

PLATON(V-311206)-Run for: kla0081

TIME: Sep 21 15:14:41 2011

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Crystal Data

Input Cell (Lattice Type: P)				Temp = 0K	Reduced Cell (Acta Cryst.(1976), A32, 297-298)			
a =	16.05900	Angstrom	alpha =	99.4400 Degree	a =	16.059	alpha =	99.44 V = 4942.7
b =	16.93100		beta =	111.6400	b =	16.931	beta =	111.64
c =	21.18500		gamma =	105.2300	c =	21.185	gamma =	105.23
V =	4942.68	Cubic-Angstrom	d(100) =	13.9692 Angstrom	Niggli Values			
			d(010) =	15.6299	257.891	286.659	448.804	
Lambda(MoKa) =	0.71073	Angstrom	d(001) =	18.8403	-58.829	-125.461	-71.425	

Orthogonalization Matrices

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

(X0) (16.05900 -4.44768 -7.81247) (X) , (X) (0.06227 0.01695 0.03098) (X0) Orthogonal Axes A0, B0 and C0
 (Y0) = (0 16.33637 -5.72812)*(Y) , (Y) = (0 0.06121 0.01861)*(Y0) are defined as:
 (Z0) (0 0 18.84033) (Z) , (Z) (0 0 0.05308) (Z0) A0 // A, C0 // C*, B0 // C0 X A0

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SPGR - Determine SpaceGroup from Observed Extinctions for: kla0081

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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
1	0.30	1.66	8565	93.3	87.1	79.9	*****			
2	0.38	1.32	8253	88.1	77.2	64.1	*****			
3	0.44	1.15	7422	81.2	64.4	46.2	*****			
4	0.48	1.04	6685	74.9	54.6	31.4	*****			
5	0.52	0.97	6189	69.6	46.6	22.9	*****			
6	0.55	0.91	5744	64.5	40.1	16.0	*****			
7	0.58	0.87	5391	60.1	33.7	11.0	****			
8	0.60	0.83	5051	55.0	27.2	5.8	**			
9	0.63	0.80	4781	49.2	21.6	3.6	*			
10	0.65	0.77	4533	48.8	19.7	2.4	*			
							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	2.43	2.43	33157	33062	28.63	3	0	-1	1.0
2	HKL:H+L=2N	2.42	2.44	33116	33103	28.33	0	3	-3	1.0
3	HKL:K+L=2N	2.44	2.42	33132	33087	28.63	3	0	-1	1.0
4	HKL:H+K+L=2N	2.41	2.45	33106	33113	28.55	-2	1	-2	1.0
5	HKL:-H+K+L=3N	2.42	2.44	22076	44143	28.96	2	0	-2	1.0
6	HKL:H-K+L=3N	2.40	2.45	22048	44171	28.63	3	0	-1	1.0
41	HKL:H=2N	2.42	2.44	33141	33078	28.63	3	0	-1	1.0
42	HKL:K=2N	2.42	2.44	33121	33098	28.55	-2	1	-2	1.0
43	HKL:L=2N	2.44	2.42	33100	33119	28.63	3	0	-1	1.0
44	HKL:H=3N	2.46	2.42	22044	44175	28.96	2	0	-2	1.0
45	HKL:K=3N	2.47	2.41	22121	44098	28.81	-4	2	0	1.0
46	HKL:L=3N	2.43	2.43	22085	44134	28.96	2	0	-2	1.0
47	-HKL, H-KL=3N	2.42	2.45	36775	29444	28.63	3	0	-1	1.0
48	-HKL:K2,KL4P2	2.44	2.36	62343	3876	28.81	-4	2	0	1.0
49	-HKL:H2,HL4P2	2.44	2.36	62314	3905	27.29	-2	-1	4	1.0
50	-HKL:H2,HK4P2	2.44	2.31	62350	3869	28.96	2	0	-2	1.1
51	HKL:H+2L=3N	2.42	2.44	22081	44138	28.96	2	0	-2	1.0

:: No Extinction Conditions Found

Possible 2-Fold Axes - 2-Axis Crit = 0.20, Exp. Error = 0.20 Deg., LATT = P

==== Transformation Matrix: Input (a,b,c) to Conventional Cell(a', b', c') ====

(a') (1.000 0.000 0.000) (a) (x') (1.000 0.000 0.000) (x) Metrically
 (b') = (0.000 1.000 0.000) (b). (y') = (0.000 1.000 0.000) (y) Anorthic
 (c') (0.000 0.000 1.000) (c) (z') (0.000 0.000 1.000) (z) FOM: 0.000

	Latt	a	b	c	Alpha	Beta	Gamma	Volume
Input Cell	P	16.059	16.931	21.185	99.44	111.64	105.23	4942.68
Reduc Cell	P	16.059	16.931	21.185	99.44	111.64	105.23	4942.67
Conv. Cell	aP	16.059	16.931	21.185	99.44	111.64	105.23	4942.68

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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