PLATON(V-311206)-Run for: xray023a TIME: Mar 4 13:35:01 2010

Crystal Data

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

a =	30.33300	Angstrom	alpha =	90	Degree	a =	6.101	alpha =	105.31	V =	3483.0
b =	6.10100		beta =	105.3100		b =	19.513	beta =	90.00		
c =	19.51300		gamma =	90		c =	30.333	gamma =	90.00		

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

V =	3482.95	Cubic-Angstrom	d(100) =	29.2565	Angstrom	Niggli Values					
			d(010) =	6.1010		37.222	380.757	920.091			
Lambda(MoKa) =	0.71073	Angstrom	d(001) =	18.8205		-156.283	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)	(	30.33300	0	-5.15224)	(X)	,	(X)	(	0.03297	0	0.00903)	(XO)	Orthogonal Axes AO, BO and CO
(YO) =	(	0	6.10100	0)*(	Y)	,	(Y) =	(	0	0.16391	0)*(	YO)	are defined as:
(ZO)	(	0	0	18.82051)	(Z)	,	(Z)	(	0	0	0.05313)	(ZO)	AO // A, CO // C*, BO // CO X AO

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SPGR - Determine SpaceGroup from Observed Extinctions for: xray023a
================================================================================
:: 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  6075  65.6  45.5  34.4  **************.........................
 2 0.38 1.32  5969  68.2  45.7  28.8  ************..........................
 3 0.44 1.15  5132  65.5  43.2  22.1  *********.............................
 4 0.48 1.04  4727  59.5  36.3  15.9  ******................................
 5 0.52 0.97  4389  55.9  31.2  11.4  *****.................................
 6 0.55 0.91  4133  51.9  27.7   7.6  ***...................................
 7 0.58 0.87  3566  51.1  27.1   7.0  ***...................................
 8 0.60 0.83  3741  48.2  23.3   5.6  **....................................
 9 0.63 0.80  3272  48.3  24.4   6.1  **....................................
10 0.65 0.77  2933  46.1  21.4   4.8  **....................................
                                    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	?	C HKL:H+K=2N	1.77	0.49	23525	23444	7.18	2	-1	-25	3.6
2		HKL:H+L=2N	1.17	1.09	23505	23464	19.14	-3	1	0	1.1
3		HKL:K+L=2N	1.17	1.09	23477	23492	19.14	-3	1	0	1.1
4		HKL:H+K+L=2N	1.27	0.99	23515	23454	19.28	-3	1	-1	1.3
5		HKL:-H+K+L=3N	1.13	1.13	15650	31319	19.78	0	0	4	1.0
6		HKL:H-K+L=3N	1.13	1.13	15641	31328	19.78	0	0	4	1.0
41		HKL:H=2N	1.08	1.18	23477	23492	19.28	-3	1	-1	0.9
42		HKL:K=2N	1.09	1.17	23311	23658	19.28	-3	1	-1	0.9
43		HKL:L=2N	1.29	0.97	23477	23492	19.28	-3	1	-1	1.3
44		HKL:H=3N	1.13	1.13	15668	31301	19.29	4	0	2	1.0
45		HKL:K=3N	1.04	1.17	15541	31428	19.28	-3	1	-1	0.9
46		HKL:L=3N	1.13	1.13	15674	31295	19.78	0	0	4	1.0
47		-HKL, H-KL=3N	1.13	1.14	26070	20899	19.78	0	0	4	1.0
48		-HKL:K2,KL4P2	1.12	1.34	43862	3107	19.29	4	0	2	0.8
49		-HKL:H2,HL4P2	1.12	1.32	43973	2996	19.29	4	0	2	0.8
50		-HKL:H2,HK4P2	1.10	1.67	44120	2849	18.71	0	2	4	0.7
51		HKL:H+2L=3N	1.13	1.13	15605	31364	19.78	0	0	4	1.0

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	6.101	0	1	0	0	1	0.000		0.							

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

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

	Latt	a	b	c	Alpha	Beta	Gamma	Volume
Input Cell	P	30.333	6.101	19.513	90.00	105.31	90.00	3482.95
Reduc Cell	P	6.101	19.513	30.333	105.31	90.00	90.00	3482.94
Conv. Cell	mP	19.513	6.101	30.333	90.00	105.31	90.00	3482.95

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	6.101	0	1 0 0	2-1 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
```

	Latt	a	b	c	Alpha	Beta	Gamma	Volume
Input Cell	C	30.333	6.101	19.513	90.00	105.31	90.00	3482.95
Reduc Cell	P	6.101	15.470	19.513	105.00	90.00	101.37	1741.45
Conv. Cell	mC	30.333	6.101	19.513	90.00	105.31	90.00	3482.95

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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 : 6 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