

PLATON(V-311206)-Run for: char324t

TIME: Jan 3 16:28:46 2011

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Crystal Data

Input Cell (Lattice Type: P)				Temp = 0K	Reduced Cell		(Acta Cryst.(1976),A32,297-298)		
a =	11.66800	Angstrom	alpha =	90.1000 Degree	a =	11.668	alpha =	90.10	V = 1930.6
b =	12.51800		beta =	95.6300	b =	12.518	beta =	95.63	
c =	13.93500		gamma =	107.5100	c =	13.935	gamma =	107.51	
V = 1930.63 Cubic-Angstrom					Niggli Values				
d(100) = 11.0677 Angstrom					136.142 156.700 194.184				
d(010) = 11.9315					-0.305 -15.951 -43.945				
d(001) = 13.8603									
Lambda(MoKa) = 0.71073 Angstrom									

Orthogonalization Matrices

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

(X0) (11.66800 -3.76632 -1.36708) (X) , (X) (0.08570 0.02704 0.00934) (X0) Orthogonal Axes A0, B0 and C0
 (Y0) = (0 11.93797 -0.45680)*(Y) , (Y) = (0 0.08377 0.00276)*(Y0) are defined as:
 (Z0) (0 0 13.86026) (Z) , (Z) (0 0 0.07215) (Z0) A0 // A, C0 // C*, B0 // C0 X A0

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SPGR - Determine SpaceGroup from Observed Extinctions for: char324t

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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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:: TRMX = 1.00 0.00 0.00 0.00 1.00 0.00 0.00 0.00 1.00

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	198	97.5	91.4	84.3	*****			
2	0.38	1.32	202	96.5	89.1	79.7	*****			
3	0.44	1.15	172	93.6	83.7	70.3	*****			
4	0.48	1.04	152	86.2	75.7	58.6	*****			
5	0.52	0.97	148	87.8	77.0	55.4	*****			
6	0.55	0.91	136	83.8	70.6	48.5	*****			
7	0.58	0.87	127	81.9	70.9	49.6	*****			
8	0.60	0.83	114	78.9	60.5	31.6	*****			
9	0.63	0.80	114	71.9	59.6	36.0	*****			
10	0.65	0.77	111	75.7	60.4	31.5	*****			
						I		I		I
						0%		50%		100%

[illegible]

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:: No Extinction Conditions Found
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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	11.668	12.518	13.935	90.10	95.63	107.51	1930.63
Reduc Cell	P	11.668	12.518	13.935	90.10	95.63	107.51	1930.62
Conv. Cell	aP	11.668	12.518	13.935	90.10	95.63	107.51	1930.63

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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