

PLATON(V-311206)-Run for: kla0143a

TIME: Oct 20 10:12:39 2011

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Crystal Data

Input Cell (Lattice Type: P)		Temp = 0K	Reduced Cell		(Acta Cryst.(1976), A32, 297-298)
a =	13.45100 Angstrom	alpha = 90 Degree	a =	13.451	alpha = 90.00 V = 8394.0
b =	26.23300	beta = 103.2900	b =	24.443	beta = 90.00
c =	24.44300	gamma = 90	c =	26.233	gamma = 103.29
V = 8393.97 Cubic-Angstrom		d(100) = 13.0908 Angstrom	Niggli Values		
		d(010) = 26.2330	180.929	597.460	688.170
Lambda(MoKa) = 0.71073 Angstrom		d(001) = 23.7884	0.000	0.000	-75.580

Orthogonalization Matrices

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

(X0) (13.45100 0 -5.61895) (X) , (X) (0.07434 0 0.01756) (X0) Orthogonal Axes A0, B0 and C0
 (Y0) = (0 26.23300 0)*(Y) , (Y) = (0 0.03812 0)*(Y0) are defined as:
 (Z0) (0 0 23.78839) (Z) , (Z) (0 0 0.04204) (Z0) A0 // A, C0 // C*, B0 // C0 X A0

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SPGR - Determine SpaceGroup from Observed Extinctions for: kla0143a

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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	11287	91.6	84.7	76.1	*****			
2	0.38	1.32	11057	88.5	77.4	63.4	*****			
3	0.44	1.15	9952	86.3	72.7	53.6	*****			
4	0.48	1.04	8941	83.4	68.3	45.6	*****			
5	0.52	0.97	8286	76.2	58.3	33.7	*****			
6	0.55	0.91	7651	73.8	56.7	33.3	*****			
7	0.58	0.87	7130	71.3	54.2	32.3	*****			
8	0.60	0.83	6776	68.2	49.4	27.6	*****			
9	0.63	0.80	6351	63.5	44.1	22.4	*****			
10	0.65	0.77	6175	60.8	39.4	18.1	*****			
						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	2.74	2.72	44048	44047	56.17	-1	6	-4	1.0
2	HKL:H+L=2N	2.73	2.73	44045	44050	68.57	3	-1	-2	1.0
3	HKL:K+L=2N	2.75	2.72	43988	44107	68.57	3	-1	-2	1.0
4	HKL:H+K+L=2N	2.71	2.75	44054	44041	71.46	-3	-1	1	1.0
5	HKL:-H+K+L=3N	2.74	2.73	29360	58735	70.24	-3	1	1	1.0
6	HKL:H-K+L=3N	2.70	2.75	29373	58722	81.54	-2	0	-2	1.0
41	HKL:H=2N	2.73	2.73	43965	44130	71.46	-3	-1	1	1.0
42	HKL:K=2N	2.67	2.80	44032	44063	71.46	-3	-1	1	1.0
43	HKL:L=2N	2.74	2.73	44041	44054	71.46	-3	-1	1	1.0
44	HKL:H=3N	2.73	2.74	29203	58892	81.54	-2	0	-2	1.0
45	HKL:K=3N	2.70	2.75	29381	58714	71.46	-3	-1	1	1.0
46	HKL:L=3N	2.71	2.75	29338	58757	81.54	-2	0	-2	1.0
47	- HKL, H-KL=3N	2.73	2.74	48965	39130	60.12	0	-4	0	1.0
48	- HKL:K2,KL4P2	2.73	2.73	82429	5666	68.05	2	0	2	1.0
49	- HKL:H2,H4P2	2.73	2.73	81134	6961	47.54	-2	-1	4	1.0
50	- HKL:H2,HK4P2	2.74	2.60	83024	5071	68.05	2	0	2	1.1
51	HKL:H+2L=3N	2.76	2.72	29370	58725	71.46	-3	-1	1	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	26.233	0	0	0	1	0	0	1	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	13.451	26.233	24.443	90.00	103.29	90.00	8393.97
Reduc Cell	P	13.451	24.443	26.233	90.00	90.00	103.29	8393.96
Conv. Cell	mP	13.451	26.233	24.443	90.00	103.29	90.00	8393.97

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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