PLATON(V-311206)-Run for: klat85 - SHELXL TIME: Nov 29 22:17:51 2011

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Crystal Data

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

a =	14.371(6)	Angstrom	alpha =	90	Degree	a =	9.736	alpha =	103.77	V =	3332.0
b =	9.736(4)		beta =	109.716(18)		b =	14.371	beta =	90.00		
c =	25.297(8)		gamma =	90		c =	24.519	gamma =	90.00		
V =	3332(2)	Cubic-Angstrom	d(100) =	13.5285	Angstrom						
			d(010) =	9.7360							
Lambda(MoKa) =	0.71073	Angstrom	d(001) =	23.8140							

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

Niggli Values: 94.790 206.526 601.175 -83.882 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)

$$\begin{pmatrix} XO \\ YO \\ ZO \end{pmatrix} = \begin{pmatrix} 14.37100 & 0 & -8.53415 \\ 0 & 9.73600 & 0 \\ 0 & 0 & 23.81400 \end{pmatrix} \begin{pmatrix} X \\ Y \\ Z \end{pmatrix}, \quad \begin{pmatrix} X \\ Y \\ Z \end{pmatrix} = \begin{pmatrix} 0.06958 & 0 & 0.02494 \\ 0 & 0.10271 & 0 \\ 0 & 0 & 0.04199 \end{pmatrix} \begin{pmatrix} XO \\ YO \\ ZO \end{pmatrix}$$

Orthogonal Axes AO, BO and CO are defined as:
AO // A, CO // C*, BO // CO X AO

Space Group Symmetry

(See e.g. G. Burns & A.M. Glazer, Space Groups for Solid State Scientists, Academic Press, 1990 or Int. Tables A)

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

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

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

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

```
          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	Cl	Cr	N
Cov.Rad(Ang):	0.68	0.35	0.99	1.35	0.68
Atom Volume :	13.87	5.08	25.80	28.10	11.80
Atom Number :	6	1	17	24	7
Atom Weight :	12.010	1.008	35.45	52.00	14.01
Scat.Fact.f0:	5.999	1.000	17.001	23.994	6.995
Scat.Fact.f':	0.003	0.000	0.148	0.321	0.006
Scat.Fact.f":	0.002	0.000	0.159	0.624	0.003
Mu/Rho(MoKa):	0.58	0.37	11.52	29.88	0.84
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

Flags	Label	Fractional Coordinates (x,y,z)			Orthogonal Coordinates (XO,YO,ZO)			Site	SSN*SSOF =	S.O.F	Move	Type
-	Cr(51)	0.41407	0.61113	0.01828	5.7946	5.9500	0.4354	1	1	1	-	Met
-	Cl(51)	0.41201	0.42576	-0.04399	6.2964	4.1452	-1.0475	1	1	1	-	D/A
-	N(501)	0.42620	0.75226	0.07995	5.4427	7.3240	1.9038	1	1	1	-	D/A
-	N(502)	0.26521	0.64211	-0.01435	3.9338	6.2516	-0.3417	1	1	1	-	D/A
-	C(501)	0.59364	0.84128	0.12708	7.4468	8.1907	3.0262	1	1	1	-	-
-	C(502)	0.17192	0.55447	-0.10927	3.4031	5.3983	-2.6022	1	1	1	-	-
-	C(503)	0.17211	0.42473	-0.02688	2.7027	4.1351	-0.6400	1	1	1	-	-
-	C(504)	0.20343	0.53927	-0.05067	3.3560	5.2503	-1.2066	1	1	1	-	-
-	C(505)	0.52349	0.67476	0.17462	6.0329	6.5694	4.1584	1	1	1	-	-
-	C(506)	0.35427	0.83370	0.08258	4.3865	8.1169	1.9666	1	1	1	-	-
-	C(507)	0.51507	0.75736	0.12752	6.3137	7.3736	3.0368	1	1	1	-	-
-	C(508)	0.25824	0.84036	0.04309	3.3434	8.1817	1.0262	1	1	1	-	-
-	C(509)	0.21775	0.74693	0.00039	3.1259	7.2721	0.0093	1	1	1	-	-
-	C(510)	0.07120	0.35125	-0.11878	2.0369	3.4197	-2.8287	1	1	1	-	-
-	C(511)	0.10588	0.46209	-0.14224	2.7354	4.4989	-3.3873	1	1	1	-	-
-	C(512)	0.10828	0.33296	-0.06154	2.0814	3.2417	-1.4656	1	1	1	-	-
-	C(513)	0.43879	0.58027	0.17508	4.8117	5.6495	4.1693	1	1	1	-	-
-	C(514)	0.68002	0.84637	0.17487	8.2802	8.2403	4.1644	1	1	1	-	-
-	C(515)	0.60992	0.68018	0.22187	6.8718	6.6222	5.2835	1	1	1	-	-

-	C(516)	0.68574	0.77049	0.22194	7.9606	7.5015	5.2853	1	1	1	- -
-	C(517)	0.20833	0.67195	-0.13666	4.1602	6.5422	-3.2543	1	1	1	- -
-	C(518)	0.37168	0.93026	0.13256	4.2101	9.0570	3.1568	1	1	1	- -
-	C(519)	0.21199	0.40373	0.03631	2.7366	3.9307	0.8647	1	1	1	- -
-	C(520)	-0.00413	0.25180	-0.15805	1.2895	2.4515	-3.7638	1	1	1	- -
-	C(521)	0.58536	0.93133	0.07686	7.7563	9.0674	1.8303	1	1	1	- -
-	C(522)	0.56182	1.08345	0.08681	7.3331	10.5484	2.0673	1	1	1	- -
-	C(523)	0.10562	0.76478	-0.03003	1.7742	7.4459	-0.7152	1	1	1	- -
-	C(524)	0.27034	0.61983	-0.17243	5.3566	6.0346	-4.1062	1	1	1	- -
-	C(525)	0.12380	0.76230	-0.17413	3.2651	7.4218	-4.1468	1	1	1	- -
-	C(526)	0.41039	0.60195	0.22945	3.9395	5.8606	5.4642	1	1	1	- -
-	C(527)	0.84369	0.89953	0.27944	9.7398	8.7578	6.6547	1	1	1	- -
-	C(528)	0.68296	0.93073	0.06348	9.2731	9.0615	1.5116	1	1	1	- -
-	C(529)	0.77326	0.78565	0.27791	8.7408	7.6490	6.6182	1	1	1	- -
-	C(530)	0.04068	0.10688	-0.15495	1.9071	1.0406	-3.6901	1	1	1	- -
-	C(531)	0.47234	0.42800	0.17250	5.3158	4.1670	4.1079	1	1	1	- -
-	C(532)	-0.10155	0.24613	-0.14493	-0.2226	2.3963	-3.4514	1	1	1	- -
-	C(533)	0.82447	0.65296	0.29842	9.3018	6.3572	7.1065	1	1	1	- -
-	C(534)	0.23933	0.25502	0.05109	3.0034	2.4829	1.2167	1	1	1	- -
-	C(535)	0.14682	0.45957	0.06511	1.5542	4.4743	1.5506	1	1	1	- -
-	Cr(51)a	0.58592	0.38887	-0.01828	8.5764	3.7860	-0.4354	1	1	1	3.665 Met
-	Cl(51)a	0.58799	0.57424	0.04399	8.0746	5.5908	1.0475	1	1	1	3.665 D/A
-	N(501)a	0.57380	0.24774	-0.07995	8.9283	2.4120	-1.9038	1	1	1	3.665 D/A
-	N(502)a	0.73479	0.35789	0.01435	10.4372	3.4844	0.3417	1	1	1	3.665 D/A
-	C(501)a	0.40636	0.15872	-0.12708	6.9242	1.5453	-3.0262	1	1	1	3.665 -
-	C(502)a	0.82808	0.44553	0.10927	10.9679	4.3377	2.6022	1	1	1	3.665 -
-	C(503)a	0.82789	0.57527	0.02688	11.6683	5.6009	0.6400	1	1	1	3.665 -
-	C(504)a	0.79657	0.46073	0.05067	11.0150	4.4857	1.2066	1	1	1	3.665 -
-	C(505)a	0.47651	0.32524	-0.17462	8.3381	3.1666	-4.1584	1	1	1	3.665 -
-	C(506)a	0.64573	0.16630	-0.08258	9.9845	1.6191	-1.9666	1	1	1	3.665 -
-	C(507)a	0.48493	0.24264	-0.12752	8.0573	2.3624	-3.0368	1	1	1	3.665 -
-	C(508)a	0.74176	0.15964	-0.04309	11.0276	1.5543	-1.0262	1	1	1	3.665 -
-	C(509)a	0.78225	0.25307	-0.00039	11.2451	2.4639	-0.0093	1	1	1	3.665 -
-	C(510)a	0.92880	0.64875	0.11878	12.3341	6.3163	2.8287	1	1	1	3.665 -
-	C(511)a	0.89412	0.53791	0.14224	11.6356	5.2371	3.3873	1	1	1	3.665 -
-	C(512)a	0.89172	0.66704	0.06154	12.2896	6.4943	1.4656	1	1	1	3.665 -
-	C(513)a	0.56121	0.41973	-0.17508	9.5593	4.0865	-4.1693	1	1	1	3.665 -
-	C(514)a	0.31998	0.15363	-0.17487	6.0908	1.4957	-4.1644	1	1	1	3.665 -
-	C(515)a	0.39008	0.31982	-0.22187	7.4992	3.1138	-5.2835	1	1	1	3.665 -
-	C(516)a	0.31426	0.22951	-0.22194	6.4104	2.2345	-5.2853	1	1	1	3.665 -
-	C(517)a	0.79167	0.32805	0.13666	10.2108	3.1938	3.2543	1	1	1	3.665 -
-	C(518)a	0.62832	0.06974	-0.13256	10.1609	0.6790	-3.1568	1	1	1	3.665 -
-	C(519)a	0.78801	0.59627	-0.03631	11.6344	5.8053	-0.8647	1	1	1	3.665 -
-	C(520)a	1.00413	0.74820	0.15805	13.0816	7.2845	3.7638	1	1	1	3.665 -
-	C(521)a	0.41464	0.06867	-0.07686	6.6147	0.6686	-1.8303	1	1	1	3.665 -
-	C(522)a	0.43818	-0.08345	-0.08681	7.0379	-0.8124	-2.0673	1	1	1	3.665 -
-	C(523)a	0.89438	0.23522	0.03003	12.5968	2.2901	0.7152	1	1	1	3.665 -
-	C(524)a	0.72966	0.38017	0.17243	9.0144	3.7014	4.1062	1	1	1	3.665 -

-	C(525)a	0.87620	0.23770	0.17413	11.1059	2.3142	4.1468	1	1	1	3.665 -
-	C(526)a	0.58961	0.39805	-0.22945	10.4315	3.8754	-5.4642	1	1	1	3.665 -
-	C(527)a	0.15631	0.10047	-0.27944	4.6312	0.9782	-6.6547	1	1	1	3.665 -
-	C(528)a	0.31704	0.06927	-0.06348	5.0979	0.6745	-1.5116	1	1	1	3.665 -
-	C(529)a	0.22674	0.21435	-0.27791	5.6302	2.0870	-6.6182	1	1	1	3.665 -
-	C(530)a	0.95932	0.89312	0.15495	12.4639	8.6954	3.6901	1	1	1	3.665 -
-	C(531)a	0.52766	0.57200	-0.17250	9.0552	5.5690	-4.1079	1	1	1	3.665 -
-	C(532)a	1.10155	0.75387	0.14493	14.5936	7.3397	3.4514	1	1	1	3.665 -
-	C(533)a	0.17553	0.34704	-0.29842	5.0692	3.3788	-7.1065	1	1	1	3.665 -
-	C(534)a	0.76067	0.74498	-0.05109	11.3676	7.2531	-1.2167	1	1	1	3.665 -
-	C(535)a	0.85318	0.54043	-0.06511	12.8168	5.2617	-1.5506	1	1	1	3.665 -

(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	Cr51	0.03309						0.03309				
2	Cl51	0.06506						0.06506				
3	N501	0.03363						0.03363				
4	N502	0.03287						0.03287				
5	C501	0.03272						0.03272				
6	C502	0.03630						0.03630				
7	C503	0.03614						0.03614				
8	C504	0.03628						0.03628				
9	C505	0.03940						0.03940				
10	C506	0.03351						0.03351				
11	C507	0.03444						0.03444				
12	C508	0.04060						0.04060				
13	C509	0.03590						0.03590				
14	C510	0.04474						0.04474				
15	C511	0.04559						0.04559				
16	C512	0.04334						0.04334				
17	C513	0.04544						0.04544				
18	C514	0.04242						0.04242				
19	C515	0.04876						0.04876				
20	C516	0.04950						0.04950				
21	C517	0.04274						0.04274				
22	C518	0.05007						0.05007				
23	C519	0.04661						0.04661				
24	C520	0.05351						0.05351				
25	C521	0.04856						0.04856				
26	C522	0.06722						0.06722				
27	C523	0.05773						0.05773				
28	C524	0.07168						0.07168				
29	C525	0.06885						0.06885				
30	C526	0.06944						0.06944				
31	C527	0.06753						0.06753				
32	C528	0.07328						0.07328				
33	C529	0.06920						0.06920				
34	C530	0.07485						0.07485				
35	C531	0.07941						0.07941				
36	C532	0.07533						0.07533				
37	C533	0.08143						0.08143				
38	C534	0.10604						0.10604				
39	C535	0.11642						0.11642				

==========

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	Cl	Cr	N
Average	0.0546	0.0561	0.0000	0.0651	0.0331	0.0332
Minimum	0.0327	0.0327	0.0000	0.0651	0.0331	0.0329
Maximum	0.1164	0.1164	0.0000	0.0651	0.0331	0.0336
Ratio	3.5581	3.5581	0.0000	1.0000	1.0000	1.0231
Number	39	35	0	1	1	2

Analysis of Bond Distance and Angle Values - Identification of Chiral Center(s) and Their (R/S)-Configuration (Cahn-Ingold-Prelog)

The Following Tests are done. Faults are Marked Under Note
-- V : Valency Check Fault for H, C
-- S : Bond Too Short
-- A : Unusual Bond Angle Values (PLEASE CHECK)

*** PLEASE NOTE: R/S ASSIGNMENTS ARE TENTATIVE *** (CIP Special rules NOT Implemented)
*** See Angew.Chem.Intern. Ed. Eng.,(1966),5,385 & (1982),21,567 for Authoritative Details for Special Cases

Flag	Label - Connected to (May be Incomplete for Polymeric Structures)					=A.N.G.L.E.S= nra	min	max	Aver	=B.O.N.D.S= min	max	nrb	tnr	Hyb	RS	Note
-	Cr(51) - Cl(51)	N(501)	N(502)	Cl(51)a	------- ------- ------- ------- -------	6	81	172	117.6	2.039	2.389	4	31			
-	Cl(51) - Cr(51)	Cr(51)a	-------	-------	------- ------- ------- ------- -------	1	99	99	98.9	2.388	2.389	2	30			
-	N(501) - Cr(51)	C(506)	C(507)	-------	------- ------- ------- ------- -------	3	115	125	119.9	1.322	2.042	3	29	sp2		
-	N(502) - Cr(51)	C(504)	C(509)	-------	------- ------- ------- ------- -------	3	116	124	119.9	1.348	2.039	3	28			
-	C(501) - C(507)	C(514)	C(521)	-------	------- ------- ------- ------- -------	3	120	121	120.0	1.397	1.515	3	20	sp2		
-	C(502) - C(504)	C(511)	C(517)	-------	------- ------- ------- ------- -------	3	119	122	120.0	1.368	1.519	3	16	sp2		
-	C(503) - C(504)	C(512)	C(519)	-------	------- ------- ------- ------- -------	3	119	121	120.0	1.366	1.519	3	16	sp2		
-	C(504) - N(502)	C(502)	C(503)	-------	------- ------- ------- ------- -------	3	120	121	120.0	1.404	1.444	3	21	sp2		
-	C(505) - C(507)	C(513)	C(515)	-------	------- ------- ------- ------- -------	3	120	121	120.0	1.404	1.529	3	20	sp2		
-	C(506) - N(501)	C(508)	C(518)	-------	------- ------- ------- ------- -------	3	114	126	120.0	1.322	1.527	3	25	sp2		
-	C(507) - N(501)	C(501)	C(505)	-------	------- ------- ------- ------- -------	3	119	121	120.0	1.397	1.430	3	24	sp2		
-	C(508) - C(506)	C(509)	-------	-------	------- ------- ------- ------- -------	1	125	125	125.4	1.382	1.406	2	19			?
-	C(509) - N(502)	C(508)	C(523)	-------	------- ------- ------- ------- -------	3	114	127	120.0	1.348	1.543	3	22	sp2		
-	C(510) - C(511)	C(512)	C(520)	-------	------- ------- ------- ------- -------	3	119	122	120.0	1.375	1.540	3	6	sp2		
-	C(511) - C(502)	C(510)	-------	-------	------- ------- ------- ------- -------	1	121	121	121.4	1.368	1.402	2	11			?
-	C(512) - C(503)	C(510)	-------	-------	------- ------- ------- ------- -------	1	122	122	121.9	1.366	1.375	2	11			?
-	C(513) - C(505)	C(526)	C(531)	-------	------- ------- ------- ------- -------	3	108	112	109.8	1.529	1.575	3	13			??
-	C(514) - C(501)	C(516)	-------	-------	------- ------- ------- ------- -------	1	120	120	120.0	1.380	1.412	2	14			?
-	C(515) - C(505)	C(516)	-------	-------	------- ------- ------- ------- -------	1	119	119	119.3	1.400	1.404	2	14			?
-	C(516) - C(514)	C(515)	C(529)	-------	------- ------- ------- ------- -------	3	117	122	120.0	1.380	1.551	3	8	sp2		
-	C(517) - C(502)	C(524)	C(525)	-------	------- ------- ------- ------- -------	3	108	113	111.1	1.519	1.554	3	10			??
-	C(518) - C(506)	-------	-------	-------	------- ------- ------- ------- -------	0	0	0	0.0	1.527	1.527	1	18			?
-	C(519) - C(503)	C(534)	C(535)	-------	------- ------- ------- ------- -------	3	111	113	112.4	1.471	1.519	3	10			?
-	C(520) - C(510)	C(530)	C(532)	-------	------- ------- ------- ------- -------	3	110	112	111.0	1.540	1.545	3	3			??
-	C(521) - C(501)	C(522)	C(528)	-------	------- ------- ------- ------- -------	3	107	112	110.2	1.515	1.558	3	13			??
-	C(522) - C(521)	-------	-------	-------	------- ------- ------- ------- -------	0	0	0	0.0	1.558	1.558	1	7			?
-	C(523) - C(509)	-------	-------	-------	------- ------- ------- ------- -------	0	0	0	0.0	1.543	1.543	1	17			?
-	C(524) - C(517)	-------	-------	-------	------- ------- ------- ------- -------	0	0	0	0.0	1.554	1.554	1	5			?
-	C(525) - C(517)	-------	-------	-------	------- ------- ------- ------- -------	0	0	0	0.0	1.540	1.540	1	5			?
-	C(526) - C(513)	-------	-------	-------	------- ------- ------- ------- -------	0	0	0	0.0	1.575	1.575	1	7			?
-	C(527) - C(529)	-------	-------	-------	------- ------- ------- ------- -------	0	0	0	0.0	1.493	1.493	1	2			?
-	C(528) - C(521)	-------	-------	-------	------- ------- ------- ------- -------	0	0	0	0.0	1.550	1.550	1	7			?
-	C(529) - C(516)	C(527)	C(533)	-------	------- ------- ------- ------- -------	3	113	115	113.6	1.491	1.551	3	4			?
-	C(530) - C(520)	-------	-------	-------	------- ------- ------- ------- -------	0	0	0	0.0	1.542	1.542	1	1			?

-	C(531) - C(513)	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	1.567	1.567	1	7		?
-	C(532) - C(520)	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	1.545	1.545	1	1		?
-	C(533) - C(529)	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	1.491	1.491	1	2		?
-	C(534) - C(519)	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	1.514	1.514	1	5		?
-	C(535) - C(519)	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	1.471	1.471	1	5		?
-	Cr(51)a- Cl(51)	Cl(51)a	N(501)a	N(502)a	-------	-------	-------	-------	-------	6	81	172	117.6	2.039	2.389	4	31		
-	Cl(51)a- Cr(51)	Cr(51)a	-------	-------	-------	-------	-------	-------	-------	1	99	99	98.9	2.388	2.389	2	30		
-	N(501)a- Cr(51)a	C(506)a	C(507)a	-------	-------	-------	-------	-------	-------	3	115	125	119.9	1.322	2.042	3	29	sp2	
-	N(502)a- Cr(51)a	C(504)a	C(509)a	-------	-------	-------	-------	-------	-------	3	116	124	119.9	1.348	2.039	3	28		
-	C(501)a- C(507)a	C(514)a	C(521)a	-------	-------	-------	-------	-------	-------	3	120	121	120.0	1.397	1.515	3	20	sp2	
-	C(502)a- C(504)a	C(511)a	C(517)a	-------	-------	-------	-------	-------	-------	3	119	122	120.0	1.368	1.519	3	16	sp2	
-	C(503)a- C(504)a	C(512)a	C(519)a	-------	-------	-------	-------	-------	-------	3	119	121	120.0	1.366	1.519	3	16	sp2	
-	C(504)a- N(502)a	C(502)a	C(503)a	-------	-------	-------	-------	-------	-------	3	120	121	120.0	1.404	1.444	3	21	sp2	
-	C(505)a- C(507)a	C(513)a	C(515)a	-------	-------	-------	-------	-------	-------	3	120	121	120.0	1.404	1.529	3	20	sp2	
-	C(506)a- N(501)a	C(508)a	C(518)a	-------	-------	-------	-------	-------	-------	3	114	126	120.0	1.322	1.527	3	25	sp2	
-	C(507)a- N(501)a	C(501)a	C(505)a	-------	-------	-------	-------	-------	-------	3	119	121	120.0	1.397	1.430	3	24	sp2	
-	C(508)a- C(506)a	C(509)a	-------	-------	-------	-------	-------	-------	-------	1	125	125	125.4	1.382	1.406	2	19		?
-	C(509)a- N(502)a	C(508)a	C(523)a	-------	-------	-------	-------	-------	-------	3	114	127	120.0	1.348	1.543	3	22	sp2	
-	C(510)a- C(511)a	C(512)a	C(520)a	-------	-------	-------	-------	-------	-------	3	119	122	120.0	1.375	1.540	3	6	sp2	
-	C(511)a- C(502)a	C(510)a	-------	-------	-------	-------	-------	-------	-------	1	121	121	121.4	1.368	1.402	2	11		?
-	C(512)a- C(503)a	C(510)a	-------	-------	-------	-------	-------	-------	-------	1	122	122	121.9	1.366	1.375	2	11		?
-	C(513)a- C(505)a	C(526)a	C(531)a	-------	-------	-------	-------	-------	-------	3	108	112	109.8	1.529	1.575	3	13		?
-	C(514)a- C(501)a	C(516)a	-------	-------	-------	-------	-------	-------	-------	1	120	120	120.0	1.380	1.412	2	14		?
-	C(515)a- C(505)a	C(516)a	-------	-------	-------	-------	-------	-------	-------	1	119	119	119.3	1.400	1.404	2	14		?
-	C(516)a- C(514)a	C(515)a	C(529)a	-------	-------	-------	-------	-------	-------	3	117	122	120.0	1.380	1.551	3	8	sp2	
-	C(517)a- C(502)a	C(524)a	C(525)a	-------	-------	-------	-------	-------	-------	3	108	113	111.1	1.519	1.554	3	10		?
-	C(518)a- C(506)a	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	1.527	1.527	1	18		?
-	C(519)a- C(503)a	C(534)a	C(535)a	-------	-------	-------	-------	-------	-------	3	111	113	112.4	1.471	1.519	3	10		?
-	C(520)a- C(510)a	C(530)a	C(532)a	-------	-------	-------	-------	-------	-------	3	110	112	111.0	1.540	1.545	3	3		?
-	C(521)a- C(501)a	C(522)a	C(528)a	-------	-------	-------	-------	-------	-------	3	107	112	110.2	1.515	1.558	3	13		?
-	C(522)a- C(521)a	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	1.558	1.558	1	7		?
-	C(523)a- C(509)a	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	1.543	1.543	1	17		?
-	C(524)a- C(517)a	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	1.554	1.554	1	5		?
-	C(525)a- C(517)a	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	1.540	1.540	1	5		?
-	C(526)a- C(513)a	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	1.575	1.575	1	7		?
-	C(527)a- C(529)a	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	1.493	1.493	1	2		?
-	C(528)a- C(521)a	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	1.550	1.550	1	7		?
-	C(529)a- C(516)a	C(527)a	C(533)a	-------	-------	-------	-------	-------	-------	3	113	115	113.6	1.491	1.551	3	4		?
-	C(530)a- C(520)a	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	1.542	1.542	1	1		?
-	C(531)a- C(513)a	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	1.567	1.567	1	7		?
-	C(532)a- C(520)a	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	1.545	1.545	1	1		?
-	C(533)a- C(529)a	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	1.491	1.491	1	2		?
-	C(534)a- C(519)a	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	1.514	1.514	1	5		?
-	C(535)a- C(519)a	-------	-------	-------	-------	-------	-------	-------	-------	0	0	0	0.0	1.471	1.471	1	5		?

Asymmetric Residue Unit (= ARU) Code List

ARU-CODE	Symmetry-Code	sym	TX	TY	TZ	Ires	x(cen)	y(cen)	z(cen)
a =[3665.01]	= 1-x,1-y,-z	= [	3	1	1	0	1]	1/2	1/2	0

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.

Analysis of the IntraMolecular Geometry in Terms of Unique Molecule(s)/Ions, with Bond Criterium: d(i-j) < R(i) + R(j) + Tol

-- Tol = 0.40 Ang. for Normal Bonds + 0.70 for (Earth)alkali-NonMetal Contacts and adjusted by -.40 Ang. for Metal-Metal Distances
-- The Bond Distance and Angle su's have been Incremented to Include the Effect of the Unit-cell su.
(Rel.Error in Dist. 0.0004 Ang. , Abs. Angle Error 0.018 Deg.)
-- Bonds below with '>' or '<' Substituted for '-' have Distances that Deviate from Expected Values(Based on the hybridisations).

Bond Lengths (Angstrom). - (Bonds are ordered on the first label, left to right and top to bottom) - su in last digit in ().

Cr(51) -	Cl(51)	2.3892	Cr(51) -	N(501)	2.0416	Cr(51) -	N(502)	2.0390	Cr(51) -	Cl(51)a	2.3878
N(501) -	C(506)	1.3222	N(501) -	C(507)	1.4300	N(502) -	C(504)	1.4438	N(502) -	C(509)	1.3481
C(501) -	C(507)	1.3970	C(501) -	C(514)	1.4116	C(501) -	C(521)	1.5148	C(502) -	C(504)	1.4042
C(502) -	C(511)	1.3679	C(502) -	C(517)	1.5188	C(503) -	C(504)	1.4112	C(503) -	C(512)	1.3660
C(503) -	C(519)	1.5190	C(505) -	C(507)	1.4084	C(505) -	C(513)	1.5289	C(505) -	C(515)	1.4044
C(506) -	C(508)	1.4059	C(506) -	C(518)	1.5269	C(508) -	C(509)	1.3816	C(509) -	C(523)	1.5435
C(510) -	C(511)	1.4016	C(510) -	C(512)	1.3754	C(510) -	C(520)	1.5397	C(513) -	C(526)	1.5755
C(513) -	C(531)	1.5671	C(514) -	C(516)	1.3800	C(515) -	C(516)	1.3996	C(516) -	C(529)	1.5515
C(517) -	C(524)	1.5539	C(517) -	C(525)	1.5399	C(519) -	C(534)	1.5137	C(519) -	C(535)	1.4711
C(520) -	C(530)	1.5419	C(520) -	C(532)	1.5450	C(521) -	C(522)	1.5584	C(521) -	C(528)	1.5499
C(527) -	C(529)	1.4929	C(529) -	C(533)	1.4906						

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

Cl(51) -	Cr(51) -	N(501)	172.32	Cl(51) -	Cr(51) -	N(502)	93.83	Cl(51) -	Cr(51) -	Cl(51)a	81.08
N(501) -	Cr(51) -	N(502)	90.99	N(501) -	Cr(51) -	Cl(51)a	94.67	N(502) -	Cr(51) -	Cl(51)a	172.45
Cr(51) -	Cl(51) -	Cr(51)a	98.92	Cr(51) -	N(501) -	C(506)	125.13	Cr(51) -	N(501) -	C(507)	119.22
C(506) -	N(501) -	C(507)	115.35	Cr(51) -	N(502) -	C(504)	119.41	Cr(51) -	N(502) -	C(509)	124.03
C(504) -	N(502) -	C(509)	116.17	C(507) -	C(501) -	C(514)	119.56	C(507) -	C(501) -	C(521)	120.68
C(514) -	C(501) -	C(521)	119.71	C(504) -	C(502) -	C(511)	118.99	C(504) -	C(502) -	C(517)	121.53
C(511) -	C(502) -	C(517)	119.47	C(504) -	C(503) -	C(512)	119.00	C(504) -	C(503) -	C(519)	119.59
C(512) -	C(503) -	C(519)	121.39	N(502) -	C(504) -	C(502)	120.59	N(502) -	C(504) -	C(503)	119.52
C(502) -	C(504) -	C(503)	119.86	C(507) -	C(505) -	C(513)	120.56	C(507) -	C(505) -	C(515)	119.83
C(513) -	C(505) -	C(515)	119.61	N(501) -	C(506) -	C(508)	126.05	N(501) -	C(506) -	C(518)	119.90
C(508) -	C(506) -	C(518)	114.04	N(501) -	C(507) -	C(501)	120.55	N(501) -	C(507) -	C(505)	119.32
C(501) -	C(507) -	C(505)	120.11	C(506) -	C(508) -	C(509)	125.36	N(502) -	C(509) -	C(508)	126.56
N(502) -	C(509) -	C(523)	119.20	C(508) -	C(509) -	C(523)	114.16	C(511) -	C(510) -	C(512)	118.59
C(511) -	C(510) -	C(520)	118.95	C(512) -	C(510) -	C(520)	122.43	C(502) -	C(511) -	C(510)	121.38
C(503) -	C(512) -	C(510)	121.94	C(505) -	C(513) -	C(526)	111.55	C(505) -	C(513) -	C(531)	108.18
C(526) -	C(513) -	C(531)	109.70	C(501) -	C(514) -	C(516)	119.96	C(505) -	C(515) -	C(516)	119.30
C(514) -	C(516) -	C(515)	121.03	C(514) -	C(516) -	C(529)	122.04	C(515) -	C(516) -	C(529)	116.88
C(502) -	C(517) -	C(524)	111.91	C(502) -	C(517) -	C(525)	112.91	C(524) -	C(517) -	C(525)	108.44
C(503) -	C(519) -	C(534)	111.28	C(503) -	C(519) -	C(535)	113.22	C(534) -	C(519) -	C(535)	112.75
C(510) -	C(520) -	C(530)	110.60	C(510) -	C(520) -	C(532)	112.01	C(530) -	C(520) -	C(532)	110.46
C(501) -	C(521) -	C(522)	111.99	C(501) -	C(521) -	C(528)	111.11	C(522) -	C(521) -	C(528)	107.50
C(516) -	C(529) -	C(527)	115.35	C(516) -	C(529) -	C(533)	112.84	C(527) -	C(529) -	C(533)	112.57

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

N(502)	Cr(51)	N(501)	C(506)	-8.10	N(502)	Cr(51)	N(501) C(507)	165.38	Cl(51)aCr(51)	N(501)	C(506)	166.89
Cl(51)aCr(51)	N(501)	C(507)		-19.63	Cl(51)	Cr(51)	N(502) C(504)	13.70	Cl(51)	Cr(51)	N(502) C(509)	-173.72
N(501)	Cr(51)	N(502)	C(504)	-160.32	N(501)	Cr(51)	N(502) C(509)	12.26	Cr(51)aCl(51)	Cr(51)	N(502)	174.38
Cr(51)aCl(51)	Cr(51)	Cl(51)a		0.00	Cr(51)	Cl(51)	Cr(51)aCl(51)a	0.00	Cr(51)	Cl(51)	Cr(51)aN(501)a	-173.56
C(514)	C(501)	C(507)	N(501)	178.96	C(514)	C(501)	C(507) C(505)	-2.25	C(521)	C(501)	C(507) N(501)	1.61
C(521)	C(501)	C(507)	C(505)	-179.61	C(507)	C(501)	C(514) C(516)	-1.08	C(521)	C(501)	C(514) C(516)	176.31
C(507)	C(501)	C(521)	C(522)	100.36	C(507)	C(501)	C(521) C(528)	-139.42	C(514)	C(501)	C(521) C(522)	-77.00
C(514)	C(501)	C(521)	C(528)	43.23	C(511)	C(502)	C(504) N(502)	-173.78	C(511)	C(502)	C(504) C(503)	4.26
C(517)	C(502)	C(504)	N(502)	5.35	C(517)	C(502)	C(504) C(503)	-176.62	C(504)	C(502)	C(511) C(510)	-1.60
C(517)	C(502)	C(511)	C(510)	179.25	C(504)	C(502)	C(517) C(524)	115.55	C(504)	C(502)	C(517) C(525)	-121.75
C(511)	C(502)	C(517)	C(524)	-65.32	C(511)	C(502)	C(517) C(525)	57.38	C(512)	C(503)	C(504) N(502)	175.60
C(512)	C(503)	C(504)	C(502)	-2.46	C(519)	C(503)	C(504) N(502)	-6.10	C(519)	C(503)	C(504) C(502)	175.84
C(504)	C(503)	C(512)	C(510)	-2.13	C(519)	C(503)	C(512) C(510)	179.61	C(504)	C(503)	C(519) C(534)	-136.57
C(504)	C(503)	C(519)	C(535)	95.21	C(512)	C(503)	C(519) C(534)	41.69	C(512)	C(503)	C(519) C(535)	-86.53
C(502)	C(504)	N(502)	Cr(51)	-98.73	C(502)	C(504)	N(502) C(509)	88.12	C(503)	C(504)	N(502) Cr(51)	83.23
C(503)	C(504)	N(502)	C(509)	-89.92	C(513)	C(505)	C(507) N(501)	0.09	C(513)	C(505)	C(507) C(501)	-178.72
C(515)	C(505)	C(507)	N(501)	-179.20	C(515)	C(505)	C(507) C(501)	2.00	C(507)	C(505)	C(513) C(526)	-128.78
C(507)	C(505)	C(513)	C(531)	110.48	C(515)	C(505)	C(513) C(526)	50.51	C(515)	C(505)	C(513) C(531)	-70.23
C(507)	C(505)	C(515)	C(516)	1.55	C(513)	C(505)	C(515) C(516)	-177.74	C(508)	C(506)	N(501) Cr(51)	-1.75
C(508)	C(506)	N(501)	C(507)	-175.45	C(518)	C(506)	N(501) Cr(51)	177.10	C(518)	C(506)	N(501) C(507)	3.39
N(501)	C(506)	C(508)	C(509)	12.09	C(518)	C(506)	C(508) C(509)	-166.82	C(501)	C(507)	N(501) Cr(51)	90.01
C(501)	C(507)	N(501)	C(506)	-95.89	C(505)	C(507)	N(501) Cr(51)	-88.78	C(505)	C(507)	N(501) C(506)	85.32
C(506)	C(508)	C(509)	N(502)	-6.98	C(506)	C(508)	C(509) C(523)	169.70	C(508)	C(509)	N(502) Cr(51)	-7.33
C(508)	C(509)	N(502)	C(504)	165.46	C(523)	C(509)	N(502) Cr(51)	176.13	C(523)	C(509)	N(502) C(504)	-11.07
C(512)	C(510)	C(511)	C(502)	-2.84	C(520)	C(510)	C(511) C(502)	179.21	C(511)	C(510)	C(512) C(503)	4.76
C(520)	C(510)	C(512)	C(503)	-177.37	C(511)	C(510)	C(520) C(530)	115.58	C(511)	C(510)	C(520) C(532)	-120.72
C(512)	C(510)	C(520)	C(530)	-62.29	C(512)	C(510)	C(520) C(532)	61.42	C(501)	C(514)	C(516) C(515)	4.71
C(501)	C(514)	C(516)	C(529)	-172.45	C(505)	C(515)	C(516) C(514)	-4.94	C(505)	C(515)	C(516) C(529)	172.36
C(514)	C(516)	C(529)	C(527)	7.33	C(514)	C(516)	C(529) C(533)	-124.01	C(515)	C(516)	C(529) C(527)	-169.95
C(515)	C(516)	C(529)	C(533)	58.72								

Statistics of Bond Length per Bond Type (NOTE: A Indicates 10 Occurrences, B Indicates 11, Etc. and * more than 35)

Bond Type	Nr	B.P.	d(min)	d(max)	d(av)	Sumrad	Note	0.0 0.5 1.0 1.5 2.0 2.5 3.0 Angstrom
Cr -- Cl	2		2.3878	2.3892	2.3885	2.34		.....2.....
Cr -- N	2		2.0390	2.0416	2.0403	2.03		.....2.....
N3 -- C3	2		1.3222	1.4300	1.3761	1.36		.....1..1.....
N -- C	2		1.3481	1.4438	1.3959	1.36		.....1.1.....
C3 -- C3	4		1.3970	1.4112	1.4052	1.36		.....4.....
C -- C	30		1.3660	1.5755	1.4846	1.36		.....2816C1.....

Selected Bond Lengths (Angstrom) - see M.F.C. Ladd & R.A. Palmer, Structure Determination by X-Ray Crystallography (1985)

Formal single bonds

C4-C4 1.54	C4-C3 1.52	C4-C2 1.46	C4-N3 1.47	C4-N2 1.47	C4-O2 1.43	C3-C3 1.46	C3-C2 1.45	C3-N3 1.40	C3-N2 1.40
C3-O2 1.36	C2-C2 1.38	C2-N3 1.33	C2-N2 1.33	C2-O2 1.36	N3-N3 1.45	N3-N2 1.45	N3-O2 1.36	N2-N2 1.45	N2-O2 1.41

Formal double bonds

C3-C3 1.34	C3-C2 1.31	C3-N2 1.32	C3-O1 1.22	C2-C2 1.28	C2-N2 1.32	C2-O1 1.16	N3-O1 1.24	N2-N2 1.25	N2-O1 1.21

Formal triple bonds

C2-C2 1.20	C2-N1 1.16	C3-C3 1.40	C2-N2 1.34

Aromatic bonds

N2-N2 1.35

The notation in the table indicates the connectivity of the atoms

For more detailed standard bond distance tabulations see: J. Chem. Soc. Perkin II, (1987), S1-S19;
J. Chem. Soc. Dalton Trans. (1989), S1 - S83 or International Tables C, (1992), 707-791.
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