

PLATON(V-311206)-Run for: kla0139

TIME: Oct 15 12:42:37 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 =	101.1400 Degree	a =	13.451	alpha =	101.14 V = 4060.2
b =	14.13400		beta =	97.0600	b =	14.134	beta =	97.06
c =	22.00500		gamma =	93.1600	c =	22.005	gamma =	93.16
V =	4060.18	Cubic-Angstrom	d(100) =	13.3052 Angstrom	Niggli Values			
			d(010) =	13.8221	180.929	199.770	484.220	
Lambda(MoKa) =	0.71073	Angstrom	d(001) =	21.3888	-60.091	-36.380	-10.480	

Orthogonalization Matrices

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

(X0) (13.45100 -0.77913 -2.70460) (X) , (X) (0.07434 0.00410 0.01025) (X0) Orthogonal Axes A0, B0 and C0
 (Y0) = (0 14.11251 -4.40731)*(Y) , (Y) = (0 0.07086 0.01460)*(Y0) are defined as:
 (Z0) (0 0 21.38880) (Z) , (Z) (0 0 0.04675) (Z0) A0 // A, C0 // C*, B0 // C0 X A0

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SPGR - Determine SpaceGroup from Observed Extinctions for: kla0139

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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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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	7001	93.7	86.4	76.8	*****			
2	0.38	1.32	6775	88.0	74.3	56.9	*****			
3	0.44	1.15	6097	86.5	71.2	50.8	*****			
4	0.48	1.04	5522	83.3	67.5	45.1	*****			
5	0.52	0.97	5070	79.3	61.9	35.9	*****			
6	0.55	0.91	4717	70.9	52.2	25.7	*****			
7	0.58	0.87	4418	65.7	46.0	22.8	*****			
8	0.60	0.83	4123	64.7	44.2	22.0	*****			
9	0.63	0.80	3949	61.6	40.2	19.8	*****			
10	0.65	0.77	3739	59.6	38.0	17.0	*****			
						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	
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1	HKL:H+K=2N	2.70	2.70	27097	27079	70.28	2	3	-7	1.0
2	HKL:H+L=2N	2.67	2.72	27092	27084	70.28	2	3	-7	1.0
3	HKL:K+L=2N	2.72	2.68	27069	27107	69.79	-1	-3	2	1.0
4	HKL:H+K+L=2N	2.73	2.66	27124	27052	66.78	-2	-2	3	1.0
5	HKL:-H+K+L=3N	2.68	2.71	18069	36107	79.91	2	2	-2	1.0
6	HKL:H-K+L=3N	2.66	2.72	18022	36154	79.91	2	2	-2	1.0
41	HKL:H=2N	2.70	2.70	27079	27097	69.79	-1	-3	2	1.0
42	HKL:K=2N	2.67	2.72	27134	27042	70.28	2	3	-7	1.0
43	HKL:L=2N	2.69	2.71	27105	27071	70.28	2	3	-7	1.0
44	HKL:H=3N	2.66	2.72	18034	36142	79.91	2	2	-2	1.0
45	HKL:K=3N	2.67	2.71	18053	36123	79.91	2	2	-2	1.0
46	HKL:L=3N	2.70	2.70	18065	36111	79.91	2	2	-2	1.0
47	-HKL, H-KL=3N	2.68	2.72	30089	24087	79.91	2	2	-2	1.0
48	-HKL:K2,KL4P2	2.70	2.69	50566	3610	55.05	0	2	0	1.0
49	-HKL:H2,HL4P2	2.70	2.69	50481	3695	47.44	-4	0	6	1.0
50	-HKL:H2,HK4P2	2.70	2.63	50930	3246	60.35	-2	4	-3	1.0
51	HKL:H+2L=3N	2.71	2.69	18062	36114	79.91	2	2	-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	13.451	14.134	22.005	101.14	97.06	93.16	4060.18
Reduc Cell	P	13.451	14.134	22.005	101.14	97.06	93.16	4060.18
Conv. Cell	aP	13.451	14.134	22.005	101.14	97.06	93.16	4060.18

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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