

PLATON(V-311206)-Run for: joer028a

TIME: Apr 4 14:59:00 2011

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Crystal Data

Input Cell (Lattice Type: P)				Temp = 0K	Reduced Cell (Acta Cryst.(1976), A32, 297-298)			
a =	15.80800	Angstrom	alpha =	106.8800 Degree	a =	15.808	alpha =	106.88 V = 4532.8
b =	17.33400		beta =	90.0400	b =	17.334	beta =	90.04
c =	17.79900		gamma =	103.1600	c =	17.799	gamma =	103.16
V = 4532.81 Cubic-Angstrom				d(100) = 15.3532 Angstrom	Niggli Values			
				d(010) = 16.1100	249.893	300.468	316.804	
Lambda(MoKa) = 0.71073 Angstrom				d(001) = 16.9883	-89.587	-0.197	-62.386	

Orthogonalization Matrices

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

(X0) (15.80800 -3.94645 -0.01243) (X) , (X) (0.06326 0.01479 0.00467) (X0) Orthogonal Axes A0, B0 and C0
 (Y0) = (0 16.87877 -5.31056)*(Y) , (Y) = (0 0.05925 0.01852)*(Y0) are defined as:
 (Z0) (0 0 16.98830) (Z) , (Z) (0 0 0.05886) (Z0) A0 // A, C0 // C*, B0 // C0 X A0

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SPGR - Determine SpaceGroup from Observed Extinctions for: joer028a

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:: 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

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Intensity Distribution

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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	7426	90.1	79.7	67.0	*****			
2	0.38	1.32	7281	88.1	74.1	55.2	*****			
3	0.44	1.15	6951	85.2	68.6	46.1	*****			
4	0.48	1.04	6171	81.9	62.8	38.2	*****			
5	0.52	0.97	5887	75.9	57.3	34.0	*****			
6	0.55	0.91	5245	74.1	57.5	35.4	*****			
7	0.58	0.87	4998	70.1	51.1	31.1	*****			
8	0.60	0.83	4742	63.9	43.6	22.5	*****			
9	0.63	0.80	4538	62.3	40.1	18.9	*****			
10	0.65	0.77	4225	56.9	33.4	12.6	*****			
						I		I		I
						0%		50%		100%

Analysis of General Reflections for Bravais Centering

Nr	Ex. Condition	Aver(I/sig(I))		Number of Refl		I/sigI Max.F				.T/F. Ratio
		.True.	.False.	.True.	.False.		H	K	L	
1	HKL:H+K=2N	2.74	2.66	29962	29970	107.69	0	3	-4	1.0
2	HKL:H+L=2N	2.79	2.61	29936	29996	77.01	-4	-2	3	1.1
3	HKL:K+L=2N	2.71	2.69	29970	29962	107.69	0	3	-4	1.0
4	HKL:H+K+L=2N	2.70	2.70	29966	29966	107.69	0	3	-4	1.0
5	HKL:-H+K+L=3N	2.70	2.70	20001	39931	107.69	0	3	-4	1.0
6	HKL:H-K+L=3N	2.77	2.66	19950	39982	107.69	0	3	-4	1.0
41 >	2X HKL:H=2N	3.88	1.47	30662	29270	58.56	-1	1	-3	2.6
42	HKL:K=2N	2.71	2.69	29996	29936	107.69	0	3	-4	1.0
43	HKL:L=2N	2.82	2.58	30020	29912	77.01	-4	-2	3	1.1
44	HKL:H=3N	2.54	2.78	19915	40017	95.09	-2	0	-2	0.9
45	HKL:K=3N	2.68	2.71	20032	39900	94.71	-2	-2	0	1.0
46	HKL:L=3N	2.68	2.71	19984	39948	107.69	0	3	-4	1.0
47	-HKL, H-KL=3N	2.74	2.65	33271	26661	107.69	0	3	-4	1.0
48	-HKL:K2,KL4P2	2.70	2.70	56357	3575	89.59	2	2	0	1.0
49	-HKL:H2,HL4P2	2.63	3.83	56258	3674	90.87	2	-3	0	0.7
50	-HKL:H2,HK4P2	2.61	3.94	56015	3917	88.63	0	2	0	0.7
51	HKL:H+2L=3N	2.68	2.71	20009	39923	107.69	0	3	-4	1.0

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

==== 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) Anorthic
 (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	15.808	17.334	17.799	106.88	90.04	103.16	4532.81
Reduc Cell	P	15.808	17.334	17.799	106.88	90.04	103.16	4532.81
Conv. Cell	aP	15.808	17.334	17.799	106.88	90.04	103.16	4532.81

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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