

PLATON(V-311206)-Run for: kla0202a

TIME: Apr 6 15:42:06 2012

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Crystal Data

Input Cell (Lattice Type: P)		Temp = 0K	Reduced Cell		(Acta Cryst.(1976), A32, 297-298)
a =	5.61700 Angstrom	alpha = 90 Degree	a =	5.617	alpha = 90.00 V = 2111.4
b =	16.00200	beta = 88.3600	b =	16.002	beta = 91.64
c =	23.50000	gamma = 90	c =	23.500	gamma = 90.00
V = 2111.39 Cubic-Angstrom		d(100) = 5.6147 Angstrom	Niggli Values		
		d(010) = 16.0020	31.551	256.064	552.250
Lambda(MoKa) = 0.71073 Angstrom		d(001) = 23.4904	0.000	-3.777	0.000

Orthogonalization Matrices

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

(X0) (5.61700 0 0.67256) (X) , (X) (0.17803 0 -0.00510) (X0) Orthogonal Axes A0, B0 and C0
 (Y0) = (0 16.00200 0)*(Y) , (Y) = (0 0.06249 0)*(Y0) are defined as:
 (Z0) (0 0 23.49037) (Z) , (Z) (0 0 0.04257) (Z0) A0 // A, C0 // C*, B0 // C0 X A0

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SPGR - Determine SpaceGroup from Observed Extinctions for: kla0202a

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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	3469	85.4	72.8	62.3	*****			
2	0.38	1.32	3362	79.8	61.8	46.8	*****			
3	0.44	1.15	3200	71.9	49.9	32.9	*****			
4	0.48	1.04	3215	69.8	45.5	27.2	*****			
5	0.52	0.97	2933	66.3	41.7	22.9	*****			
6	0.55	0.91	2729	63.5	39.5	18.7	*****			
7	0.58	0.87	2784	63.0	37.5	18.8	*****			
8	0.60	0.83	2579	61.2	34.3	15.0	*****			
9	0.63	0.80	2400	57.3	30.5	12.0	*****			
10	0.65	0.77	2232	57.3	33.0	12.6	*****			
							I	I	I	
							0%	50%	100%	

Nr	Ex. Condition	Aver(I/sig(I)) .True.	.False.	Number .True.	of Refl. .False.	I/sigI Max.F	H	K	L	T/F. Ratio
1	HKL:H+K=2N	1.61	1.54	23474	23501	52.26	0	-3	1	1.0
2	HKL:H+L=2N	1.53	1.62	23512	23463	106.38	-1	1	0	0.9
3	HKL:K+L=2N	1.53	1.62	23523	23452	106.38	-1	1	0	0.9
4	HKL:H+K+L=2N	1.60	1.54	23488	23487	76.93	1	1	1	1.0
5	HKL:-H+K+L=3N	1.55	1.58	15649	31326	106.38	-1	1	0	1.0
6	HKL:H-K+L=3N	1.54	1.59	15673	31302	106.38	-1	1	0	1.0
41	HKL:H=2N	1.58	1.57	23464	23511	106.38	-1	1	0	1.0
42	HKL:K=2N	1.55	1.60	23457	23518	106.38	-1	1	0	1.0
43	HKL:L=2N	1.58	1.57	23491	23484	76.93	1	1	1	1.0
44	HKL:H=3N	1.56	1.58	15726	31249	106.38	-1	1	0	1.0
45	HKL:K=3N	1.53	1.59	15693	31282	106.38	-1	1	0	1.0
46	HKL:L=3N	1.57	1.58	15663	31312	78.69	1	1	2	1.0
47	-HKL, H-KL=3N	1.55	1.61	26101	20874	106.38	-1	1	0	1.0
48	-HKL:K2,KL4P2	1.56	1.74	44070	2905	73.36	0	2	0	0.9
49	-HKL:H2,H4P2	1.56	1.75	44073	2902	39.52	2	0	0	0.9
50	-HKL:H2,HK4P2	1.57	1.60	44194	2781	73.36	0	2	0	1.0
51	HKL:H+2L=3N	1.56	1.58	15665	31310	106.38	-1	1	0	1.0
:: No Extinction Conditions Found										

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

Nr	D	Rows			Products			Angle Between Two Direct Axes										
		N	Direct	Recip	Dot	Delta		1	2	3	4	5	6	7	8	9		
1	16.002	0	0	1	0	0	1	0	1	0.000	0.							

==== 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) Monoclinic
 (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	5.617	16.002	23.500	90.00	88.36	90.00	2111.39
Reduc Cell	P	5.617	16.002	23.500	90.00	91.64	90.00	2111.40
Conv. Cell	mP	5.617	16.002	23.500	90.00	91.64	90.00	2111.39

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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