PLATON(V-311206)-Run for: kla0156 TIME: Nov 20 11:35:57 2011

Crystal Data

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

a =	13.79300	Angstrom	alpha =	90	Degree	a =	9.989	alpha =	98.90	V =	1933.2
b =	9.98900		beta =	98.9000		b =	13.793	beta =	90.00		
c =	14.20200		gamma =	90		c =	14.202	gamma =	90.00		
V =	1933.17	Cubic-Angstrom	d(100) =	13.6269	Angstrom						
			d(010) =	9.9890							
Lambda(MoKa) =	0.71073	Angstrom	d(001) =	14.0310							

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

Niggli Values		
99.780	190.247	201.697
-30.306	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)

$$\begin{pmatrix} XO \\ YO \\ ZO \end{pmatrix} = \begin{pmatrix} 13.79300 & 0 & -2.19720 \\ 0 & 9.98900 & 0 \\ 0 & 0 & 14.03101 \end{pmatrix} \begin{pmatrix} X \\ Y \\ Z \end{pmatrix} , \quad \begin{pmatrix} X \\ Y \\ Z \end{pmatrix} = \begin{pmatrix} 0.07250 & 0 & 0.01135 \\ 0 & 0.10011 & 0 \\ 0 & 0 & 0.07127 \end{pmatrix} \begin{pmatrix} XO \\ YO \\ ZO \end{pmatrix}$$

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: kla0156
================================================================================
:: 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  2916  90.8  84.8  78.6  ******************************.........
 2 0.38 1.32  2847  89.0  80.0  68.6  *************************.............
 3 0.44 1.15  2520  88.4  78.0  63.8  *************************.............
 4 0.48 1.04  2315  87.3  76.7  61.9  *************************.............
 5 0.52 0.97  2124  84.0  71.2  52.5  ********************..................
 6 0.55 0.91  1903  79.7  63.9  42.1  ****************.......................
 7 0.58 0.87  1830  78.3  63.1  44.6  ******************.....................
 8 0.60 0.83  1695  74.2  55.8  37.0  ***************........................
 9 0.63 0.80  1670  69.1  51.1  33.3  *************..........................
10 0.65 0.77  1489  70.8  54.9  36.7  ***************........................
                                    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	4.10	4.08	11284	11239	38.03	0	1	3	1.0
2	HKL:H+L=2N	4.20	3.98	11265	11258	38.03	0	1	3	1.1
3	HKL:K+L=2N	4.08	4.10	11274	11249	36.68	1	-1	4	1.0
4	HKL:H+K+L=2N	4.42	3.76	11257	11266	36.75	1	2	-2	1.2
5	HKL:-H+K+L=3N	3.98	4.14	7504	15019	38.03	0	1	3	1.0
6	HKL:H-K+L=3N	4.14	4.06	7485	15038	38.03	0	1	3	1.0
41	HKL:H=2N	4.09	4.09	11254	11269	36.75	1	2	-2	1.0
42	HKL:K=2N	3.96	4.22	11213	11310	38.03	0	1	3	0.9
43	HKL:L=2N	4.13	4.05	11282	11241	38.03	0	1	3	1.0
44	HKL:H=3N	4.11	4.08	7504	15019	36.75	1	2	-2	1.0
45	HKL:K=3N	3.78	4.25	7602	14921	38.03	0	1	3	0.9
46	HKL:L=3N	3.96	4.16	7538	14985	36.75	1	2	-2	1.0
47	-HKL, H-KL=3N	4.10	4.08	12475	10048	38.03	0	1	3	1.0
48	-HKL:K2,KL4P2	4.10	3.95	20961	1562	36.48	-1	2	0	1.0
49	-HKL:H2,HL4P2	4.06	4.42	20785	1738	35.19	0	0	2	0.9
50	-HKL:H2,HK4P2	4.11	3.79	20862	1661	34.79	2	0	2	1.1
51	HKL:H+2L=3N	4.08	4.09	7497	15026	36.73	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

			Rows			Products		Angle Between Two Direct Axes							
Nr	D	N	Direct			Recip Dot	Delta	1	2	3	4	5	6	7	8	9
1	9.989	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	13.793	9.989	14.202	90.00	98.90	90.00	1933.17
Reduc Cell	P	9.989	13.793	14.202	98.90	90.00	90.00	1933.17
Conv. Cell	mP	13.793	9.989	14.202	90.00	98.90	90.00	1933.17

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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