

PLATON(V-311206)-Run for: klat497

TIME: Dec 17 18:32:13 2007

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Crystal Data

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Input Cell (Lattice Type: P)		Temp = 0K	Reduced Cell		(Acta Cryst.(1976),A32,297-298)
a =	15.14600 Angstrom	alpha =	90 Degree	a =	15.146 alpha = 90.00 V = 9088.4
b =	30.96300	beta =	96.8500	b =	19.519 beta = 90.00
c =	19.51900	gamma =	90	c =	30.963 gamma = 96.85
V =	9088.40 Cubic-Angstrom	d(100) =	15.0379 Angstrom	Niggli Values	
Lambda(MoKa) =	0.71073 Angstrom	d(010) =	30.9630	229.401	380.991 958.707
		d(001) =	19.3797	0.000	0.000 -35.261

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Orthogonalization Matrices

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

(XO) (15.14600 0 -2.32804) (X) , (X) (0.06602 0 0.00793) (XO) Orthogonal Axes AO, BO and CO
 (YO) = (0 30.96300 0)*(Y) , (Y) = (0 0.03230 0)*(YO) are defined as:
 (ZO) (0 0 19.37967) (Z) , (Z) (0 0 0.05160) (ZO) AO // A, CO // C*, BO // CO X AO

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SPGR - Determine SpaceGroup from Observed Extinctions for: klat497

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:: Reflection Data are READ from File : latt.hkl - (OBS-Data)

:: TRMX = 1.00 0.00 0.00 0.00 1.00 0.00 0.00 0.00 1.00

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:: TRMX = 1.00 0.00 0.00 0.00 1.00 0.00 0.00 0.00 1.00

Intensity Distribution

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sh st/l Ang # 0.25 1.0 2.0 0 Percent Distr. for I gt 2.0 s(I) 100

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sh	st/l	Ang	#	0.25	1.0	2.0	0 Percent	Distr. for I	gt 2.0	s(I)	100
1	0.30	1.66	3121	77.2	53.3	33.0	*****			
2	0.38	1.32	2975	64.1	32.5	11.5	*****			
3	0.44	1.15	2665	59.3	29.8	8.0	***			
4	0.48	1.04	2418	61.9	34.1	9.8	****			
5	0.52	0.97	2211	57.3	33.0	11.0	****			
6	0.55	0.91	2080	55.6	33.8	10.3	****			
7	0.58	0.87	1867	52.6	33.2	12.9	*****			
8	0.60	0.83	1753	57.2	35.8	14.8	*****			
9	0.63	0.80	1711	55.0	33.8	14.0	*****			
10	0.65	0.77	1585	55.5	35.1	15.9	*****			
							I		I		I
							0%		50%		100%

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 Analysis of General Reflections for Bravais Centering

Nr	Ex. Condition	Aver(I/sig(I))		Number of Refl		I/sigI Max.F	.T/F.			
		.True.	.False.	.True.	.False.		H	K	L	Ratio
1	HKL:H+K=2N	0.97	0.97	11757	11759	27.88	1	-8	-4	1.0
2	HKL:H+L=2N	0.98	0.96	11771	11745	33.71	1	-7	-4	1.0
3	HKL:K+L=2N	0.96	0.97	11762	11754	33.71	1	-7	-4	1.0
4	HKL:H+K+L=2N	0.98	0.96	11749	11767	27.88	1	-8	-4	1.0
5	HKL:-H+K+L=3N	0.98	0.97	7874	15642	44.44	0	4	0	1.0
6	HKL:H-K+L=3N	0.97	0.97	7846	15670	44.44	0	4	0	1.0
41	HKL:H=2N	0.97	0.97	11767	11749	33.71	1	-7	-4	1.0
42	HKL:K=2N	0.96	0.97	11752	11764	33.71	1	-7	-4	1.0
43	HKL:L=2N	0.97	0.97	11742	11774	27.71	0	6	3	1.0
44	HKL:H=3N	0.96	0.97	7814	15702	33.71	1	-7	-4	1.0
45	HKL:K=3N	0.97	0.97	7829	15687	44.44	0	4	0	1.0
46	HKL:L=3N	0.98	0.96	7862	15654	33.71	1	-7	-4	1.0
47	-HKL, H-KL=3N	0.97	0.97	13081	10435	44.44	0	4	0	1.0
48	-HKL:K2, KL4P2	0.97	0.95	21699	1817	16.18	-3	14	4	1.0
49	-HKL:H2, HL4P2	0.97	1.04	22547	969	13.60	4	-1	-2	0.9
50	-HKL:H2, HK4P2	0.97	0.93	20918	2598	27.71	0	6	3	1.1
51	HKL:H+2L=3N	0.96	0.97	7836	15680	33.71	1	-7	-4	1.0

:: No Extinction Conditions Found

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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/>

:: Input Xtal Data from File latt.ins - Data Type SPF

:: NORMAL END of PLATON : 5 Pages on:
:: latt.lis (ASCII, 132 Characters Wide)
:: latt.lps (PostScript Version of .lis)
:: latt.pdf (PDF Version of .lis)

:: SPGR.PAR on :latt.par