PLATON(V-311206)-Run for: kla0131a TIME: Sep 17 11:26:35 2011

Crystal Data

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

a =	17.90400	Angstrom	alpha =	78.0800	Degree	a =	17.904	alpha =	78.08	V =	6747.1
b =	17.93700		beta =	77.9900		b =	17.937	beta =	77.99		
c =	22.91100		gamma =	71.5300		c =	22.911	gamma =	71.53		
V =	6747.10	Cubic-Angstrom	d(100) =	16.7800	Angstrom	Niggli Values					
			d(010) =	16.8165		320.553	321.736	524.914			
Lambda(MoKa) =	0.71073	Angstrom	d(001) =	22.1506		84.881	85.355	101.741			

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

Orthogonalization Matrices

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

$$\begin{pmatrix} XO \\ YO \\ ZO \end{pmatrix} = \begin{pmatrix} 17.90400 & 5.68259 & 4.76738 \\ 0 & 17.01306 & 3.39680 \\ 0 & 0 & 22.15057 \end{pmatrix} \begin{pmatrix} X \\ Y \\ Z \end{pmatrix} , \quad \begin{pmatrix} X \\ Y \\ Z \end{pmatrix} = \begin{pmatrix} 0.05585 & -0.01866 & -0.00916 \\ 0 & 0.05878 & -0.00901 \\ 0 & 0 & 0.04515 \end{pmatrix} \begin{pmatrix} XO \\ YO \\ ZO \end{pmatrix}$$

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: kla0131a
================================================================================
:: 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 10954  91.0  80.0  62.8  ************************.............
 2 0.38 1.32 10481  84.7  71.8  48.1  ******************.....................
 3 0.44 1.15  9319  76.5  59.6  34.5  **************.........................
 4 0.48 1.04  8387  69.5  50.5  28.3  ***********.............................
 5 0.52 0.97  7779  65.1  44.2  23.2  *********...............................
 6 0.55 0.91  7086  60.1  37.8  16.9  *******.................................
 7 0.58 0.87  6744  52.4  27.9   9.9  ****....................................
 8 0.60 0.83  6472  45.9  19.3   5.3  **......................................
 9 0.63 0.80  6042  35.2  11.6   3.0  *.......................................
10 0.65 0.77  5684  40.4  12.9   4.2  **......................................
                                   I                   I                   I
                                   0%                 50%                100%
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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	1.48	1.52	41812	41870	64.89	-3	-2	0	1.0
2	HKL:H+L=2N	1.50	1.50	41831	41851	64.89	-3	-2	0	1.0
3	HKL:K+L=2N	1.49	1.51	41819	41863	63.91	-2	-3	0	1.0
4	HKL:H+K+L=2N	1.54	1.45	41863	41819	64.89	-3	-2	0	1.1
5	HKL:-H+K+L=3N	1.49	1.50	27864	55818	64.89	-3	-2	0	1.0
6	HKL:H-K+L=3N	1.48	1.51	27911	55771	64.89	-3	-2	0	1.0
41	HKL:H=2N	1.51	1.49	41842	41840	64.89	-3	-2	0	1.0
42	HKL:K=2N	1.51	1.49	41748	41934	63.91	-2	-3	0	1.0
43	HKL:L=2N	1.62	1.38	41879	41803	39.71	-3	0	-1	1.2
44	HKL:H=3N	1.50	1.50	27860	55822	63.91	-2	-3	0	1.0
45	HKL:K=3N	1.51	1.49	27837	55845	64.89	-3	-2	0	1.0
46	HKL:L=3N	1.50	1.50	27898	55784	60.25	-1	1	4	1.0
47	-HKL, H-KL=3N	1.49	1.51	46472	37210	64.89	-3	-2	0	1.0
48	-HKL:K2,KL4P2	1.48	1.71	77888	5794	54.73	3	0	2	0.9
49	-HKL:H2,HL4P2	1.48	1.71	77693	5989	48.06	2	3	0	0.9
50	-HKL:H2,HK4P2	1.49	1.57	77733	5949	51.94	2	4	2	0.9
51	HKL:H+2L=3N	1.49	1.50	27901	55781	63.91	-2	-3	0	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	20.948	0	1-1 0	1-1 0	2	0.142	0.								

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

(a') (-1.000-1.000 0.000) (a) (x') (-0.500-0.500 0.000) (x) Metrically
(b') = (1.000-1.000 0.000) (b). (y') = (0.500-0.500 0.000) (y) Monoclinic
(c') (0.000 0.000 1.000) (c) (z') (0.000 0.000 1.000) (z) FOM: 0.142

	Latt	a	b	c	Alpha	Beta	Gamma	Volume
Input Cell	P	17.904	17.937	22.911	78.08	77.99	71.53	6747.10
Reduc Cell	P	17.904	17.937	22.911	78.08	77.99	71.53	6747.10
Conv. Cell	mC	29.082	20.948	22.911	89.94	104.80	89.89	13494.21

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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