A)	-------	-------	-------	-------	-------	3	118	123	120.0	0.960	1.527	3	20	sp2		
-	C(16)	- C(15)	C(17)	C(21)	-------	-------	-------	-------	-------	3	117	122	120.0	1.393	1.543	3	15	sp2		
-	C(17)	- C(16)	C(18)	H(17A)	-------	-------	-------	-------	-------	3	111	125	120.0	0.960	1.393	3	20	sp2		
-	C(18)	- C(17)	C(19)	C(22)	-------	-------	-------	-------	-------	3	107	128	120.0	1.373	1.405	3	25	sp2		
-	C(19)	- N(2)	C(14)	C(18)	-------	-------	-------	-------	-------	3	117	124	120.0	1.373	1.444	3	28	sp2		
-	C(20)	- C(14)	H(20A)	H(20B)	H(20C)	-------	-------	-------	-------	6	109	109	109.5	0.960	1.588	4	19	sp3		
-	C(21)	- C(16)	H(21A)	H(21B)	H(21C)	-------	-------	-------	-------	6	109	109	109.5	0.960	1.543	4	11	sp3		
-	C(22)	- C(18)	H(22A)	H(22B)	H(22C)	-------	-------	-------	-------	6	109	109	109.5	0.960	1.405	4	19	sp3		
-	H(1A)	- C(1)	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.960	0.960	1	9			
-	H(1B)	- C(1)	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.960	0.960	1	9			
-	H(1C)	- C(1)	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.960	0.960	1	9			
-	H(3A)	- C(3)	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.960	0.960	1	8			
-	H(4A)	- C(4)	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.960	0.960	1	7			
-	H(6A)	- C(6)	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.960	0.960	1	6			

-	H(8A) - C(8)	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.960	0.960	1	6		
-	H(11A) - C(11)	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.960	0.960	1	5		
-	H(11B) - C(11)	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.960	0.960	1	5		
-	H(11C) - C(11)	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.960	0.960	1	5		
-	H(12A) - C(12)	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.960	0.960	1	2		
-	H(12B) - C(12)	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.960	0.960	1	2		
-	H(12C) - C(12)	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.960	0.960	1	2		
-	H(13A) - C(13)	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.960	0.960	1	5		
-	H(13B) - C(13)	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.960	0.960	1	5		
-	H(13C) - C(13)	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.960	0.960	1	5		
-	H(15A) - C(15)	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.960	0.960	1	4		
-	H(17A) - C(17)	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.960	0.960	1	4		
-	H(20A) - C(20)	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.960	0.960	1	3		
-	H(20B) - C(20)	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.960	0.960	1	3		
-	H(20C) - C(20)	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.960	0.960	1	3		
-	H(21A) - C(21)	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.960	0.960	1	1		
-	H(21B) - C(21)	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.960	0.960	1	1		
-	H(21C) - C(21)	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.960	0.960	1	1		
-	H(22A) - C(22)	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.960	0.960	1	3		
-	H(22B) - C(22)	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.960	0.960	1	3		
-	H(22C) - C(22)	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.960	0.960	1	3		

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

N: ADDSYM finds additional (pseudo)symmetry in the structure (please check!)
N: No S.U.'s (esd) on observed/calculated parameters.

N: Number of Isotropic Non-H Atoms 27
N: Number of moved primary input atoms: 54
N: Number of Ignored Lines on INPUT   4
          of which blank in column 1   4

:: Input Xtal Data from File i10466.eld - Data Type SPF

:: NORMAL END of PLATON :   11 Pages on:
:: i10466.lis (ASCII, 132 Characters Wide)
:: i10466.lps (PostScript Version of .lis)
:: i10466.pdf (PDF   Version of .lis)

PLATON(V-311206)-Run for: i10466 in P2(1)2(1)2(1) New: Pnma TIME: Oct 14 11:18:27 2008

Crystal Data

Input Cell (Lattice Type: P) - Temp = 150K				Reduced Cell (Acta Cryst.(1976),A32,297-298)				
a = 23.0321(9)	Angstrom	alpha =	90 Degree	a = 7.966	alpha =	90.00	V =	2228.3
b = 12.1449(5)		beta =	90	b = 12.145	beta =	90.00		
c = 7.9660(3)		gamma =	90	c = 23.032	gamma =	90.00		
V = 2228.27(15)	Cubic-Angstrom	d(100) =	23.0321 Angstrom		Niggli Values			
		d(010) =	12.1449		63.457	147.499	530.478	
Lambda(MoKa) = 0.71073	Angstrom	d(001) =	7.9660		0.000	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)

$$(XO) = \begin{pmatrix} 23.03210 & 0 & 0 \\ 0 & 12.14490 & 0 \\ 0 & 0 & 7.96600 \end{pmatrix} (X), \quad (X) = \begin{pmatrix} 0.04342 & 0 & 0 \\ 0 & 0.08234 & 0 \\ 0 & 0 & 0.12553 \end{pmatrix} (XO)$$

$$(YO) = \quad (Y), \quad (Y) = \quad (YO)$$

$$(ZO) \quad (Z) \quad (Z) \quad (ZO)$$

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 Pnma No: 62, Laue: mmm [Hall: -P 2ac 2n]

Lattice Type oP, Centric, Orthorhombic, Order 8(4) [Schoenflies: D2h^16]

Nr	***** Symmetry Operation(s) *****		
1	X ,	Y ,	Z
2	1/2 - X ,	- Y ,	1/2 + Z
3	1/2 + X ,	1/2 - Y ,	1/2 - Z
4	- X ,	1/2 + Y ,	- Z
5	- X ,	- Y ,	- Z
6	1/2 + X ,	Y ,	1/2 - Z
7	1/2 - X ,	1/2 + Y ,	1/2 + Z
8	X ,	1/2 - 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	Al	Cl	N	O
Cov.Rad(Ang):	0.68	0.35	1.35	0.99	0.68	0.68
Atom Volume :	13.87	5.08	39.60	25.80	11.80	11.39
Atom Number :	6	1	13	17	7	8
Atom Weight :	12.010	1.008	26.98	35.45	14.01	16.00
Scat.Fact.f0:	5.999	1.000	12.994	17.001	6.995	7.999
Scat.Fact.f':	0.003	0.000	0.064	0.148	0.006	0.011
Scat.Fact.f":	0.002	0.000	0.051	0.159	0.003	0.006
Mu/Rho(MoKa):	0.58	0.37	5.11	11.52	0.84	1.22
Elem. Type :	--	--	--	HL	--	--

```
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
```

Flags	Label	Fractional Coordinates (x,y,z)			Orthogonal Coordinates (XO,YO,ZO)			Site	SSN	*SSOF =	S.O.F	Move	Type
-	Cl(1)	0.12405	0.39507	0.17757	2.8570	4.7980	1.4145		1	1	1	4.555	D/A
-	Al	0.09786	1/4	0.31467	2.2539	3.0362	2.5067	.m.	2	1/2	1	4.555	Met
-	N(1)	0.13012	1/4	0.68552	2.9969	3.0362	5.4609	.m.	2	1/2	1	4.555	D/A
-	N(2)	0.20686	1/4	0.53700	4.7644	3.0362	4.2777	.m.	2	1/2	1	4.555	D/A
-	C(1)	0.01335	1/4	0.35814	0.3075	3.0362	2.8529	.m.	2	1/2	1	4.555	-
-	C(2)	0.14832	1/4	0.52986	3.4161	3.0362	4.2209	.m.	2	1/2	1	4.555	-
-	C(3)	0.17691	1/4	0.79763	4.0746	3.0362	6.3539	.m.	2	1/2	1	4.555	-
-	C(4)	0.22462	1/4	0.70304	5.1735	3.0362	5.6004	.m.	2	1/2	1	4.555	-
-	C(5)	0.04356	0.14968	0.77645	1.0033	1.8179	6.1852		1	1	1	4.555	-
-	C(6)	-0.01356	0.15214	0.84145	-0.3124	1.8477	6.7030		1	1	1	4.555	-
-	C(7)	-0.04031	1/4	0.87590	-0.9284	3.0362	6.9774	.m.	2	1/2	1	4.555	-
-	C(10)	0.07033	1/4	0.74476	1.6198	3.0362	5.9328	.m.	2	1/2	1	4.555	-
-	C(11)	0.07243	0.04381	0.73849	1.6682	0.5321	5.8829		1	1	1	4.555	-
-	C(12)	-0.10052	1/4	0.95140	-2.3152	3.0362	7.5789	.m.	2	1/2	1	4.555	-
-	C(14)	0.26526	0.14881	0.33522	6.1094	1.8073	2.6703		1	1	1	4.555	-
-	C(15)	0.30251	0.14490	0.19965	6.9674	1.7598	1.5904		1	1	1	4.555	-
-	C(16)	0.32134	1/4	0.12976	7.4011	3.0362	1.0337	.m.	2	1/2	1	4.555	-
-	C(19)	0.24650	1/4	0.39657	5.6774	3.0362	3.1591	.m.	2	1/2	1	4.555	-
-	C(20)	0.24767	0.04253	0.41488	5.7044	0.5165	3.3049		1	1	1	4.555	-

-	C(21)	0.36132	0.28184	-0.02523	8.3220	3.4229	-0.2010		1	1	1	4.555	-
-	H(1A)	0.00310	0.18559	0.42109	0.0713	2.2540	3.3544		1	1	1	4.555	-
-	H(1C)	-0.00712	1/4	0.25332	-0.1640	3.0362	2.0179	.m.	2	1/2	1	4.555	-
-	H(3A)	0.17510	1/4	0.91764	4.0329	3.0362	7.3099	.m.	2	1/2	1	4.555	-
-	H(4A)	0.26376	1/4	0.74261	6.0749	3.0362	5.9156	.m.	2	1/2	1	4.555	-
-	H(6A)	-0.03375	0.08431	0.86161	-0.7774	1.0239	6.8635		1	1	1	4.555	-
-	H(11A)	0.11069	0.05757	0.69571	2.5494	0.6992	5.5420		1	1	1	4.555	-
-	H(11B)	0.07509	0.00065	0.83902	1.7295	0.0078	6.6836		1	1	1	4.555	-
-	H(11C)	0.05023	0.00451	0.65611	1.1569	0.0547	5.2266		1	1	1	4.555	-
-	H(12A)	-0.11741	0.30549	0.97261	-2.7042	3.7101	7.7478		1	1	1	4.555	-
-	H(12B)	-0.12461	0.19449	0.87433	-2.8700	2.3621	6.9649		1	1	1	4.555	-
-	H(12C)	-0.09753	0.19446	1.05488	-2.2463	2.3617	8.4032		1	1	1	4.555	-
-	H(15A)	0.31546	0.07645	0.15406	7.2656	0.9285	1.2273		1	1	1	4.555	-
-	H(20A)	0.25891	-0.02316	0.36286	5.9632	-0.2813	2.8905		1	1	1	4.555	-
-	H(20B)	0.24148	0.04747	0.52058	5.5619	0.5766	4.1469		1	1	1	4.555	-
-	H(20C)	0.20113	0.03601	0.41466	4.6324	0.4373	3.3032		1	1	1	4.555	-
-	H(21A)	0.36782	0.35788	-0.05229	8.4717	4.3464	-0.4165		1	1	1	4.555	-
-	H(21B)	0.39777	1/4	-0.00103	9.1615	3.0362	-0.0082	.m.	2	1/2	1	4.555	-
-	H(21C)	0.34324	1/4	-0.11879	7.9055	3.0362	-0.9463	.m.	2	1/2	1	4.555	-
-	H(22B)	0.28790	0.01018	0.44368	6.6309	0.1236	3.5344		1	1	1	5.555	-
-	H(22C)	0.23284	0.00064	0.32888	5.3628	0.0078	2.6199		1	1	1	5.555	-
-	Cl(1)a	0.12405	0.10493	0.17757	2.8570	1.2744	1.4145		1	1	1	5.555	D/A
-	C(5)a	0.04356	0.35032	0.77645	1.0033	4.2545	6.1852		1	1	1	5.555	-
-	C(6)a	-0.01356	0.34786	0.84145	-0.3124	4.2247	6.7030		1	1	1	5.555	-
-	C(11)a	0.07243	0.45619	0.73849	1.6682	5.5404	5.8829		1	1	1	5.555	-
-	C(14)a	0.26526	0.35119	0.33522	6.1094	4.2652	2.6703		1	1	1	5.555	-
-	C(15)a	0.30251	0.35510	0.19965	6.9674	4.3127	1.5904		1	1	1	5.555	-
-	C(20)a	0.24767	0.45747	0.41488	5.7044	5.5559	3.3049		1	1	1	5.555	-
-	C(21)a	0.36132	0.21816	-0.02523	8.3220	2.6495	-0.2010		1	1	1	5.555	-
-	H(1A)a	0.00310	0.31441	0.42109	0.0713	3.8185	3.3544		1	1	1	5.555	-
-	H(6A)a	-0.03375	0.41569	0.86161	-0.7774	5.0485	6.8635		1	1	1	5.555	-
-	H(11A)a	0.11069	0.44243	0.69571	2.5494	5.3733	5.5420		1	1	1	5.555	-
-	H(11B)a	0.07509	0.49935	0.83902	1.7295	6.0646	6.6836		1	1	1	5.555	-
-	H(11C)a	0.05023	0.49549	0.65611	1.1569	6.0177	5.2266		1	1	1	5.555	-
-	H(12A)a	-0.11741	0.19451	0.97261	-2.7042	2.3623	7.7478		1	1	1	5.555	-
-	H(12B)a	-0.12461	0.30551	0.87433	-2.8700	3.7104	6.9649		1	1	1	5.555	-
-	H(12C)a	-0.09753	0.30554	1.05488	-2.2463	3.7108	8.4032		1	1	1	5.555	-
-	H(15A)a	0.31546	0.42355	0.15406	7.2656	5.1440	1.2273		1	1	1	5.555	-
-	H(20A)a	0.25891	0.52316	0.36286	5.9632	6.3537	2.8905		1	1	1	5.555	-
-	H(20B)a	0.24148	0.45253	0.52058	5.5619	5.4959	4.1469		1	1	1	5.555	-
-	H(20C)a	0.20113	0.46399	0.41466	4.6324	5.6351	3.3032		1	1	1	5.555	-
-	H(21A)a	0.36782	0.14212	-0.05229	8.4717	1.7260	-0.4165		1	1	1	5.555	-
-	H(22B)a	0.28790	0.48982	0.44368	6.6309	5.9488	3.5344		1	1	1	4.555	-
-	H(22C)a	0.23284	0.49936	0.32888	5.3628	6.0647	2.6199		1	1	1	4.555	-

Predicted Volume = 2446.4[2412.0] Ang**3, 298[150]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	Cl1	0.03547						0.03547				
2	Al	0.02254						0.02254				
3	N1	0.02171						0.02171				
4	N2	0.02001						0.02001				
5	C1	0.02257						0.02257				
6	C2	0.01817						0.01817				
7	C3	0.02207						0.02207				
8	C4	0.02055						0.02055				
9	C5	0.02618						0.02618				
10	C6	0.02299						0.02299				
11	C7	0.02934						0.02934				
12	C10	0.01783						0.01783				
13	C11	0.02895						0.02895				
14	C12	0.04158						0.04158				
15	C14	0.02252						0.02252				
16	C15	0.03162						0.03162				
17	C16	0.04094						0.04094				
18	C19	0.02068						0.02068				
19	C20	0.04834						0.04834				
20	C21	0.04667						0.04667				

==========

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	Al	Cl	N	O
Average	0.0280	0.0288	0.0000	0.0225	0.0355	0.0209	0.0000

Minimum	0.0178	0.0178	0.0000	0.0225	0.0355	0.0200	0.0000
Maximum	0.0483	0.0483	0.0000	0.0225	0.0355	0.0217	0.0000
Ratio	2.7112	2.7112	0.0000	1.0000	1.0000	1.0850	0.0000
Number	20	16	0	1	1	2	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
-	Cl(1)	- Al	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	2.159	2.159	1	44			
-	Al	- Cl(1)	C(1)	C(2)	Cl(1)a	-------	-------	-------	-------	6	105	114	109.4	1.977	2.159	4	43			
-	N(1)	- C(2)	C(3)	C(10)	-------	-------	-------	-------	-------	3	111	128	120.0	1.309	1.456	3	42	sp2		
-	N(2)	- C(2)	C(4)	C(19)	-------	-------	-------	-------	-------	3	110	127	120.0	1.349	1.444	3	41			
-	C(1)	- Al	H(1A)	H(1C)	H(1A)a	-------	-------	-------	-------	6	109	110	109.5	0.959	1.977	4	36	sp3		
-	C(2)	- Al	N(1)	N(2)	-------	-------	-------	-------	-------	3	106	127	120.0	1.309	2.071	3	37	sp2		
-	C(3)	- N(1)	C(4)	H(3A)	-------	-------	-------	-------	-------	3	106	127	120.0	0.957	1.400	3	34	sp2		
-	C(4)	- N(2)	C(3)	H(4A)	-------	-------	-------	-------	-------	3	107	126	120.0	0.955	1.384	3	32	sp2		
-	C(5)	- C(6)	C(10)	C(11)	-------	-------	-------	-------	-------	3	117	122	120.0	1.389	1.479	3	30	sp2		
-	C(6)	- C(5)	C(7)	H(6A)	-------	-------	-------	-------	-------	3	120	121	120.0	0.960	1.414	3	26	sp2		
-	C(7)	- C(6)	C(12)	C(6)a	-------	-------	-------	-------	-------	3	120	121	120.0	1.366	1.512	3	20	sp2		
-	C(10)	- N(1)	C(5)	C(5)a	-------	-------	-------	-------	-------	3	119	123	120.0	1.389	1.456	3	35	sp2		
-	C(11)	- C(5)	H(11A)	H(11B)	H(11C)	-------	-------	-------	-------	6	109	110	109.5	0.959	1.479	4	25	sp3		
-	C(12)	- C(7)	H(12A)	H(12B)	H(12C)	H(12A)a	H(12B)a	H(12C)a	-------	21	48	151	98.7	0.796	1.512	7	16			?
-	C(14)	- C(15)	C(19)	C(20)	-------	-------	-------	-------	-------	3	118	122	120.0	1.380	1.494	3	28	sp2		
-	C(15)	- C(14)	C(16)	H(15A)	-------	-------	-------	-------	-------	3	117	122	120.0	0.955	1.459	3	23	sp2		
-	C(16)	- C(15)	C(21)	C(15)a	C(21)a	-------	-------	-------	-------	6	28	133	104.3	1.459	1.588	4	18			A
-	C(19)	- N(2)	C(14)	C(14)a	-------	-------	-------	-------	-------	3	118	124	120.0	1.391	1.444	3	31	sp2		
-	C(20)	- C(14)	H(20A)	H(20B)	H(20C)	H(22B)	H(22C)	-------	-------	15	46	150	100.4	0.856	1.494	6	22			?
-	C(21)	- C(16)	H(21A)	H(21B)	H(21C)	C(21)a	-------	-------	-------	10	66	164	102.9	0.773	1.588	5	14			A
-	H(1A)	- C(1)	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.959	0.959	1	13			
-	H(1C)	- C(1)	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.959	0.959	1	13			
-	H(3A)	- C(3)	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.957	0.957	1	12			
-	H(4A)	- C(4)	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.955	0.955	1	11			
-	H(6A)	- C(6)	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.960	0.960	1	10			
-	H(11A)	- C(11)	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.960	0.960	1	9			
-	H(11B)	- C(11)	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.959	0.959	1	9			
-	H(11C)	- C(11)	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.959	0.959	1	9			
-	H(12A)	- C(12)	H(12B)a	H(12C)a	-------	-------	-------	-------	-------	3	84	157	108.3	0.796	0.800	3	2			VA
-	H(12B)	- C(12)	H(12A)a	-------	-------	-------	-------	-------	-------	1	48	48	47.9	0.800	1.067	2	1			VA
-	H(12C)	- C(12)	H(12A)a	-------	-------	-------	-------	-------	-------	1	48	48	47.9	0.799	1.067	2	1			VA
-	H(15A)	- C(15)	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.955	0.955	1	8			
-	H(20A)	- C(20)	H(22B)	H(22C)	-------	-------	-------	-------	-------	3	64	129	86.3	0.719	1.012	3	7			VA

-	H(20B) - C(20)	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.856	0.856	1	5				
-	H(20C) - C(20)	H(22C)	-------	-------	-------	-------	-------	-------	-------	1	50	50	50.3	1.075	1.089	2	6				VA
-	H(21A) - C(21)	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.960	0.960	1	3				
-	H(21B) - C(21)	C(21)a	-------	-------	-------	-------	-------	-------	-------	1	48	48	48.4	0.944	0.944	2	4				VA
-	H(21C) - C(21)	C(21)a	-------	-------	-------	-------	-------	-------	-------	1	49	49	48.7	0.937	0.937	2	4				VA
-	H(22B) - C(20)	H(20A)	-------	-------	-------	-------	-------	-------	-------	1	54	54	54.5	1.012	1.032	2	6				VA
-	H(22C) - C(20)	H(20A)	H(20C)	-------	-------	-------	-------	-------	-------	3	64	119	83.8	0.719	1.089	3	7				VA
-	Cl(1)a - Al	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	2.159	2.159	1	44				
-	C(5)a - C(10)	C(6)a	C(11)a	-------	-------	-------	-------	-------	-------	3	117	122	120.0	1.389	1.479	3	30	sp2			
-	C(6)a - C(7)	C(5)a	H(6A)a	-------	-------	-------	-------	-------	-------	3	120	121	120.0	0.960	1.414	3	26	sp2			
-	C(11)a - C(5)a	H(11A)a	H(11B)a	H(11C)a	-------	-------	-------	-------	-------	6	109	110	109.5	0.959	1.479	4	25	sp3			
-	C(14)a - C(19)	C(15)a	C(20)a	-------	-------	-------	-------	-------	-------	3	118	122	120.0	1.380	1.494	3	28	sp2			
-	C(15)a - C(16)	C(14)a	H(15A)a	-------	-------	-------	-------	-------	-------	3	117	122	120.0	0.955	1.459	3	23	sp2			
-	C(20)a - C(14)a	H(20A)a	H(20B)a	H(20C)a	H(22B)a	H(22C)a	-------	-------	-------	15	46	150	100.4	0.856	1.494	6	22				?
-	C(21)a - C(16)	C(21)	H(21B)	H(21C)	H(21A)a	-------	-------	-------	-------	10	66	164	102.9	0.773	1.588	5	14				?
-	H(1A)a - C(1)	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.959	0.959	1	13				
-	H(6A)a - C(6)a	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.960	0.960	1	10				
-	H(11A)a- C(11)a	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.960	0.960	1	9				
-	H(11B)a- C(11)a	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.959	0.959	1	9				
-	H(11C)a- C(11)a	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.959	0.959	1	9				
-	H(12A)a- C(12)	H(12B)	H(12C)	-------	-------	-------	-------	-------	-------	3	84	157	108.3	0.796	0.800	3	2				V
-	H(12B)a- C(12)	H(12A)	-------	-------	-------	-------	-------	-------	-------	1	48	48	47.9	0.800	1.067	2	1				V
-	H(12C)a- C(12)	H(12A)	-------	-------	-------	-------	-------	-------	-------	1	48	48	47.9	0.799	1.067	2	1				V
-	H(15A)a- C(15)a	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.955	0.955	1	8				
-	H(20A)a- C(20)a	H(22B)a	H(22C)a	-------	-------	-------	-------	-------	-------	3	64	129	86.3	0.719	1.012	3	7				V
-	H(20B)a- C(20)a	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.856	0.856	1	5				
-	H(20C)a- C(20)a	H(22C)a	-------	-------	-------	-------	-------	-------	-------	1	50	50	50.3	1.075	1.089	2	6				V
-	H(21A)a- C(21)a	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	0.960	0.960	1	3				
-	H(22B)a- C(20)a	H(20A)a	-------	-------	-------	-------	-------	-------	-------	1	54	54	54.5	1.012	1.032	2	6				V
-	H(22C)a- C(20)a	H(20A)a	H(20C)a	-------	-------	-------	-------	-------	-------	3	64	119	83.8	0.719	1.089	3	7				V

Asymmetric Residue Unit (= ARU) Code List

ARU-CODE	Symmetry-Code	sym	TX	TY	TZ	Ires	x(cen)	y(cen)	z(cen)
a =[8555.01]	= x,1/2-y,z	= [8	0	0	0	1]	0.147	1/4	0.462

Note: Symmetry Operations Refer to the Coordinates listed in the Fractional Coordinate Table given above

X(J) = X(sym) + TX , Y(J) = Y(sym) + TY , Z(J) = Z(sym) + TZ,

SYM - Number of the Symmetry Operator.
Ires - Residue Number.
TX, TY, TZ - Unit Cell Translations.

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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/

Page - Index

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

N: ADDSYM finds additional (pseudo)symmetry in the structure (please check!)
N: No S.U.'s (esd) on observed/calculated parameters.

N: Number of Isotropic Non-H Atoms 20
N: Number of moved primary input atoms: 40
N: Input Data following TRNS [e.g. (CELL/CESD)/SPGR/COORDS/UIJ)] have been
    transformed according to the specified Cell Transformation Matrix:
                      0.00000   0.00000 -1.00000
                      0.00000 -1.00000   0.00000
                     -1.00000   0.00000   0.00000
N: INPUT data (COORDINATES) have been transformed
     according to additive coordinate shift vector:
                   0.25010   0.25030   0.00100
N: Number of deleted ATOMS from input stream 14
W: Number of valency check faults for H & C 16
W: Number of unusual bond angle faults 11
W: Number of (Carbon) Atoms with no sp(x) assignment   4
N: Number of Ignored Lines on INPUT 29
          of which blank in column 1   0

:: Input Xtal Data from File i10466.eld - Data Type SPF

:: NORMAL END of PLATON :   22 Pages on:
:: i10466.lis (ASCII, 132 Characters Wide)
:: i10466.lps (PostScript Version of .lis)
:: i10466.pdf (PDF   Version of .lis)

:: SHELXL Style Output on :i10466.res