

PLATON(V-311206)-Run for: kla0168t

TIME: Dec 13 17:17:45 2011

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Crystal Data

Input Cell (Lattice Type: P)		Temp = 0K	Reduced Cell		(Acta Cryst.(1976), A32, 297-298)
a =	14.89500 Angstrom	alpha = 90 Degree	a =	14.895	alpha = 90.00 V = 4623.7
b =	15.80000	beta = 96.1400	b =	15.800	beta = 96.14
c =	19.76000	gamma = 90	c =	19.760	gamma = 90.00
V = 4623.66 Cubic-Angstrom		d(100) = 14.8096 Angstrom	Niggli Values		
		d(010) = 15.8000	221.861	249.640	390.458
Lambda(MoKa) = 0.71073 Angstrom		d(001) = 19.6466	0.000	-31.480	0.000

Orthogonalization Matrices

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

(X0) (14.89500 0 -2.11349) (X) , (X) (0.06714 0 0.00722) (X0) Orthogonal Axes A0, B0 and C0
 (Y0) = (0 15.80000 0)*(Y) , (Y) = (0 0.06329 0)*(Y0) are defined as:
 (Z0) (0 0 19.64665) (Z) , (Z) (0 0 0.05090) (Z0) A0 // A, C0 // C*, B0 // C0 X A0

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SPGR - Determine SpaceGroup from Observed Extinctions for: kla0168t

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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	530	94.7	90.0	85.1	*****			
2	0.38	1.32	522	91.2	82.2	69.7	*****			
3	0.44	1.15	466	88.6	76.8	65.0	*****			
4	0.48	1.04	423	87.0	74.7	53.7	*****			
5	0.52	0.97	382	84.0	71.7	52.1	*****			
6	0.55	0.91	356	77.2	64.0	48.9	*****			
7	0.58	0.87	338	74.9	60.1	40.8	*****			
8	0.60	0.83	322	72.4	57.8	38.2	*****			
9	0.63	0.80	293	64.2	50.2	30.0	*****			
10	0.65	0.77	266	52.6	40.2	25.9	*****			
						I		I		I
						0%		50%		100%

Analysis of General Reflections for Bravais Centering

Nr	Ex. Condition	Aver(I/sig(I))		Number of Refl		I/sigI Max.F				.T/F. L Ratio
		.True.	.False.	.True.	.False.		H	K	L	
1	HKL:H+K=2N	5.04	4.75	2039	2038	110.74	0	3	3	1.1
2	HKL:H+L=2N	4.86	4.94	2049	2028	111.22	3	-1	2	1.0
3	HKL:K+L=2N	5.29	4.51	2025	2052	111.22	3	-1	2	1.2
4	HKL:H+K+L=2N	4.97	4.82	2050	2027	101.20	2	3	2	1.0
5	HKL:-H+K+L=3N	4.96	4.87	1361	2716	111.22	3	-1	2	1.0
6	HKL:H-K+L=3N	4.84	4.93	1353	2724	101.20	2	3	2	1.0
41	HKL:H=2N	4.93	4.86	2050	2027	111.22	3	-1	2	1.0
42	HKL:K=2N	4.76	5.04	2044	2033	111.22	3	-1	2	0.9
43	HKL:L=2N	4.96	4.84	2030	2047	110.74	0	3	3	1.0
44	HKL:H=3N	5.07	4.81	1364	2713	101.20	2	3	2	1.1
45	HKL:K=3N	4.82	4.94	1348	2729	111.22	3	-1	2	1.0
46	HKL:L=3N	4.88	4.91	1349	2728	111.22	3	-1	2	1.0
47	-HKL, H-KL=3N	4.82	5.00	2267	1810	99.20	4	-2	1	1.0
48	-HKL:K2,KL4P2	4.93	4.62	3625	452	53.76	2	0	2	1.1
49	-HKL:H2,HL4P2	4.91	4.83	3557	520	87.55	0	2	2	1.0
50	-HKL:H2,HK4P2	4.87	5.10	3574	503	99.20	4	-2	1	1.0
51	HKL:H+2L=3N	4.98	4.86	1359	2718	111.22	3	-1	2	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	15.800	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	14.895	15.800	19.760	90.00	96.14	90.00	4623.66
Reduc Cell	P	14.895	15.800	19.760	90.00	96.14	90.00	4623.66
Conv. Cell	mP	14.895	15.800	19.760	90.00	96.14	90.00	4623.66

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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