PLATON(V-311206)-Run for: kla0150 TIME: Nov 7 13:07:53 2011

Crystal Data

Input Cell (Lattice Type: P) - Temp = 0K						Reduced Cell (Acta Cryst.(1976),A32,297-298)					
a =	9.83300	Angstrom	alpha =	90	Degree	a =	9.833	alpha =	90.00	V =	3315.8
b =	31.94200		beta =	90		b =	10.557	beta =	90.00		
c =	10.55700		gamma =	90		c =	31.942	gamma =	90.00		
V =	3315.80	Cubic-Angstrom	d(100) =	9.8330	Angstrom	Niggli Values					
			d(010) =	31.9420		96.688	111.450	1020.291			
Lambda(MoKa) =	0.71073	Angstrom	d(001) =	10.5570		0.000	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)

(XO)	(	9.83300	0	0)	(X)	,	(X)	(	0.10170	0	0)	(XO)
(YO) =	(	0	31.94200	0)*(	(Y)	,	(Y) =	(	0	0.03131	0)*(	(YO)
(ZO)	(	0	0	10.55700)	(Z)	,	(Z)	(	0	0	0.09472)	(ZO)

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: kla0150
================================================================================
:: 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  2764  95.1  93.6  93.0  ************************************...
 2 0.38 1.32  2773  97.3  95.4  93.1  ************************************...
 3 0.44 1.15  2661  97.1  94.8  91.9  ************************************...
 4 0.48 1.04  2232  95.9  92.4  87.6  ********************************.....
 5 0.52 0.97  2145  96.1  90.5  81.2  ******************************........
 6 0.55 0.91  2042  92.7  84.8  71.0  ****************************............
 7 0.58 0.87  1786  89.8  75.4  59.5  ************************................
 8 0.60 0.83  1789  85.7  69.6  52.3  **********************..................
 9 0.63 0.80  1661  85.2  70.0  52.8  **********************..................
10 0.65 0.77  1616  78.8  60.0  40.7  ****************.......................
                                    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	E C	HKL:H+K=2N	6.45	0.00	22511	0	0.00	0	0	0	99.0
2		HKL:H+L=2N	6.54	6.37	11271	11240	16.72	-4	6	-1	1.0
3		HKL:K+L=2N	6.54	6.37	11271	11240	16.72	-4	6	-1	1.0
4		HKL:H+K+L=2N	6.28	6.62	11221	11290	16.72	-4	6	-1	0.9
5		HKL:-H+K+L=3N	6.43	6.47	7480	15031	16.49	2	4	-4	1.0
6		HKL:H-K+L=3N	6.43	6.47	7514	14997	16.72	-4	6	-1	1.0
41		HKL:H=2N	6.46	6.45	11297	11214	16.37	3	-7	1	1.0
42		HKL:K=2N	6.46	6.45	11297	11214	16.37	3	-7	1	1.0
43		HKL:L=2N	6.28	6.62	11221	11290	16.72	-4	6	-1	0.9
44		HKL:H=3N	6.37	6.50	7525	14986	16.72	-4	6	-1	1.0
45		HKL:K=3N	6.43	6.47	7494	15017	16.49	2	4	-4	1.0
46		HKL:L=3N	6.10	6.63	7522	14989	16.72	-4	6	-1	0.9
47		-HKL, H-KL=3N	6.51	6.38	12489	10022	16.09	2	-10	-4	1.0
48		-HKL:K2,KL4P2	6.44	6.68	21078	1433	15.89	2	10	-4	1.0
49		-HKL:H2,HL4P2	6.46	6.44	21022	1489	15.69	2	-20	0	1.0
50		-HKL:H2,HK4P2	6.43	6.60	19565	2946	16.72	-4	6	-1	1.0
51		HKL:H+2L=3N	6.42	6.47	7515	14996	16.37	3	-7	1	1.0

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

			Rows			Products		Angle Between Two Direct Axes							
Nr	D	N	Direct			Recip Dot	Delta	1	2	3	4	5	6	7	8	9
1	9.833	2	1	0	0	2	0-1 2 0.000	0.	90.	90.						
2	10.557	2	0	1	0	0	1 0 1 0.000	90.	0.	90.						
3	31.942	2	1	0	2	0	0 1 2 0.000	90.	90.	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)	Orthorhombic
(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	C	9.833	31.942	10.557	90.00	90.00	90.00	3315.80
Reduc Cell	P	9.833	10.557	16.711	90.00	107.11	90.00	1657.90
Conv. Cell	oC	9.833	31.942	10.557	90.00	90.00	90.00	3315.80

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

			Rows		Products		Angle Between Two Direct Axes								
Nr	D	N	Direct	Recip	Dot	Delta	1	2	3	4	5	6	7	8	9
1	9.833	0	1 0 0	2 0-1	2	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	C	9.833	31.942	10.557	90.00	90.00	90.00	3315.80
Reduc Cell	P	9.833	10.557	16.711	90.00	107.11	90.00	1657.90
Conv. Cell	mC	31.942	9.833	10.557	90.00	90.00	90.00	3315.80

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

Nr	D	N	Rows Direct			Products Recip Dot			Delta	Angle Between Two Direct Axes 1	2	3	4	5	6	7	8	9
1	10.557	0	0	1	0	0	1	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 1.000 0.000) (x)  Metrically
(b') = ( 0.000 0.000-1.000) (b).  (y') = ( 0.000 0.000-1.000) (y)  Monoclinic
(c')   (-0.500 0.500 0.000) (c)   (z')   ( 0.000 2.000 0.000) (z)  FOM:  0.000
```

	Latt	a	b	c	Alpha	Beta	Gamma	Volume
Input Cell	C	9.833	31.942	10.557	90.00	90.00	90.00	3315.80
Reduc Cell	P	9.833	10.557	16.711	90.00	107.11	90.00	1657.90
Conv. Cell	mP	9.833	10.557	16.711	90.00	107.11	90.00	1657.90

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

Nr	D	N	Rows Direct			Products Recip Dot			Delta	Angle Between Two Direct Axes 1	2	3	4	5	6	7	8	9
1	31.942	0	1	0	2	0	0	1	2	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	C	9.833	31.942	10.557	90.00	90.00	90.00	3315.80
Reduc Cell	P	9.833	10.557	16.711	90.00	107.11	90.00	1657.90
Conv. Cell	mC	9.833	31.942	10.557	90.00	90.00	90.00	3315.80

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

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

```
(a')   ( 1.000 0.000 0.000) (a)   (x')   ( 1.000-1.000 0.000) (x)  Metrically
(b') = ( 0.000 0.000 1.000) (b).  (y') = ( 0.000 0.000 1.000) (y)  Anorthic
(c')   (-0.500-0.500 0.000) (c)   (z')   ( 0.000-2.000 0.000) (z)  FOM:  0.000
```

	Latt	a	b	c	Alpha	Beta	Gamma	Volume
Input Cell	C	9.833	31.942	10.557	90.00	90.00	90.00	3315.80
Reduc Cell	P	9.833	10.557	16.711	90.00	107.11	90.00	1657.90
Conv. Cell	aP	9.833	10.557	16.711	90.00	107.11	90.00	1657.90

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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 : 9 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