PLATON(V-311206)-Run for: klat481 in P6(3)/m TIME: Dec 5 13:22:30 2007

Crystal Data

Input Cell (Lattice Type: P) - Temp = 170K

a =	19.1096(16)	Angstrom	alpha =	90	Degree	a =	19.110	alpha =	90.00
b =	19.1096(16)		beta =	90		b =	19.110	beta =	90.00
c =	20.555(2)		gamma =	120		c =	20.555	gamma =	120.00
V =	6500.6(10)	Cubic-Angstrom	d(100) =	16.5494	Angstrom				
			d(010) =	16.5494					
Lambda(MoKa) =	0.71073	Angstrom	d(001) =	20.5550					

Reduced Cell (Acta Cryst.(1976),A32,297-298) V = 6500.6

Niggli Values

365.177	365.177	422.508
0.000	0.000	-182.589

Orthogonalization Matrices

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

$$\begin{pmatrix} XO \\ YO \\ ZO \end{pmatrix} = \begin{pmatrix} 19.10960 & -9.55480 & 0 \\ 0 & 16.54940 & 0 \\ 0 & 0 & 20.55500 \end{pmatrix} \begin{pmatrix} X \\ Y \\ Z \end{pmatrix} , \quad \begin{pmatrix} X \\ Y \\ Z \end{pmatrix} = \begin{pmatrix} 0.05233 & 0.03021 & 0 \\ 0 & 0.06043 & 0 \\ 0 & 0 & 0.04865 \end{pmatrix} \begin{pmatrix} XO \\ YO \\ ZO \end{pmatrix}$$

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 P63/m No: 176, Laue: 6/m [Hall: -P 6c]

Lattice Type hP, Centric, Hexagonal, Order 12(6) [Schoenflies: C6h^2]

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

11	X - Y ,	X ,	- Z
12	- Y ,	X - Y ,	1/2 - Z

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

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         Site    = Site Symmetry; SSN = Site Symmetry Number; SSOF = SHELX Site Occupation Factor (= S.O.F / SSN).
*******  Move    = Transformation on Input Data: N.IJK (N = SymOp, IJK = Translation) i.e. 1.555 = nomove
SYMBOLS: Type    = D/A = Potential Donor or Acceptor atom, D-H = H on Donor atom, MET = Metal.
*******  El Type = AK = Alkali Metal, AE = Alkaline Earth, HL = Halogen, AN = Actinide, LN = Lanthanide, TR = Transition Element.
         ARU     = Asymmetric Residue Unit encoded as sklm.nn, with s = symmetry op, klm = translation, nn = residue #.
         RESIDUE = collection of ARU's constituting an isolated unit (= molecule, ion).
         FLAGS   : d = determined, c = calculated, R = riding G = group
```

Atom Types :	C	H	Cr	Li	N	Na	O
Cov.Rad(Ang):	0.68	0.35	1.35	0.68	0.68	0.97	0.68
Atom Volume :	13.87	5.08	28.10	22.60	11.80	26.00	11.39
Atom Number :	6	1	24	3	7	11	8
Atom Weight :	12.010	1.008	52.00	6.94	14.01	22.99	16.00
Scat.Fact.f0:	5.999	1.000	23.994	3.000	6.995	10.992	7.999
Scat.Fact.f':	0.003	0.000	0.321	0.000	0.006	0.036	0.011
Scat.Fact.f":	0.002	0.000	0.624	0.000	0.003	0.025	0.006
Mu/Rho(MoKa):	0.58	0.37	29.88	0.20	0.84	3.04	1.22
Elem. Type :	--	--	TR	AK	--	AK	--

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
-	Cr	0.26497	0.41257	1/4	1.1214	6.8278	5.1387	..m	2	1/2	1	10.555	Met
-	Na	1/3	2/3	1/4	0	11.0329	5.1387	-6..	6	1/6	1	10.555	Met
-	N(1)	0.25257	0.33180	0.17951	1.6562	5.4911	3.6898		1	1	1	10.555	D/A
-	N(2)	0.29939	0.56156	0.15351	0.3556	9.2935	3.1554		1	1	1	10.555	D/A
-	C(1)	0.27146	0.36255	0.11339	1.7234	6.0000	2.3307		1	1	1	10.555	-
-	C(2)	0.20802	0.35314	0.07238	0.6010	5.8443	1.4878		1	1	1	10.555	-
-	C(3)	0.22659	0.38160	0.00880	0.6839	6.3153	0.1809		1	1	1	10.555	-
-	C(4)	0.30757	0.41861	-0.01169	1.8778	6.9277	-0.2403		1	1	1	10.555	-
-	C(5)	0.36773	0.42799	0.02813	2.9378	7.0830	0.5782		1	1	1	10.555	-
-	C(6)	0.35041	0.40020	0.09315	2.8724	6.6231	1.9147		1	1	1	10.555	-
-	C(7)	0.41902	0.41196	0.13794	4.0711	6.8177	2.8354		1	1	1	10.555	-
-	C(8)	0.47343	0.50464	0.14727	4.2253	8.3515	3.0271		1	1	1	10.555	-
-	C(9)	0.46354	0.36997	0.11220	5.3231	6.1228	2.3063		1	1	1	10.555	-
-	C(10)	0.12385	0.31630	0.09470	-0.6555	5.2346	1.9466		1	1	1	10.555	-
-	C(11)	0.05977	0.24430	0.05271	-1.1921	4.0430	1.0835		1	1	1	10.555	-
-	C(12)	0.09471	0.37946	0.09539	-1.8158	6.2798	1.9607		1	1	1	10.555	-
-	C(14)	0.22700	0.20328	0.13140	2.3956	3.3642	2.7009		1	1	1	10.555	-
-	C(15)	0.23446	0.25637	0.18915	2.0309	4.2428	3.8880		1	1	1	10.555	-
-	C(16)	0.22172	0.22073	1/4	2.1279	3.6529	5.1387	..m	2	1/2	1	10.555	-

-	C(17)	0.28429	0.50331	0.18314	0.6236	8.3295	3.7644		1	1	1	10.555 -
-	Li	1/3	2/3	0.10858	0	11.0329	2.2319	3..	3	1/3	1	10.555 Met
-	H(3A)	0.18542	0.37615	-0.02017	-0.0507	6.2251	-0.4146		1	1	1	10.555 -
-	H(4A)	0.32034	0.43770	-0.05517	1.9394	7.2437	-1.1340		1	1	1	10.555 -
-	H(5A)	0.42173	0.45324	0.01253	3.7285	7.5008	0.2576		1	1	1	10.555 -
-	H(7A)	0.39516	0.38770	0.18115	3.8470	6.4162	3.7235		1	1	1	10.555 -
-	H(8A)	0.44079	0.52712	0.16406	3.3868	8.7235	3.3723		1	1	1	10.555 -
-	H(8B)	0.51667	0.51543	0.17825	4.9485	8.5301	3.6639		1	1	1	10.555 -
-	H(8C)	0.49715	0.52984	0.10538	4.4378	8.7685	2.1661		1	1	1	10.555 -
-	H(9A)	0.42566	0.31181	0.10847	5.1549	5.1603	2.2296		1	1	1	10.555 -
-	H(9B)	0.48641	0.39191	0.06932	5.5505	6.4859	1.4249		1	1	1	10.555 -
-	H(9C)	0.50714	0.37922	0.14229	6.0679	6.2759	2.9248		1	1	1	10.555 -
-	H(10A)	0.12103	0.29647	0.14018	-0.5199	4.9064	2.8814		1	1	1	10.555 -
-	H(11A)	0.07503	0.20250	0.04943	-0.5011	3.3513	1.0160		1	1	1	10.555 -
-	H(11B)	0.00657	0.22153	0.07334	-1.9911	3.6662	1.5075		1	1	1	10.555 -
-	H(11C)	0.05762	0.26380	0.00907	-1.4195	4.3657	0.1864		1	1	1	10.555 -
-	H(12A)	0.13243	0.42663	0.12104	-1.5457	7.0605	2.4880		1	1	1	10.555 -
-	H(12B)	0.09271	0.39632	0.05072	-2.0151	6.5589	1.0425		1	1	1	10.555 -
-	H(12C)	0.04073	0.35506	0.11482	-2.6142	5.8760	2.3601		1	1	1	10.555 -
-	H(14A)	0.23686	0.23415	0.09105	2.2890	3.8750	1.8715		1	1	1	10.555 -
-	H(14B)	0.26682	0.18550	0.13554	3.3264	3.0699	2.7860		1	1	1	10.555 -
-	H(14C)	0.17251	0.15599	0.13041	1.8061	2.5815	2.6806		1	1	1	10.555 -
-	H(16A)	0.22085	0.18807	1/4	2.4234	3.1124	5.1387	..m	2	1/2	1	10.555 -
-	Cr_a	0.58743	0.85240	1/4	3.0810	14.1067	5.1387	..m	2	1/2	1	12.665 Met
-	N(1)a	0.66820	0.92077	0.17951	3.9713	15.2382	3.6898		1	1	1	12.665 D/A
-	N(2)a	0.43844	0.73783	0.15351	1.3286	12.2106	3.1554		1	1	1	12.665 D/A
-	C(1)a	0.63745	0.90891	0.11339	3.4970	15.0419	2.3307		1	1	1	12.665 -
-	C(2)a	0.64686	0.85488	0.07238	4.1930	14.1477	1.4878		1	1	1	12.665 -
-	C(3)a	0.61840	0.84499	0.00880	3.7437	13.9841	0.1809		1	1	1	12.665 -
-	C(4)a	0.58139	0.88896	-0.01169	2.6163	14.7118	-0.2403		1	1	1	12.665 -
-	C(5)a	0.57201	0.93974	0.02813	1.9519	15.5521	0.5782		1	1	1	12.665 -
-	C(6)a	0.59980	0.95021	0.09315	2.3829	15.7254	1.9147		1	1	1	12.665 -
-	C(7)a	0.58804	1.00706	0.13794	1.6150	16.6662	2.8354		1	1	1	12.665 -
-	C(8)a	0.49536	0.96879	0.14727	0.2095	16.0329	3.0271		1	1	1	12.665 -
-	C(9)a	0.63003	1.09357	0.11220	1.5908	18.0979	2.3063		1	1	1	12.665 -
-	C(10)a	0.68370	0.80755	0.09470	5.3493	13.3645	1.9466		1	1	1	12.665 -
-	C(11)a	0.75570	0.81547	0.05271	6.6495	13.4955	1.0835		1	1	1	12.665 -
-	C(12)a	0.62054	0.71525	0.09539	5.0242	11.8370	1.9607		1	1	1	12.665 -
-	C(14)a	0.79672	1.02372	0.13140	5.4436	16.9419	2.7009		1	1	1	12.665 -
-	C(15)a	0.74363	0.97809	0.18915	4.8650	16.1868	3.8880		1	1	1	12.665 -
-	C(16)a	0.77927	1.00099	1/4	5.3273	16.5658	5.1387	..m	2	1/2	1	12.665 -
-	C(17)a	0.49669	0.78098	0.18314	2.0294	12.9247	3.7644		1	1	1	12.665 -
-	H(3A)a	0.62385	0.80927	-0.02017	4.1891	13.3929	-0.4146		1	1	1	12.665 -

-	H(4A)a	0.56230	0.88264	-0.05517	2.3119	14.6072	-1.1340		1	1	1	12.665	-
-	H(5A)a	0.54676	0.96849	0.01253	1.1946	16.0279	0.2576		1	1	1	12.665	-
-	H(7A)a	0.61230	1.00746	0.18115	2.0747	16.6729	3.7235		1	1	1	12.665	-
-	H(8A)a	0.47288	0.91367	0.16406	0.3066	15.1207	3.3723		1	1	1	12.665	-
-	H(8B)a	0.48457	1.00124	0.17825	-0.3067	16.5699	3.6639		1	1	1	12.665	-
-	H(8C)a	0.47016	0.96731	0.10538	-0.2579	16.0084	2.1661		1	1	1	12.665	-
-	H(9A)a	0.68819	1.11385	0.10847	2.5084	18.4335	2.2296		1	1	1	12.665	-
-	H(9B)a	0.60809	1.09450	0.06932	1.1626	18.1133	1.4249		1	1	1	12.665	-
-	H(9C)a	0.62078	1.12792	0.14229	1.0858	18.6664	2.9248		1	1	1	12.665	-
-	H(10A)a	0.70353	0.82456	0.14018	5.5657	13.6460	2.8814		1	1	1	12.665	-
-	H(11A)a	0.79750	0.87253	0.04943	6.9031	14.4398	1.0160		1	1	1	12.665	-
-	H(11B)a	0.77847	0.78504	0.07334	7.3753	12.9919	1.5075		1	1	1	12.665	-
-	H(11C)a	0.73620	0.79382	0.00907	6.4837	13.1372	0.1864		1	1	1	12.665	-
-	H(12A)a	0.57337	0.70580	0.12104	4.2131	11.6806	2.4880		1	1	1	12.665	-
-	H(12B)a	0.60368	0.69639	0.05072	4.8822	11.5248	1.0425		1	1	1	12.665	-
-	H(12C)a	0.64494	0.68567	0.11482	5.7731	11.3474	2.3601		1	1	1	12.665	-
-	H(14A)a	0.76585	1.00271	0.09105	5.0544	16.5942	1.8715		1	1	1	12.665	-
-	H(14B)a	0.81450	1.08132	0.13554	5.2330	17.8952	2.7860		1	1	1	12.665	-
-	H(14C)a	0.84401	1.01652	0.13041	6.4160	16.8228	2.6806		1	1	1	12.665	-
-	H(16A)a	0.81193	1.03278	1/4	5.6477	17.0919	5.1387	..m	2	1/2	1	12.665	-
-	Cr_b	0.14760	0.73503	1/4	-4.2025	12.1643	5.1387	..m	2	1/2	1	8.565	Met
-	N(1)b	0.07923	0.74743	0.17951	-5.6275	12.3695	3.6898		1	1	1	8.565	D/A
-	N(2)b	0.26217	0.70061	0.15351	-1.6842	11.5947	3.1554		1	1	1	8.565	D/A
-	C(1)b	0.09109	0.72854	0.11339	-5.2204	12.0569	2.3307		1	1	1	8.565	-
-	C(2)b	0.14512	0.79198	0.07238	-4.7940	13.1068	1.4878		1	1	1	8.565	-
-	C(3)b	0.15501	0.77341	0.00880	-4.4276	12.7995	0.1809		1	1	1	8.565	-
-	C(4)b	0.11104	0.69243	-0.01169	-4.4941	11.4593	-0.2403		1	1	1	8.565	-
-	C(5)b	0.06026	0.63227	0.02813	-4.8897	10.4637	0.5782		1	1	1	8.565	-
-	C(6)b	0.04979	0.64959	0.09315	-5.2552	10.7503	1.9147		1	1	1	8.565	-
-	C(7)b	-0.00706	0.58098	0.13794	-5.6861	9.6149	2.8354		1	1	1	8.565	-
-	C(8)b	0.03121	0.52657	0.14727	-4.4349	8.7144	3.0271		1	1	1	8.565	-
-	C(9)b	-0.09357	0.53646	0.11220	-6.9139	8.8781	2.3063		1	1	1	8.565	-
-	C(10)b	0.19245	0.87615	0.09470	-4.6938	14.4998	1.9466		1	1	1	8.565	-
-	C(11)b	0.18453	0.94023	0.05271	-5.4574	15.5602	1.0835		1	1	1	8.565	-
-	C(12)b	0.28475	0.90529	0.09539	-3.2084	14.9820	1.9607		1	1	1	8.565	-
-	C(14)b	-0.02372	0.77300	0.13140	-7.8391	12.7927	2.7009		1	1	1	8.565	-
-	C(15)b	0.02191	0.76554	0.18915	-6.8959	12.6692	3.8880		1	1	1	8.565	-
-	C(16)b	-0.00099	0.77828	1/4	-7.4552	12.8801	5.1387	..m	2	1/2	1	8.565	-
-	C(17)b	0.21902	0.71571	0.18314	-2.6531	11.8446	3.7644		1	1	1	8.565	-
-	H(3A)b	0.19073	0.81458	-0.02017	-4.1384	13.4808	-0.4146		1	1	1	8.565	-
-	H(4A)b	0.11736	0.67966	-0.05517	-4.2513	11.2480	-1.1340		1	1	1	8.565	-
-	H(5A)b	0.03151	0.57827	0.01253	-4.9231	9.5700	0.2576		1	1	1	8.565	-
-	H(7A)b	-0.00746	0.60484	0.18115	-5.9217	10.0097	3.7235		1	1	1	8.565	-
-	H(8A)b	0.08633	0.55921	0.16406	-3.6934	9.2546	3.3723		1	1	1	8.565	-

-	H(8B)b	-0.00124	0.48333	0.17825	-4.6418	7.9988	3.6639		1	1	1	8.565 -
-	H(8C)b	0.03269	0.50285	0.10538	-4.1799	8.3219	2.1661		1	1	1	8.565 -
-	H(9A)b	-0.11385	0.57434	0.10847	-7.6633	9.5050	2.2296		1	1	1	8.565 -
-	H(9B)b	-0.09450	0.51359	0.06932	-6.7131	8.4996	1.4249		1	1	1	8.565 -
-	H(9C)b	-0.12792	0.49286	0.14229	-7.1537	8.1565	2.9248		1	1	1	8.565 -
-	H(10A)b	0.17544	0.87897	0.14018	-5.0458	14.5464	2.8814		1	1	1	8.565 -
-	H(11A)b	0.12747	0.92497	0.04943	-6.4020	15.3077	1.0160		1	1	1	8.565 -
-	H(11B)b	0.21496	0.99343	0.07334	-5.3842	16.4407	1.5075		1	1	1	8.565 -
-	H(11C)b	0.20618	0.94238	0.00907	-5.0642	15.5958	0.1864		1	1	1	8.565 -
-	H(12A)b	0.29420	0.86757	0.12104	-2.6674	14.3578	2.4880		1	1	1	8.565 -
-	H(12B)b	0.30361	0.90729	0.05072	-2.8671	15.0151	1.0425		1	1	1	8.565 -
-	H(12C)b	0.31433	0.95927	0.11482	-3.1589	15.8753	2.3601		1	1	1	8.565 -
-	H(14A)b	-0.00271	0.76314	0.09105	-7.3434	12.6295	1.8715		1	1	1	8.565 -
-	H(14B)b	-0.08132	0.73318	0.13554	-8.5594	12.1337	2.7860		1	1	1	8.565 -
-	H(14C)b	-0.01652	0.82749	0.13041	-8.2222	13.6945	2.6806		1	1	1	8.565 -
-	H(16A)b	-0.03278	0.77915	1/4	-8.0710	12.8945	5.1387	..m	2	1/2	1	8.565 -
-	N(1)c	0.07923	0.74743	0.32049	-5.6275	12.3695	6.5877		1	1	1	5.565 D/A
-	N(2)c	0.26217	0.70061	0.34649	-1.6842	11.5947	7.1221		1	1	1	5.565 D/A
-	C(1)c	0.09109	0.72854	0.38661	-5.2204	12.0569	7.9468		1	1	1	5.565 -
-	C(2)c	0.14512	0.79198	0.42762	-4.7940	13.1068	8.7897		1	1	1	5.565 -
-	C(3)c	0.15501	0.77341	0.49120	-4.4276	12.7995	10.0966		1	1	1	5.565 -
-	C(4)c	0.11104	0.69243	0.51169	-4.4941	11.4593	10.5178		1	1	1	5.565 -
-	C(5)c	0.06026	0.63227	0.47187	-4.8897	10.4637	9.6993		1	1	1	5.565 -
-	C(6)c	0.04979	0.64959	0.40685	-5.2552	10.7503	8.3628		1	1	1	5.565 -
-	C(7)c	-0.00706	0.58098	0.36206	-5.6861	9.6149	7.4421		1	1	1	5.565 -
-	C(8)c	0.03121	0.52657	0.35273	-4.4349	8.7144	7.2504		1	1	1	5.565 -
-	C(9)c	-0.09357	0.53646	0.38780	-6.9139	8.8781	7.9712		1	1	1	5.565 -
-	C(10)c	0.19245	0.87615	0.40530	-4.6938	14.4998	8.3309		1	1	1	5.565 -
-	C(11)c	0.18453	0.94023	0.44729	-5.4574	15.5602	9.1940		1	1	1	5.565 -
-	C(12)c	0.28475	0.90529	0.40461	-3.2084	14.9820	8.3168		1	1	1	5.565 -
-	C(14)c	-0.02372	0.77300	0.36860	-7.8391	12.7927	7.5766		1	1	1	5.565 -
-	C(15)c	0.02191	0.76554	0.31085	-6.8959	12.6692	6.3895		1	1	1	5.565 -
-	C(17)c	0.21902	0.71571	0.31686	-2.6531	11.8446	6.5131		1	1	1	5.565 -
-	Li_c	1/3	2/3	0.39142	0	11.0329	8.0456	3..	3	1/3	1	5.565 Met
-	H(3A)c	0.19073	0.81458	0.52017	-4.1384	13.4808	10.6921		1	1	1	5.565 -
-	H(4A)c	0.11736	0.67966	0.55517	-4.2513	11.2480	11.4115		1	1	1	5.565 -
-	H(5A)c	0.03151	0.57827	0.48747	-4.9231	9.5700	10.0199		1	1	1	5.565 -
-	H(7A)c	-0.00746	0.60484	0.31885	-5.9217	10.0097	6.5540		1	1	1	5.565 -
-	H(8A)c	0.08633	0.55921	0.33594	-3.6934	9.2546	6.9052		1	1	1	5.565 -
-	H(8B)c	-0.00124	0.48333	0.32175	-4.6418	7.9988	6.6136		1	1	1	5.565 -
-	H(8C)c	0.03269	0.50285	0.39462	-4.1799	8.3219	8.1114		1	1	1	5.565 -
-	H(9A)c	-0.11385	0.57434	0.39153	-7.6633	9.5050	8.0479		1	1	1	5.565 -
-	H(9B)c	-0.09450	0.51359	0.43068	-6.7131	8.4996	8.8526		1	1	1	5.565 -
-	H(9C)c	-0.12792	0.49286	0.35771	-7.1537	8.1565	7.3527		1	1	1	5.565 -

-	H(10A)c	0.17544	0.87897	0.35982	-5.0458	14.5464	7.3961	1	1	1	5.565 -
-	H(11A)c	0.12747	0.92497	0.45057	-6.4020	15.3077	9.2615	1	1	1	5.565 -
-	H(11B)c	0.21496	0.99343	0.42666	-5.3842	16.4407	8.7700	1	1	1	5.565 -
-	H(11C)c	0.20618	0.94238	0.49093	-5.0642	15.5958	10.0911	1	1	1	5.565 -
-	H(12A)c	0.29420	0.86757	0.37896	-2.6674	14.3578	7.7895	1	1	1	5.565 -
-	H(12B)c	0.30361	0.90729	0.44928	-2.8671	15.0151	9.2349	1	1	1	5.565 -
-	H(12C)c	0.31433	0.95927	0.38518	-3.1589	15.8753	7.9174	1	1	1	5.565 -
-	H(14A)c	-0.00271	0.76314	0.40895	-7.3434	12.6295	8.4060	1	1	1	5.565 -
-	H(14B)c	-0.08132	0.73318	0.36446	-8.5594	12.1337	7.4915	1	1	1	5.565 -
-	H(14C)c	-0.01652	0.82749	0.36959	-8.2222	13.6945	7.5969	1	1	1	5.565 -
-	N(1)d	0.25257	0.33180	0.32049	1.6562	5.4911	6.5877	1	1	1	- D/A
-	N(2)d	0.29939	0.56156	0.34649	0.3556	9.2935	7.1221	1	1	1	- D/A
-	C(1)d	0.27146	0.36255	0.38661	1.7234	6.0000	7.9468	1	1	1	- -
-	C(2)d	0.20802	0.35314	0.42762	0.6010	5.8443	8.7897	1	1	1	- -
-	C(3)d	0.22659	0.38160	0.49120	0.6839	6.3153	10.0966	1	1	1	- -
-	C(4)d	0.30757	0.41861	0.51169	1.8778	6.9277	10.5178	1	1	1	- -
-	C(5)d	0.36773	0.42799	0.47187	2.9378	7.0830	9.6993	1	1	1	- -
-	C(6)d	0.35041	0.40020	0.40685	2.8724	6.6231	8.3628	1	1	1	- -
-	C(7)d	0.41902	0.41196	0.36206	4.0711	6.8177	7.4421	1	1	1	- -
-	C(8)d	0.47343	0.50464	0.35273	4.2253	8.3515	7.2504	1	1	1	- -
-	C(9)d	0.46354	0.36997	0.38780	5.3231	6.1228	7.9712	1	1	1	- -
-	C(10)d	0.12385	0.31630	0.40530	-0.6555	5.2346	8.3309	1	1	1	- -
-	C(11)d	0.05977	0.24430	0.44729	-1.1921	4.0430	9.1940	1	1	1	- -
-	C(12)d	0.09471	0.37946	0.40461	-1.8158	6.2798	8.3168	1	1	1	- -
-	C(14)d	0.22700	0.20328	0.36860	2.3956	3.3642	7.5766	1	1	1	- -
-	C(15)d	0.23446	0.25637	0.31085	2.0309	4.2428	6.3895	1	1	1	- -
-	C(17)d	0.28429	0.50331	0.31686	0.6236	8.3295	6.5131	1	1	1	- -
-	H(3A)d	0.18542	0.37615	0.52017	-0.0507	6.2251	10.6921	1	1	1	- -
-	H(4A)d	0.32034	0.43770	0.55517	1.9394	7.2437	11.4115	1	1	1	- -
-	H(5A)d	0.42173	0.45324	0.48747	3.7285	7.5008	10.0199	1	1	1	- -
-	H(7A)d	0.39516	0.38770	0.31885	3.8470	6.4162	6.5540	1	1	1	- -
-	H(8A)d	0.44079	0.52712	0.33594	3.3868	8.7235	6.9052	1	1	1	- -
-	H(8B)d	0.51667	0.51543	0.32175	4.9485	8.5301	6.6136	1	1	1	- -
-	H(8C)d	0.49715	0.52984	0.39462	4.4378	8.7685	8.1114	1	1	1	- -
-	H(9A)d	0.42566	0.31181	0.39153	5.1549	5.1603	8.0479	1	1	1	- -
-	H(9B)d	0.48641	0.39191	0.43068	5.5505	6.4859	8.8526	1	1	1	- -
-	H(9C)d	0.50714	0.37922	0.35771	6.0679	6.2759	7.3527	1	1	1	- -
-	H(10A)d	0.12103	0.29647	0.35982	-0.5199	4.9064	7.3961	1	1	1	- -
-	H(11A)d	0.07503	0.20250	0.45057	-0.5011	3.3513	9.2615	1	1	1	- -
-	H(11B)d	0.00657	0.22153	0.42666	-1.9911	3.6662	8.7700	1	1	1	- -
-	H(11C)d	0.05762	0.26380	0.49093	-1.4195	4.3657	10.0911	1	1	1	- -
-	H(12A)d	0.13243	0.42663	0.37896	-1.5457	7.0605	7.7895	1	1	1	- -
-	H(12B)d	0.09271	0.39632	0.44928	-2.0151	6.5589	9.2349	1	1	1	- -
-	H(12C)d	0.04073	0.35506	0.38518	-2.6142	5.8760	7.9174	1	1	1	- -

-	H(14A)d	0.23686	0.23415	0.40895	2.2890	3.8750	8.4060	1	1	1	- -
-	H(14B)d	0.26682	0.18550	0.36446	3.3264	3.0699	7.4915	1	1	1	- -
-	H(14C)d	0.17251	0.15599	0.36959	1.8061	2.5815	7.5969	1	1	1	- -
-	N(1)e	0.66820	0.92077	0.32049	3.9713	15.2382	6.5877	1	1	1	3.665 D/A
-	N(2)e	0.43844	0.73783	0.34649	1.3286	12.2106	7.1221	1	1	1	3.665 D/A
-	C(1)e	0.63745	0.90891	0.38661	3.4970	15.0419	7.9468	1	1	1	3.665 -
-	C(2)e	0.64686	0.85488	0.42762	4.1930	14.1477	8.7897	1	1	1	3.665 -
-	C(3)e	0.61840	0.84499	0.49120	3.7437	13.9841	10.0966	1	1	1	3.665 -
-	C(4)e	0.58139	0.88896	0.51169	2.6163	14.7118	10.5178	1	1	1	3.665 -
-	C(5)e	0.57201	0.93974	0.47187	1.9519	15.5521	9.6993	1	1	1	3.665 -
-	C(6)e	0.59980	0.95021	0.40685	2.3829	15.7254	8.3628	1	1	1	3.665 -
-	C(7)e	0.58804	1.00706	0.36206	1.6150	16.6662	7.4421	1	1	1	3.665 -
-	C(8)e	0.49536	0.96879	0.35273	0.2095	16.0329	7.2504	1	1	1	3.665 -
-	C(9)e	0.63003	1.09357	0.38780	1.5908	18.0979	7.9712	1	1	1	3.665 -
-	C(10)e	0.68370	0.80755	0.40530	5.3493	13.3645	8.3309	1	1	1	3.665 -
-	C(11)e	0.75570	0.81547	0.44729	6.6495	13.4955	9.1940	1	1	1	3.665 -
-	C(12)e	0.62054	0.71525	0.40461	5.0242	11.8370	8.3168	1	1	1	3.665 -
-	C(14)e	0.79672	1.02372	0.36860	5.4436	16.9419	7.5766	1	1	1	3.665 -
-	C(15)e	0.74363	0.97809	0.31085	4.8650	16.1868	6.3895	1	1	1	3.665 -
-	C(17)e	0.49669	0.78098	0.31686	2.0294	12.9247	6.5131	1	1	1	3.665 -
-	H(3A)e	0.62385	0.80927	0.52017	4.1891	13.3929	10.6921	1	1	1	3.665 -
-	H(4A)e	0.56230	0.88264	0.55517	2.3119	14.6072	11.4115	1	1	1	3.665 -
-	H(5A)e	0.54676	0.96849	0.48747	1.1946	16.0279	10.0199	1	1	1	3.665 -
-	H(7A)e	0.61230	1.00746	0.31885	2.0747	16.6729	6.5540	1	1	1	3.665 -
-	H(8A)e	0.47288	0.91367	0.33594	0.3066	15.1207	6.9052	1	1	1	3.665 -
-	H(8B)e	0.48457	1.00124	0.32175	-0.3067	16.5699	6.6136	1	1	1	3.665 -
-	H(8C)e	0.47016	0.96731	0.39462	-0.2579	16.0084	8.1114	1	1	1	3.665 -
-	H(9A)e	0.68819	1.11385	0.39153	2.5084	18.4335	8.0479	1	1	1	3.665 -
-	H(9B)e	0.60809	1.09450	0.43068	1.1626	18.1133	8.8526	1	1	1	3.665 -
-	H(9C)e	0.62078	1.12792	0.35771	1.0858	18.6664	7.3527	1	1	1	3.665 -
-	H(10A)e	0.70353	0.82456	0.35982	5.5657	13.6460	7.3961	1	1	1	3.665 -
-	H(11A)e	0.79750	0.87253	0.45057	6.9031	14.4398	9.2615	1	1	1	3.665 -
-	H(11B)e	0.77847	0.78504	0.42666	7.3753	12.9919	8.7700	1	1	1	3.665 -
-	H(11C)e	0.73620	0.79382	0.49093	6.4837	13.1372	10.0911	1	1	1	3.665 -
-	H(12A)e	0.57337	0.70580	0.37896	4.2131	11.6806	7.7895	1	1	1	3.665 -
-	H(12B)e	0.60368	0.69639	0.44928	4.8822	11.5248	9.2349	1	1	1	3.665 -
-	H(12C)e	0.64494	0.68567	0.38518	5.7731	11.3474	7.9174	1	1	1	3.665 -
-	H(14A)e	0.76585	1.00271	0.40895	5.0544	16.5942	8.4060	1	1	1	3.665 -
-	H(14B)e	0.81450	1.08132	0.36446	5.2330	17.8952	7.4915	1	1	1	3.665 -
-	H(14C)e	0.84401	1.01652	0.36959	6.4160	16.8228	7.5969	1	1	1	3.665 -

Disordered Atoms with S.O.F < 0.5

-	<O(1)	0.32600	0.67542	0.01740	-0.2238	11.1778	0.3577	1	1/3	1/3	10.555 D/A
-	<C(18)	0.27711	0.60806	-0.02299	-0.5144	10.0630	-0.4726	1	1/3	1/3	10.555 -
-	<C(19)	0.31771	0.61959	-0.08330	0.1513	10.2538	-1.7122	1	1/3	1/3	10.555 -
-	<C(20)	0.39169	0.69406	-0.08019	0.8534	11.4863	-1.6483	1	1/3	1/3	10.555 -
-	<C(21)	0.39682	0.72857	-0.01795	0.6217	12.0574	-0.3690	1	1/3	1/3	10.555 -
-	<H(18A)	0.26827	0.55760	-0.00210	-0.2012	9.2279	-0.0432	1	1/3	1/3	10.555 -
-	<H(18B)	0.22387	0.60382	-0.03008	-1.4913	9.9929	-0.6183	1	1/3	1/3	10.555 -
-	<H(19A)	0.32833	0.57465	-0.09131	0.7836	9.5101	-1.8769	1	1/3	1/3	10.555 -
-	<H(19B)	0.28393	0.62086	-0.11929	-0.5064	10.2749	-2.4520	1	1/3	1/3	10.555 -
-	<H(20B)	0.39337	0.73103	-0.11468	0.5323	12.0981	-2.3572	1	1/3	1/3	10.555 -
-	<H(20C)	0.43777	0.68482	-0.08670	1.8223	11.3334	-1.7821	1	1/3	1/3	10.555 -
-	<H(21A)	0.40095	0.78208	-0.02262	0.1894	12.9430	-0.4650	1	1/3	1/3	10.555 -
-	<H(21B)	0.44535	0.73586	0.00537	1.4795	12.1780	0.1104	1	1/3	1/3	10.555 -
-	<O(1)a	0.32458	0.65058	0.01740	-0.0136	10.7667	0.3577	1	1/3	1/3	12.665 D/A
-	<C(18)a	0.39194	0.66905	-0.02299	1.0972	11.0724	-0.4726	1	1/3	1/3	12.665 -
-	<C(19)a	0.38041	0.69812	-0.08330	0.5991	11.5535	-1.7122	1	1/3	1/3	12.665 -
-	<C(20)a	0.30594	0.69763	-0.08019	-0.8193	11.5454	-1.6483	1	1/3	1/3	12.665 -
-	<C(21)a	0.27143	0.66825	-0.01795	-1.1981	11.0591	-0.3690	1	1/3	1/3	12.665 -
-	<H(18A)a	0.44240	0.71067	-0.00210	1.6638	11.7612	-0.0432	1	1/3	1/3	12.665 -
-	<H(18B)a	0.39618	0.62005	-0.03008	1.6464	10.2615	-0.6183	1	1/3	1/3	12.665 -
-	<H(19A)a	0.42535	0.75368	-0.09131	0.9270	12.4729	-1.8769	1	1/3	1/3	12.665 -
-	<H(19B)a	0.37914	0.66307	-0.11929	0.9097	10.9734	-2.4520	1	1/3	1/3	12.665 -
-	<H(20B)a	0.26897	0.66234	-0.11468	-1.1886	10.9613	-2.3572	1	1/3	1/3	12.665 -
-	<H(20C)a	0.31518	0.75295	-0.08670	-1.1713	12.4609	-1.7821	1	1/3	1/3	12.665 -
-	<H(21A)a	0.21792	0.61887	-0.02262	-1.7488	10.2419	-0.4650	1	1/3	1/3	12.665 -
-	<H(21B)a	0.26414	0.70949	0.00537	-1.7314	11.7416	0.1104	1	1/3	1/3	12.665 -
-	<O(1)b	0.34942	0.67400	0.01740	0.2373	11.1543	0.3577	1	1/3	1/3	8.565 D/A
-	<C(18)b	0.33095	0.72289	-0.02299	-0.5827	11.9634	-0.4726	1	1/3	1/3	8.565 -
-	<C(19)b	0.30188	0.68229	-0.08330	-0.7503	11.2915	-1.7122	1	1/3	1/3	8.565 -
-	<C(20)b	0.30237	0.60831	-0.08019	-0.0341	10.0672	-1.6483	1	1/3	1/3	8.565 -
-	<C(21)b	0.33175	0.60318	-0.01795	0.5763	9.9823	-0.3690	1	1/3	1/3	8.565 -
-	<H(18A)b	0.28933	0.73173	-0.00210	-1.4626	12.1097	-0.0432	1	1/3	1/3	8.565 -
-	<H(18B)b	0.37995	0.77613	-0.03008	-0.1551	12.8445	-0.6183	1	1/3	1/3	8.565 -
-	<H(19A)b	0.24632	0.67167	-0.09131	-1.7106	11.1157	-1.8769	1	1/3	1/3	8.565 -
-	<H(19B)b	0.33693	0.71607	-0.11929	-0.4033	11.8505	-2.4520	1	1/3	1/3	8.565 -
-	<H(20B)b	0.33766	0.60663	-0.11468	0.6563	10.0394	-2.3572	1	1/3	1/3	8.565 -
-	<H(20C)b	0.24705	0.56223	-0.08670	-0.6510	9.3046	-1.7821	1	1/3	1/3	8.565 -
-	<H(21A)b	0.38113	0.59905	-0.02262	1.5594	9.9139	-0.4650	1	1/3	1/3	8.565 -
-	<H(21B)b	0.29051	0.55465	0.00537	0.2520	9.1791	0.1104	1	1/3	1/3	8.565 -
-	<O(1)c	0.34942	0.67400	0.48260	0.2373	11.1543	9.9198	1	1/3	1/3	5.565 D/A
-	<C(18)c	0.33095	0.72289	0.52299	-0.5827	11.9634	10.7501	1	1/3	1/3	5.565 -
-	<C(19)c	0.30188	0.68229	0.58330	-0.7503	11.2915	11.9897	1	1/3	1/3	5.565 -
-	<C(20)c	0.30237	0.60831	0.58019	-0.0341	10.0672	11.9258	1	1/3	1/3	5.565 -
-	<C(21)c	0.33175	0.60318	0.51795	0.5763	9.9823	10.6465	1	1/3	1/3	5.565 -

-	<H(18A)c	0.28933	0.73173	0.50210	-1.4626	12.1097	10.3207	1	1/3	1/3	5.565	-
-	<H(18B)c	0.37995	0.77613	0.53008	-0.1551	12.8445	10.8958	1	1/3	1/3	5.565	-
-	<H(19A)c	0.24632	0.67167	0.59131	-1.7106	11.1157	12.1544	1	1/3	1/3	5.565	-
-	<H(19B)c	0.33693	0.71607	0.61929	-0.4033	11.8505	12.7295	1	1/3	1/3	5.565	-
-	<H(20B)c	0.33766	0.60663	0.61468	0.6563	10.0394	12.6347	1	1/3	1/3	5.565	-
-	<H(20C)c	0.24705	0.56223	0.58670	-0.6510	9.3046	12.0596	1	1/3	1/3	5.565	-
-	<H(21A)c	0.38113	0.59905	0.52262	1.5594	9.9139	10.7425	1	1/3	1/3	5.565	-
-	<H(21B)c	0.29051	0.55465	0.49463	0.2520	9.1791	10.1671	1	1/3	1/3	5.565	-
-	<O(1)d	0.32600	0.67542	0.48260	-0.2238	11.1778	9.9198	1	1/3	1/3	-	D/A
-	<C(18)d	0.27711	0.60806	0.52299	-0.5144	10.0630	10.7501	1	1/3	1/3	-	-
-	<C(19)d	0.31771	0.61959	0.58330	0.1513	10.2538	11.9897	1	1/3	1/3	-	-
-	<C(20)d	0.39169	0.69406	0.58019	0.8534	11.4863	11.9258	1	1/3	1/3	-	-
-	<C(21)d	0.39682	0.72857	0.51795	0.6217	12.0574	10.6465	1	1/3	1/3	-	-
-	<H(18A)d	0.26827	0.55760	0.50210	-0.2012	9.2279	10.3207	1	1/3	1/3	-	-
-	<H(18B)d	0.22387	0.60382	0.53008	-1.4913	9.9929	10.8958	1	1/3	1/3	-	-
-	<H(19A)d	0.32833	0.57465	0.59131	0.7836	9.5101	12.1544	1	1/3	1/3	-	-
-	<H(19B)d	0.28393	0.62086	0.61929	-0.5064	10.2749	12.7295	1	1/3	1/3	-	-
-	<H(20B)d	0.39337	0.73103	0.61468	0.5323	12.0981	12.6347	1	1/3	1/3	-	-
-	<H(20C)d	0.43777	0.68482	0.58670	1.8223	11.3334	12.0596	1	1/3	1/3	-	-
-	<H(21A)d	0.40095	0.78208	0.52262	0.1894	12.9430	10.7425	1	1/3	1/3	-	-
-	<H(21B)d	0.44535	0.73586	0.49463	1.4795	12.1780	10.1671	1	1/3	1/3	-	-
-	<O(1)e	0.32458	0.65058	0.48260	-0.0136	10.7667	9.9198	1	1/3	1/3	3.665	D/A
-	<C(18)e	0.39194	0.66905	0.52299	1.0972	11.0724	10.7501	1	1/3	1/3	3.665	-
-	<C(19)e	0.38041	0.69812	0.58330	0.5991	11.5535	11.9897	1	1/3	1/3	3.665	-
-	<C(20)e	0.30594	0.69763	0.58019	-0.8193	11.5454	11.9258	1	1/3	1/3	3.665	-
-	<C(21)e	0.27143	0.66825	0.51795	-1.1981	11.0591	10.6465	1	1/3	1/3	3.665	-
-	<H(18A)e	0.44240	0.71067	0.50210	1.6638	11.7612	10.3207	1	1/3	1/3	3.665	-
-	<H(18B)e	0.39618	0.62005	0.53008	1.6464	10.2615	10.8958	1	1/3	1/3	3.665	-
-	<H(19A)e	0.42535	0.75368	0.59131	0.9270	12.4729	12.1544	1	1/3	1/3	3.665	-
-	<H(19B)e	0.37914	0.66307	0.61929	0.9097	10.9734	12.7295	1	1/3	1/3	3.665	-
-	<H(20B)e	0.26897	0.66234	0.61468	-1.1886	10.9613	12.6347	1	1/3	1/3	3.665	-
-	<H(20C)e	0.31518	0.75295	0.58670	-1.1713	12.4609	12.0596	1	1/3	1/3	3.665	-
-	<H(21A)e	0.21792	0.61887	0.52262	-1.7488	10.2419	10.7425	1	1/3	1/3	3.665	-
-	<H(21B)e	0.26414	0.70949	0.49463	-1.7314	11.7416	10.1671	1	1/3	1/3	3.665	-

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-y,1+x-y,z	= [3	1	1	0	1]	1	1	0
b =[5565.01]	= -x+y,1-x,z	= [5	0	1	0	1]	0	1	0
c =[8565.01]	= -x+y,1-x,1/2-z	= [8	0	1	0	1]	0	1	1/2
d =[10555.01]	= x,y,1/2-z	= [10	0	0	0	1]	0	0	1/2
e =[12665.01]	= 1-y,1+x-y,1/2-z	= [12	1	1	0	1]	1	1	1/2

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.

NOTE: Atoms preceded by > * or < indicate disordered positions (SOF : < 50%, 50%, > 50%)

Disordered 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	Cr	Li	N	Na	O
1	-6..	1/3	2/3	1/4	1745.97	1	2	101.0	139.0	3.0	2.0	12.0	1.0	2.0
Unit Cell Weight =					3491.94			202	278	6	4	24	2	4
Calculated Analysis (Percent) =								69.5	8.0	8.9	0.8	9.6	1.3	1.8

Moiety_Formula = C101 H138.98 Cr3 Li2 N12 Na O2

Sum_Formula = C101 H138.98 Cr3 Li2 N12 Na O2

Formula_Weight = 1745.97 [Note: Based on SHELXL97 Atomic Weights]

Formula_Z = 2

SpaceGroup_Z = 12 ===> Z' = 2 / 12 = 0.167

Calculated Density = 0.8920(1) g cm-3 [= Mg m-3]

F(000) = 1867.8 [1870.33]

mu(MoKa) = 2.89 cm-1 = 0.289 mm-1

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

Resonant Scattering = 1.91 Percent - (Girard,E. et al. (2003). Acta Cryst. D59, 1914-1922)

Predicted Volume = 4853.3[4794.3] Ang**3, 298[170]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

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

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

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

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

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

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

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

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

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

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

N: No S.U.’s (esd) on observed/calculated parameters.
N: DISORDERED structure - ATOMS with Pop. .LT. 1.0 are not moved or as a group.

N: Number of moved primary input atoms: 55
W: Low density (check!) of 0.892 gcm-3
N: Number of Ignored Lines on INPUT 3
         of which blank in column 1 3
W: Number of unusual anisotropic displacement parameters 1
N: Total Potential Solvent Accessible Void Vol .... 1847.3 Ang^3
N: Electron Count / Cell =   352 - To be included in D(calc), F000 & Mol.Wght.

:: Input Xtal Data from File klat481s.ins - Data Type RES

:: NORMAL END of PLATON :   45 Pages on:
:: klat481s.lis (ASCII, 132 Characters Wide)
:: klat481s.lps (PostScript Version of .lis)
:: klat481s.pdf (PDF   Version of .lis)

:: SQUEEZE xyz on :klat481s.sqz
:: SQUEEZE CIF on :klat481s.sqf