PLATON(V-311206)-Run for: xray025 TIME: Apr 27 13:54:18 2010

Crystal Data

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

a =	8.79600	Angstrom	alpha =	90	Degree	a =	8.796	alpha =	90.00	V =	2550.3
b =	23.08000		beta =	94.1400		b =	12.595	beta =	90.00		
c =	12.59500		gamma =	90		c =	23.080	gamma =	94.14		
V =	2550.26	Cubic-Angstrom	d(100) =	8.7730	Angstrom						
			d(010) =	23.0800							
Lambda(MoKa) =	0.71073	Angstrom	d(001) =	12.5621							

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

Niggli Values: 77.370 158.634 532.686 / 0.000 0.000 -7.998

Orthogonalization Matrices

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

$$\begin{pmatrix} XO \\ YO \\ ZO \end{pmatrix} = \begin{pmatrix} 8.79600 & 0 & -0.90928 \\ 0 & 23.08000 & 0 \\ 0 & 0 & 12.56214 \end{pmatrix} \begin{pmatrix} X \\ Y \\ Z \end{pmatrix}, \quad \begin{pmatrix} X \\ Y \\ Z \end{pmatrix} = \begin{pmatrix} 0.11369 & 0 & 0.00823 \\ 0 & 0.04333 & 0 \\ 0 & 0 & 0.07960 \end{pmatrix} \begin{pmatrix} XO \\ YO \\ ZO \end{pmatrix}$$

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

SPGR - Determine SpaceGroup from Observed Extinctions for: xray025

:: 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	2208	100.0	100.0	100.0	**********
2	0.38	1.32	2140	99.8	99.4	99.0	**********
3	0.44	1.15	1950	98.4	97.0	95.1	**********..
4	0.48	1.04	1748	97.1	92.4	86.7	**********.....
5	0.52	0.97	1581	95.6	89.9	81.8	**********.....
6	0.55	0.91	1556	93.1	83.5	68.2	**********.....
7	0.58	0.87	1411	88.5	75.5	59.5	**********.....
8	0.60	0.83	1263	83.4	68.0	48.2	**********.....
9	0.63	0.80	1278	78.0	56.4	35.9	**********.....
10	0.65	0.77	1191	75.2	53.4	30.1	**********.....

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	7.09	0.00	17246	0	0.00	0	0	0	99.0
2		HKL:H+L=2N	7.06	7.11	8643	8603	20.28	-1	3	-2	1.0
3		HKL:K+L=2N	7.06	7.11	8643	8603	20.28	-1	3	-2	1.0
4		HKL:H+K+L=2N	7.09	7.08	8626	8620	19.09	2	-4	-1	1.0
5		HKL:-H+K+L=3N	7.06	7.10	5765	11481	20.28	-1	3	-2	1.0
6		HKL:H-K+L=3N	7.09	7.08	5766	11480	19.46	1	1	2	1.0
41		HKL:H=2N	7.06	7.11	8599	8647	20.28	-1	3	-2	1.0
42		HKL:K=2N	7.06	7.11	8599	8647	20.28	-1	3	-2	1.0
43		HKL:L=2N	7.09	7.08	8626	8620	19.09	2	-4	-1	1.0
44		HKL:H=3N	7.36	6.95	5685	11561	20.28	-1	3	-2	1.1
45		HKL:K=3N	7.07	7.09	5763	11483	19.46	1	1	2	1.0
46		HKL:L=3N	6.99	7.13	5775	11471	20.28	-1	3	-2	1.0
47		-HKL, H-KL=3N	7.10	7.06	9592	7654	19.46	1	1	2	1.0
48		-HKL:K2,KL4P2	7.08	7.10	16185	1061	17.65	-2	4	2	1.0
49		-HKL:H2,HL4P2	7.08	7.18	16114	1132	18.54	-2	0	4	1.0
50		-HKL:H2,HK4P2	7.12	6.85	15182	2064	18.64	0	6	-2	1.0
51		HKL:H+2L=3N	7.05	7.10	5746	11500	20.28	-1	3	-2	1.0

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

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	23.080	0	1-2 0	0 1 0	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
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	Latt	a	b	c	Alpha	Beta	Gamma	Volume
Input Cell	C	8.796	23.080	12.595	90.00	94.14	90.00	2550.26
Reduc Cell	P	8.796	12.350	12.595	88.53	85.86	69.14	1275.13
Conv. Cell	mC	8.796	23.080	12.595	90.00	94.14	90.00	2550.26

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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