

PLATON(V-311206)-Run for: kla0159

TIME: Nov 25 19:03:04 2011

(C) 1980-2007 A.L.Spek

Crystal Data

Input Cell (Lattice Type: P)		Temp = 0K	Reduced Cell		(Acta Cryst.(1976), A32, 297-298)
a =	13.70300 Angstrom	alpha = 90 Degree	a =	13.703	alpha = 90.00 V = 5094.9
b =	19.26900	beta = 99.0300	b =	19.269	beta = 99.03
c =	19.53800	gamma = 90	c =	19.538	gamma = 90.00
V = 5094.94 Cubic-Angstrom		d(100) = 13.5332 Angstrom	Niggli Values		
		d(010) = 19.2690	187.772	371.294	381.733
Lambda(MoKa) = 0.71073 Angstrom		d(001) = 19.2959	0.000	-42.021	0.000

Orthogonalization Matrices

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

(X0) (13.70300 0 -3.06652) (X) , (X) (0.07298 0 0.01160) (X0) Orthogonal Axes A0, B0 and C0
 (Y0) = (0 19.26900 0)*(Y) , (Y) = (0 0.05190 0)*(Y0) are defined as:
 (Z0) (0 0 19.29585) (Z) , (Z) (0 0 0.05182) (Z0) A0 // A, C0 // C*, B0 // C0 X A0

=====

SPGR - Determine SpaceGroup from Observed Extinctions for: kla0159

=====

:: 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

:: 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

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	9007	90.3	82.3	71.5	*****			
2	0.38	1.32	8790	88.7	77.8	62.2	*****			
3	0.44	1.15	7836	85.3	72.5	54.5	*****			
4	0.48	1.04	7204	79.9	64.5	43.8	*****			
5	0.52	0.97	6515	78.1	62.6	41.8	*****			
6	0.55	0.91	6011	76.3	60.1	40.7	*****			
7	0.58	0.87	5858	72.7	55.2	35.6	*****			
8	0.60	0.83	5462	67.9	49.3	29.1	*****			
9	0.63	0.80	5030	65.5	45.5	24.9	*****			
10	0.65	0.77	4799	63.0	41.1	19.1	*****			
						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. Ratio
		.True.	.False.	.True.	.False.		H	K	L	
1	HKL:H+K=2N	2.70	2.79	35120	35132	95.66	-1	-4	1	1.0
2	HKL:H+L=2N	2.84	2.65	35140	35112	64.96	-2	-3	1	1.1
3	HKL:K+L=2N	2.73	2.76	35152	35100	95.66	-1	-4	1	1.0
4	HKL:H+K+L=2N	2.79	2.70	35175	35077	67.68	0	7	-2	1.0
5	HKL:-H+K+L=3N	2.81	2.71	23404	46848	95.66	-1	-4	1	1.0
6	HKL:H-K+L=3N	2.76	2.73	23361	46891	95.66	-1	-4	1	1.0
41	HKL:H=2N	2.73	2.76	35159	35093	95.66	-1	-4	1	1.0
42	HKL:K=2N	2.73	2.76	35149	35103	67.68	0	7	-2	1.0
43	HKL:L=2N	2.73	2.76	35117	35135	95.66	-1	-4	1	1.0
44	HKL:H=3N	2.69	2.77	23388	46864	95.66	-1	-4	1	1.0
45	HKL:K=3N	2.60	2.81	23435	46817	95.66	-1	-4	1	0.9
46	HKL:L=3N	2.71	2.76	23394	46858	95.66	-1	-4	1	1.0
47	-HKL, H-KL=3N	2.79	2.69	38998	31254	95.66	-1	-4	1	1.0
48	-HKL:K2,KL4P2	2.74	2.72	65742	4510	47.65	-2	0	2	1.0
49	-HKL:H2,HL4P2	2.73	2.89	65642	4610	67.05	0	7	2	0.9
50	-HKL:H2,HK4P2	2.75	2.62	65674	4578	45.53	0	6	0	1.1
51	HKL:H+2L=3N	2.70	2.76	23408	46844	95.66	-1	-4	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	19.269	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	13.703	19.269	19.538	90.00	99.03	90.00	5094.94
Reduc Cell	P	13.703	19.269	19.538	90.00	99.03	90.00	5094.93
Conv. Cell	mP	13.703	19.269	19.538	90.00	99.03	90.00	5094.94

=====

***** N O T I C E *****

=====

- 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