PLATON(V-311206)-Run for: kla0132 TIME: Sep 18 11:32:21 2011

Crystal Data

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

a =	9.15000	Angstrom	alpha =	66.9600	Degree	a =	9.150	alpha =	66.96	V =	1282.5
b =	11.35100		beta =	80.9900		b =	11.351	beta =	80.99		
c =	13.59900		gamma =	84.2600		c =	13.599	gamma =	84.26		
V =	1282.55	Cubic-Angstrom	d(100) =	9.0289	Angstrom						
			d(010) =	10.4361							
Lambda(MoKa) =	0.71073	Angstrom	d(001) =	12.4108							

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

Niggli Values: 83.722 128.845 184.933 / 60.414 19.486 10.387

Orthogonalization Matrices

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

$$\begin{pmatrix} XO \\ YO \\ ZO \end{pmatrix} = \begin{pmatrix} 9.15000 & 1.13526 & 2.12970 \\ 0 & 11.29409 & 5.13504 \\ 0 & 0 & 12.41083 \end{pmatrix} \begin{pmatrix} X \\ Y \\ Z \end{pmatrix}, \quad \begin{pmatrix} X \\ Y \\ Z \end{pmatrix} = \begin{pmatrix} 0.10929 & -0.01099 & -0.01421 \\ 0 & 0.08854 & -0.03663 \\ 0 & 0 & 0.08057 \end{pmatrix} \begin{pmatrix} XO \\ YO \\ ZO \end{pmatrix}$$

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

```
SPGR - Determine SpaceGroup from Observed Extinctions for: kla0132
==========================================================================
:: 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  2104  99.5  98.3  94.7  ************************************..
 2 0.38 1.32  2032  98.5  96.5  89.8  **********************************....
 3 0.44 1.15  1791  97.2  92.8  83.1  ********************************.......
 4 0.48 1.04  1737  95.9  89.0  74.3  ******************************..........
 5 0.52 0.97  1526  93.1  83.3  65.8  ************************..............
 6 0.55 0.91  1413  89.4  82.0  63.1  ************************..............
 7 0.58 0.87  1353  87.3  76.1  58.6  ***********************.................
 8 0.60 0.83  1229  88.5  78.3  58.5  ***********************.................
 9 0.63 0.80  1201  83.3  73.5  54.5  **********************..................
10 0.65 0.77  1086  81.9  68.0  48.5  ******************.....................
                                    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	5.41	5.29	8149	8169	40.91	2	1	1	1.0
2	HKL:H+L=2N	5.42	5.28	8167	8151	40.91	2	1	1	1.0
3	HKL:K+L=2N	5.53	5.17	8150	8168	40.24	-1	-3	0	1.1
4	HKL:H+K+L=2N	5.38	5.32	8152	8166	40.04	1	1	1	1.0
5	HKL:-H+K+L=3N	5.38	5.34	5447	10871	40.24	-1	-3	0	1.0
6	HKL:H-K+L=3N	5.30	5.37	5462	10856	41.03	2	0	2	1.0
41	HKL:H=2N	5.34	5.36	8126	8192	40.24	-1	-3	0	1.0
42	HKL:K=2N	5.34	5.36	8175	8143	40.91	2	1	1	1.0
43	HKL:L=2N	5.30	5.40	8147	8171	40.91	2	1	1	1.0
44	HKL:H=3N	5.45	5.30	5375	10943	41.03	2	0	2	1.0
45	HKL:K=3N	5.39	5.33	5371	10947	40.91	2	1	1	1.0
46	HKL:L=3N	5.29	5.38	5401	10917	41.03	2	0	2	1.0
47	-HKL, H-KL=3N	5.36	5.34	9102	7216	40.24	-1	-3	0	1.0
48	-HKL:K2,KL4P2	5.32	5.72	15184	1134	41.03	2	0	2	0.9
49	-HKL:H2,HL4P2	5.34	5.47	15336	982	38.44	2	0	0	1.0
50	-HKL:H2,HK4P2	5.36	5.24	15272	1046	41.03	2	0	2	1.0
51	HKL:H+2L=3N	5.38	5.34	5429	10889	40.91	2	1	1	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	9.150	11.351	13.599	66.96	80.99	84.26	1282.55
Reduc Cell	P	9.150	11.351	13.599	66.96	80.99	84.26	1282.54
Conv. Cell	aP	9.150	11.351	13.599	66.96	80.99	84.26	1282.55

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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