PLATON(V-311206)-Run for: kla0167t TIME: Dec 13 13:28:28 2011

Crystal Data

Input Cell (Lattice Type: P) - Temp = 0K

a =	11.22400	Angstrom	alpha =	69.6100	Degree	a =	11.224	alpha =	69.61	V =	1875.5
b =	12.65900		beta =	85.6700		b =	12.659	beta =	85.67		
c =	15.68700		gamma =	64.3300		c =	15.687	gamma =	64.33		
V =	1875.51	Cubic-Angstrom	d(100) =	10.0758	Angstrom						
			d(010) =	10.6825							
Lambda(MoKa) =	0.71073	Angstrom	d(001) =	14.6454							

Reduced Cell (Acta Cryst.(1976),A32,297-298)

Niggli Values: 125.978 160.250 246.082 / 69.188 13.293 61.549

Orthogonalization Matrices

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

$$\begin{pmatrix} XO \\ YO \\ ZO \end{pmatrix} = \begin{pmatrix} 11.22400 & 5.48372 & 1.18438 \\ 0 & 11.40961 & 5.49473 \\ 0 & 0 & 14.64538 \end{pmatrix} \begin{pmatrix} X \\ Y \\ Z \end{pmatrix} , \quad \begin{pmatrix} X \\ Y \\ Z \end{pmatrix} = \begin{pmatrix} 0.08909 & -0.04282 & 0.00886 \\ 0 & 0.08765 & -0.03288 \\ 0 & 0 & 0.06828 \end{pmatrix} \begin{pmatrix} XO \\ YO \\ ZO \end{pmatrix}$$

Orthogonal Axes AO, BO and CO are defined as:
AO // A, CO // C*, BO // CO X AO

SPGR - Determine SpaceGroup from Observed Extinctions for: kla0167t

:: 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	725	96.3	92.3	86.1	**********.....
2	0.38	1.32	685	93.1	85.0	74.3	**********.....
3	0.44	1.15	619	87.7	74.8	60.1	**********.....
4	0.48	1.04	564	84.2	67.6	50.0	**********.....
5	0.52	0.97	520	81.2	62.5	39.4	**********.....
6	0.55	0.91	463	77.8	56.4	34.8	**********.....
7	0.58	0.87	468	72.9	50.6	26.9	**********.....
8	0.60	0.83	432	65.7	44.7	21.3	**********.....
9	0.63	0.80	404	61.9	35.6	13.6	**********.....
10	0.65	0.77	391	58.6	32.7	11.0	**********.....

I I I
0% 50% 100%

Analysis of General Reflections for Bravais Centering

Nr	Ex. Condition	Aver(I/sig(I)) .True.	Aver(I/sig(I)) .False.	Number of Refl .True.	Number of Refl .False.	I/sigI Max.F	H	K	L	.T/F. Ratio
1	HKL:H+K=2N	3.36	3.46	2780	2773	118.24	-1	-2	-3	1.0
2	HKL:H+L=2N	3.39	3.43	2773	2780	79.95	-1	-2	-2	1.0
3	HKL:K+L=2N	3.52	3.29	2768	2785	118.24	-1	-2	-3	1.1
4	HKL:H+K+L=2N	3.40	3.42	2781	2772	100.35	1	-1	-1	1.0
5	HKL:-H+K+L=3N	3.52	3.35	1861	3692	118.24	-1	-2	-3	1.0
6	HKL:H-K+L=3N	3.32	3.45	1855	3698	118.24	-1	-2	-3	1.0
41	HKL:H=2N	3.41	3.41	2784	2769	118.24	-1	-2	-3	1.0
42	HKL:K=2N	3.42	3.40	2781	2772	100.35	1	-1	-1	1.0
43	HKL:L=2N	3.32	3.50	2784	2769	118.24	-1	-2	-3	0.9
44	HKL:H=3N	3.23	3.50	1862	3691	118.24	-1	-2	-3	0.9
45	HKL:K=3N	3.30	3.46	1853	3700	118.24	-1	-2	-3	1.0
46	HKL:L=3N	3.46	3.38	1828	3725	100.35	1	-1	-1	1.0
47	-HKL, H-KL=3N	3.42	3.39	3100	2453	118.24	-1	-2	-3	1.0
48	-HKL:K2,KL4P2	3.39	3.75	5302	251	69.24	1	2	0	0.9
49	-HKL:H2,HL4P2	3.36	5.04	5399	154	65.93	2	2	0	0.7
50	-HKL:H2,HK4P2	3.44	3.03	5108	445	44.46	6	4	0	1.1
51	HKL:H+2L=3N	3.35	3.44	1853	3700	118.24	-1	-2	-3	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
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	Latt	a	b	c	Alpha	Beta	Gamma	Volume
Input Cell	P	11.224	12.659	15.687	69.61	85.67	64.33	1875.51
Reduc Cell	P	11.224	12.659	15.687	69.61	85.67	64.33	1875.51
Conv. Cell	aP	11.224	12.659	15.687	69.61	85.67	64.33	1875.51

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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