

PLATON(V-311206)-Run for: kla0138

TIME: Oct 10 10:33:49 2011

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Crystal Data

Input Cell (Lattice Type: P)		Temp = 0K	Reduced Cell		(Acta Cryst.(1976), A32, 297-298)
a =	16.94000 Angstrom	alpha = 90 Degree	a =	13.156	alpha = 97.76 V = 3830.6
b =	13.15600	beta = 97.7600	b =	16.940	beta = 90.00
c =	17.34700	gamma = 90	c =	17.347	gamma = 90.00
V = 3830.59 Cubic-Angstrom		d(100) = 16.7849 Angstrom	Niggli Values		
		d(010) = 13.1560	173.080	286.964	300.918
Lambda(MoKa) = 0.71073 Angstrom		d(001) = 17.1881	-39.678	0.000	0.000

Orthogonalization Matrices

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

(X0) (16.94000 0 -2.34226) (X) , (X) (0.05903 0 0.00804) (X0) Orthogonal Axes A0, B0 and C0
 (Y0) = (0 13.15600 0)*(Y) , (Y) = (0 0.07601 0)*(Y0) are defined as:
 (Z0) (0 0 17.18814) (Z) , (Z) (0 0 0.05818) (Z0) A0 // A, C0 // C*, B0 // C0 X A0

SPGR - Determine SpaceGroup from Observed Extinctions for: k1a0138

:: 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

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	2156	99.0	97.4	95.1	*****	..		
2	0.38	1.32	2163	98.9	96.9	92.6	*****	...		
3	0.44	1.15	2283	98.6	94.7	86.2	*****			
4	0.48	1.04	2218	97.1	92.9	84.3	*****			
5	0.52	0.97	2273	96.7	91.9	81.9	*****			
6	0.55	0.91	2190	93.6	86.7	74.7	*****			
7	0.58	0.87	2040	92.8	84.7	73.6	*****			
8	0.60	0.83	2043	88.4	78.6	68.0	*****			
9	0.63	0.80	2081	83.7	68.9	54.6	*****			
10	0.65	0.77	2136	77.3	59.9	41.6	*****			
						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. Ratio
		.True.	.False.	.True.	.False.		H	K	L	
=====										
1	HKL:H+K=2N	4.51	4.72	11644	11768	17.94	2	-3	0	1.0
2	HKL:H+L=2N	4.46	4.78	11943	11469	17.88	1	-4	2	0.9
3	HKL:K+L=2N	4.59	4.65	11723	11689	17.94	2	-3	0	1.0
4	HKL:H+K+L=2N	4.56	4.67	11655	11757	17.94	2	-3	0	1.0
5	HKL:-H+K+L=3N	4.61	4.63	7784	15628	17.94	2	-3	0	1.0
6	HKL:H-K+L=3N	4.59	4.63	7752	15660	17.94	2	-3	0	1.0
41	HKL:H=2N	4.64	4.60	11948	11464	17.88	1	-4	2	1.0
42	HKL:K=2N	4.68	4.55	12196	11216	17.94	2	-3	0	1.0
43	HKL:L=2N	4.67	4.57	11731	11681	17.44	-3	3	-7	1.0
44	HKL:H=3N	4.59	4.64	7807	15605	17.94	2	-3	0	1.0
45	HKL:K=3N	4.86	4.48	8470	14942	17.88	1	-4	2	1.1
46	HKL:L=3N	4.65	4.60	7819	15593	17.88	1	-4	2	1.0
47	-HKL, H-KL=3N	4.60	4.64	12967	10445	17.94	2	-3	0	1.0
48	-HKL:K2,KL4P2	4.62	4.65	21876	1536	17.55	0	4	-2	1.0
49	-HKL:H2,HL4P2	4.62	4.57	21636	1776	17.94	2	-3	0	1.0
50	-HKL:H2,HK4P2	4.62	4.64	21671	1741	16.72	2	0	-2	1.0
51	HKL:H+2L=3N	4.57	4.65	7751	15661	17.94	2	-3	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	13.156	0	1	0	0	1	0	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	16.940	13.156	17.347	90.00	97.76	90.00	3830.59
Reduc Cell	P	13.156	16.940	17.347	97.76	90.00	90.00	3830.59
Conv. Cell	mP	16.940	13.156	17.347	90.00	97.76	90.00	3830.59

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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