PLATON(V-311206)-Run for: test TIME: Sep 30 11:57:46 2011

Crystal Data

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

a =	12.67200	Angstrom	alpha =	90	Degree	a =	12.672	alpha =	90.00	V =	6025.7
b =	21.52900		beta =	90		b =	21.529	beta =	90.00		
c =	22.54600		gamma =	101.5800		c =	22.546	gamma =	101.58		
V =	6025.70	Cubic-Angstrom	d(100) =	12.4141	Angstrom	Niggli Values					
			d(010) =	21.0908		160.580	463.498	508.322			
Lambda(MoKa) =	0.71073	Angstrom	d(001) =	22.5460		0.000	0.000	-54.764			

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)

$$(XO) = \begin{pmatrix} 12.67200 & -4.32164 & 0 \\ 0 & 21.09078 & 0 \\ 0 & 0 & 22.54600 \end{pmatrix} (X) \quad , \quad (X) = \begin{pmatrix} 0.07891 & 0.01617 & 0 \\ 0 & 0.04741 & 0 \\ 0 & 0 & 0.04435 \end{pmatrix} (XO)$$

$$(YO) = \begin{pmatrix} 0 & 21.09078 & 0 \\ 0 & 0 & 22.54600 \end{pmatrix} (Y) \quad , \quad (Y) = \begin{pmatrix} 0 & 0.04741 & 0 \\ 0 & 0 & 0.04435 \end{pmatrix} (YO)$$

$$(ZO) = \begin{pmatrix} 0 & 0 & 22.54600 \end{pmatrix} (Z) \quad , \quad (Z) = \begin{pmatrix} 0 & 0 & 0.04435 \end{pmatrix} (ZO)$$

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: test
================================================================================
:: 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   549  96.0  87.6  82.7  *********************************.......
 2 0.38 1.32   573  93.9  82.5  74.0  ****************************..........
 3 0.44 1.15   540  89.1  76.7  62.6  ************************................
 4 0.48 1.04   503  85.7  74.0  56.3  ***********************.................
 5 0.52 0.97   480  81.0  71.2  55.2  **********************..................
 6 0.55 0.91   464  78.7  64.4  47.4  ******************.....................
 7 0.58 0.87   442  78.1  64.0  41.4  *****************.......................
 8 0.60 0.83   419  70.6  59.2  35.1  **************.........................
 9 0.63 0.80   385  71.2  49.6  24.9  **********.............................
10 0.65 0.77   393  65.9  45.8  24.9  **********.............................
                                    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	3.90	4.03	2502	2518	111.39	2	-1	-2	1.0
2		HKL:H+L=2N	4.18	3.76	2516	2504	96.39	3	-2	-2	1.1
3		HKL:K+L=2N	3.92	4.02	2510	2510	111.39	2	-1	-2	1.0
4		HKL:H+K+L=2N	3.96	3.98	2515	2505	111.39	2	-1	-2	1.0
5		HKL:-H+K+L=3N	4.05	3.93	1676	3344	111.39	2	-1	-2	1.0
6		HKL:H-K+L=3N	3.95	3.98	1667	3353	111.39	2	-1	-2	1.0
41		HKL:H=2N	4.07	3.87	2527	2493	99.03	1	-4	-1	1.1
42		HKL:K=2N	4.09	3.85	2521	2499	111.39	2	-1	-2	1.1
43		HKL:L=2N	4.03	3.91	2509	2511	99.03	1	-4	-1	1.0
44		HKL:H=3N	4.06	3.92	1680	3340	111.39	2	-1	-2	1.0
45		HKL:K=3N	3.86	4.02	1673	3347	111.39	2	-1	-2	1.0
46		HKL:L=3N	3.77	4.07	1683	3337	111.39	2	-1	-2	0.9
47		-HKL, H-KL=3N	4.02	3.91	2779	2241	111.39	2	-1	-2	1.0
48	E tw2	-HKL:K2,KL4P2	3.97	0.00	5020	0	0.00	0	0	0	99.0
49		-HKL:H2,HL4P2	4.00	3.53	4697	323	39.88	2	-16	0	1.1
50		-HKL:H2,HK4P2	3.99	3.32	4865	155	36.26	4	-2	-3	1.2
51		HKL:H+2L=3N	3.78	4.06	1663	3357	111.39	2	-1	-2	0.9

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	22.546	0	0	0	1	0 0 1	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 0.000-1.000) (b). (y') = (0.000 0.000-1.000) (y) Monoclinic
(c') (0.000-1.000 0.000) (c) (z') (0.000-1.000 0.000) (z) FOM: 0.000

	Latt	a	b	c	Alpha	Beta	Gamma	Volume
Input Cell	P	12.672	21.529	22.546	90.00	90.00	101.58	6025.70
Reduc Cell	P	12.672	21.529	22.546	90.00	90.00	101.58	6025.71
Conv. Cell	mP	12.672	22.546	21.529	90.00	101.58	90.00	6025.70

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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