PLATON(V-311206)-Run for: joer040 TIME: Jun 9 13:19:28 2011

Crystal Data

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

a =	15.32700	Angstrom	alpha =	90	Degree	a =	15.163	alpha =	96.22	V =	3744.8
b =	15.16300		beta =	96.2200		b =	15.327	beta =	90.00		
c =	16.20900		gamma =	90		c =	16.209	gamma =	90.00		

V =	3744.85	Cubic-Angstrom	d(100) =	15.2368	Angstrom	Niggli Values
			d(010) =	15.1630		229.917 234.917 262.732
Lambda(MoKa) =	0.71073	Angstrom	d(001) =	16.1136		-26.917 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)

$$(XO) = \begin{pmatrix} 15.32700 & 0 & -1.75619 \\ 0 & 15.16300 & 0 \\ 0 & 0 & 16.11358 \end{pmatrix} (X) \quad , \quad (X) = \begin{pmatrix} 0.06524 & 0 & 0.00711 \\ 0 & 0.06595 & 0 \\ 0 & 0 & 0.06206 \end{pmatrix} (XO)$$

$$(YO) = \begin{pmatrix} 0 & 15.16300 & 0 \end{pmatrix} (Y) \quad , \quad (Y) = \begin{pmatrix} 0 & 0.06595 & 0 \end{pmatrix} (YO)$$

$$(ZO) = \begin{pmatrix} 0 & 0 & 16.11358 \end{pmatrix} (Z) \quad , \quad (Z) = \begin{pmatrix} 0 & 0 & 0.06206 \end{pmatrix} (ZO)$$

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

```
SPGR - Determine SpaceGroup from Observed Extinctions for: joer040
================================================================================
:: 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  6585  95.0  90.4  85.4  **********************************......
 2 0.38 1.32  6483  93.7  86.4  76.6  ******************************.........
 3 0.44 1.15  5769  92.7  84.2  72.4  *****************************...........
 4 0.48 1.04  5270  91.1  83.3  68.7  ****************************............
 5 0.52 0.97  4809  87.1  78.2  64.0  ***************************.............
 6 0.55 0.91  4474  85.0  75.3  61.1  *************************...............
 7 0.58 0.87  4133  83.8  73.1  58.8  *************************...............
 8 0.60 0.83  3896  79.9  68.7  53.6  ***********************.................
 9 0.63 0.80  3700  77.9  65.1  48.6  *********************...................
10 0.65 0.77  3470  75.4  61.6  44.8  ********************....................
                                    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	HKL:H+K=2N	5.38	5.49	25649	25576	103.21	-1	0	4	1.0
2	HKL:H+L=2N	5.40	5.47	25602	25623	103.21	-1	0	4	1.0
3	HKL:K+L=2N	5.48	5.39	25628	25597	102.34	-1	-1	-4	1.0
4	HKL:H+K+L=2N	5.43	5.43	25613	25612	103.21	-1	0	4	1.0
5	HKL:-H+K+L=3N	5.42	5.44	17071	34154	103.21	-1	0	4	1.0
6	HKL:H-K+L=3N	5.46	5.42	17072	34153	102.34	-1	-1	-4	1.0
41	HKL:H=2N	5.42	5.45	25628	25597	103.21	-1	0	4	1.0
42	HKL:K=2N	5.33	5.54	25588	25637	102.34	-1	-1	-4	1.0
43	HKL:L=2N	5.97	4.90	25615	25610	98.76	2	-2	3	1.2
44	HKL:H=3N	5.33	5.48	17078	34147	103.21	-1	0	4	1.0
45	HKL:K=3N	5.30	5.50	17069	34156	102.34	-1	-1	-4	1.0
46	HKL:L=3N	5.46	5.42	17063	34162	103.21	-1	0	4	1.0
47	-HKL, H-KL=3N	5.43	5.43	28451	22774	102.34	-1	-1	-4	1.0
48	-HKL:K2,KL4P2	5.39	6.07	47987	3238	95.04	0	0	2	0.9
49	-HKL:H2,HL4P2	5.38	6.17	47838	3387	95.04	0	0	2	0.9
50	-HKL:H2,HK4P2	5.44	5.39	47832	3393	82.28	4	-2	3	1.0
51	HKL:H+2L=3N	5.46	5.42	17076	34149	103.21	-1	0	4	1.0

:: No Extinction Conditions Found

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	15.163	0	1 0 0			1 0 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 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	P	15.327	15.163	16.209	90.00	96.22	90.00	3744.85
Reduc Cell	P	15.163	15.327	16.209	96.22	90.00	90.00	3744.86
Conv. Cell	mP	15.327	15.163	16.209	90.00	96.22	90.00	3744.85

==========

********** N O T I C E **********

==========

- 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