PLATON(V-311206)-Run for: jain003 TIME: Jul 31 16:37:06 2007

Crystal Data

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

a =	7.42400	Angstrom	alpha =	90	Degree	a =	7.424	alpha =	90.00	V =	1728.8
b =	13.60900		beta =	94.7900		b =	13.609	beta =	94.79		
c =	17.17100		gamma =	90		c =	17.171	gamma =	90.00		

V =	1728.78	Cubic-Angstrom	d(100) =	7.3981	Angstrom	Niggli Values	
			d(010) =	13.6090		55.116	185.205	294.843
Lambda(MoKa) =	0.71073	Angstrom	d(001) =	17.1110		0.000	-10.645	0.000

Orthogonalization Matrices

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

(XO)	(	7.42400	0	-1.43385)	(X)	,	(X)	(	0.13470	0	0.01129)	(XO)
(YO) =	(	0	13.60900	0)*(Y)	,	(Y) =	(	0	0.07348	0)*(YO)		
(ZO)	(	0	0	17.11103)	(Z)	,	(Z)	(	0	0	0.05844)	(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: jain003

:: 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	3026	99.6	99.4	99.3	**********
2	0.38	1.32	2690	99.6	99.2	98.5	**********.
3	0.44	1.15	2382	99.2	98.8	97.8	**********.
4	0.48	1.04	2018	99.8	99.1	98.2	**********.
5	0.52	0.97	1953	99.1	98.5	97.1	**********.
6	0.55	0.91	1695	98.6	97.3	94.3	**********..
7	0.58	0.87	1744	98.2	96.3	92.5	**********...
8	0.60	0.83	1497	97.9	96.3	93.3	**********...
9	0.63	0.80	1521	97.2	96.0	93.0	**********...
10	0.65	0.77	706	98.0	97.5	96.2	**********..

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	22.46	22.36	9660	9656	82.97	3	2	-4	1.0
2	HKL:H+L=2N	22.26	22.57	9661	9655	82.97	3	2	-4	1.0
3	HKL:K+L=2N	22.63	22.19	9665	9651	82.69	1	2	-7	1.0
4	HKL:H+K+L=2N	22.30	22.53	9673	9643	82.97	3	2	-4	1.0
5	HKL:-H+K+L=3N	22.66	22.29	6422	12894	82.97	3	2	-4	1.0
6	HKL:H-K+L=3N	22.52	22.36	6428	12888	82.69	1	2	-7	1.0
41	HKL:H=2N	22.11	22.71	9590	9726	82.97	3	2	-4	1.0
42	HKL:K=2N	22.18	22.65	9670	9646	82.51	1	3	-3	1.0
43	HKL:L=2N	22.63	22.19	9657	9659	82.69	1	2	-7	1.0
44	HKL:H=3N	22.91	22.17	6367	12949	82.69	1	2	-7	1.0
45	HKL:K=3N	22.49	22.37	6429	12887	82.97	3	2	-4	1.0
46	HKL:L=3N	22.08	22.58	6469	12847	82.97	3	2	-4	1.0
47	-HKL, H-KL=3N	22.63	22.14	10700	8616	82.51	1	3	-3	1.0
48	-HKL:K2,KL4P2	22.37	23.01	18089	1227	82.26	2	0	6	1.0
49	-HKL:H2,HL4P2	22.50	21.03	18156	1160	79.83	0	2	2	1.1
50	-HKL:H2,HK4P2	22.42	22.31	17988	1328	82.26	2	0	6	1.0
51	HKL:H+2L=3N	22.25	22.50	6438	12878	82.97	3	2	-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	13.609	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 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	P	7.424	13.609	17.171	90.00	94.79	90.00	1728.78
Reduc Cell	P	7.424	13.609	17.171	90.00	94.79	90.00	1728.79
Conv. Cell	mP	7.424	13.609	17.171	90.00	94.79	90.00	1728.78

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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