PLATON(V-311206)-Run for: klat855a TIME: Nov 29 22:07:35 2011

Crystal Data

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

a =	9.73600	Angstrom	alpha =	76.2300	Degree	a =	9.736	alpha =	103.77	V =	3332.0
b =	14.37100		beta =	90		b =	14.371	beta =	90.00		
c =	24.51900		gamma =	90		c =	24.519	gamma =	90.00		
V =	3332.00	Cubic-Angstrom	d(100) =	9.7360	Angstrom						
			d(010) =	13.9580							
Lambda(MoKa) =	0.71073	Angstrom	d(001) =	23.8143							

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

Niggli Values

94.790	206.526	601.181
-83.871	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)

$$\begin{pmatrix} XO \\ YO \\ ZO \end{pmatrix} = \begin{pmatrix} 9.73600 & 0 & 0 \\ 0 & 14.37100 & 5.83613 \\ 0 & 0 & 23.81430 \end{pmatrix} \begin{pmatrix} X \\ Y \\ Z \end{pmatrix}, \quad \begin{pmatrix} X \\ Y \\ Z \end{pmatrix} = \begin{pmatrix} 0.10271 & 0 & 0 \\ 0 & 0.06958 & -0.01705 \\ 0 & 0 & 0.04199 \end{pmatrix} \begin{pmatrix} XO \\ YO \\ ZO \end{pmatrix}$$

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

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SPGR - Determine SpaceGroup from Observed Extinctions for: klat855a
================================================================================
:: 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  4348  90.8  84.8  78.1  ******************************.........
 2 0.38 1.32  4282  88.2  77.9  64.2  ************************..............
 3 0.44 1.15  3854  84.1  72.6  55.3  ********************..................
 4 0.48 1.04  3458  82.8  67.6  45.1  ******************......................
 5 0.52 0.97  3092  75.7  55.5  33.2  *************..........................
 6 0.55 0.91  3023  69.3  47.5  23.8  **********.............................
 7 0.58 0.87  2722  65.0  40.4  14.8  ******.................................
 8 0.60 0.83  2658  62.2  37.8  13.7  *****..................................
 9 0.63 0.80  2424  57.1  33.0   9.7  ****...................................
10 0.65 0.77  2384  56.6  29.7   6.9  ***....................................
                                    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	2.34	2.33	17063	16963	14.84	-2	-1	4	1.0
2	HKL:H+L=2N	2.34	2.33	17037	16989	14.74	-1	1	6	1.0
3	HKL:K+L=2N	2.45	2.22	17050	16976	14.84	-2	-1	4	1.1
4	HKL:H+K+L=2N	2.37	2.31	16994	17032	15.00	-1	1	-1	1.0
5	HKL:-H+K+L=3N	2.31	2.35	11355	22671	15.00	-1	1	-1	1.0
6	HKL:H-K+L=3N	2.32	2.35	11338	22688	14.74	-1	1	6	1.0
41	HKL:H=2N	2.28	2.39	17030	16996	15.00	-1	1	-1	1.0
42	HKL:K=2N	2.32	2.35	17037	16989	15.00	-1	1	-1	1.0
43	HKL:L=2N	2.32	2.36	17003	17023	15.00	-1	1	-1	1.0
44	HKL:H=3N	2.20	2.40	11347	22679	15.00	-1	1	-1	0.9
45	HKL:K=3N	2.33	2.34	11368	22658	15.00	-1	1	-1	1.0
46	HKL:L=3N	2.35	2.33	11369	22657	15.00	-1	1	-1	1.0
47	-HKL, H-KL=3N	2.32	2.36	18901	15125	14.74	-1	1	6	1.0
48	-HKL:K2,KL4P2	2.34	2.37	32060	1966	14.45	-1	2	0	1.0
49	-HKL:H2,HL4P2	2.34	2.28	32331	1695	14.84	-2	-1	4	1.0
50	-HKL:H2,HK4P2	2.32	2.59	32224	1802	13.90	0	6	4	0.9
51	HKL:H+2L=3N	2.35	2.33	11337	22689	14.74	-1	1	6	1.0

:: No Extinction Conditions Found

Possible 2-Fold Axes - 2-Axis Crit = 0.20, Exp. Error = 0.20 Deg., LATT = P

Nr	D	N	Rows Direct	Rows Recip	Products Dot	Products Delta	Angle Between Two Direct Axes 1	2	3	4	5	6	7	8	9
1	9.736	0	1 0 0	1 0 0	1	0.000	0.								

==== Transformation Matrix: Input (a,b,c) to Conventional Cell(a', b', c') ====

```
(a')   ( 0.000 1.000 0.000) (a)   (x')   ( 0.000 1.000 0.000) (x)  Metrically
(b') = ( 1.000 0.000 0.000) (b).  (y') = ( 1.000 0.000 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	9.736	14.371	24.519	76.23	90.00	90.00	3332.00
Reduc Cell	P	9.736	14.371	24.519	103.77	90.00	90.00	3332.01
Conv. Cell	mP	14.371	9.736	24.519	90.00	103.77	90.00	3332.00

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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