

PLATON(V-311206)-Run for: klat84 - SHELXL

TIME: Aug 8 10:33:14 2011

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Crystal Data

Input Cell (Lattice Type: P)		Temp = 200K	Reduced Cell		(Acta Cryst.(1976), A32, 297-298)
a =	18.701(3) Angstrom	alpha = 90 Degree	a =	13.666	alpha = 101.46 V = 5896.2
b =	13.666(2)	beta = 101.455(3)	b =	18.701	beta = 90.00
c =	23.540(4)	gamma = 90	c =	23.540	gamma = 90.00
V = 5896.2(16) Cubic-Angstrom		d(100) = 18.3285 Angstrom	Niggli Values		
		d(010) = 13.6660	186.760	349.727	554.132
Lambda(MoKa) = 0.71073 Angstrom		d(001) = 23.0711	-87.427	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)

(X0) (18.70100 0 -4.67500) (X) , (X) (0.05347 0 0.01084) (X0) Orthogonal Axes A0, B0 and C0
 (Y0) = (0 13.66600 0)*(Y) , (Y) = (0 0.07317 0)*(Y0) are defined as:
 (Z0) (0 0 23.07111) (Z) , (Z) (0 0 0.04334) (Z0) A0 // A, C0 // C*, B0 // C0 X A0

Space Group Symmetry

(See e.g. G. Burns & A.M. Glazer, Space Groups for Solid State Scientists, Academic Press, 1990 or Int. Tables A)

Space Group P21/c No: 14, Laue: 2/m [Hall: -P 2ybc]

Lattice Type mP, Centric, Monoclinic, Order 4(2) [Schoenflies: C2h^5]

Nr ***** Symmetry Operation(s) *****

1	X ,	Y ,	Z
2	- X ,	1/2 + Y ,	1/2 - Z
3	- X ,	- Y ,	- Z
4	X ,	1/2 - Y ,	1/2 + Z

ADDSYM - CHECK (cf. MISSYM (C): Le Page, Y., J. Appl. Cryst. (1987), 20, 264-269; J. Appl. Cryst. (1988), 21, 983-984)

- ADDSYM Search on ALL NON-H Chemical Types [Max NonFit 20 Perc]
 - Number of Input Atoms Included in Search 69 (Unitcell 276)
 - Density based on Input Atom Set = 1.142 g.cm-3 - Vol / Non-H atom = 21.4 Ang+3
 - The Structure Implies the Following Symmetry Elements Subject to the Criteria:
 Criteria: 1.00 Deg (Metric), 0.25 Ang (Rot.), 0.45 Ang (Inv), 0.45 Ang (Transl)

Symm. Elem	Input Cell	Reduced Cell	Row	(Ang) d	(Deg) Typ	(%) Dot	(Ang) Angle	(%) Fit	(Ang) MaxDev.	Input Cell x	Input Cell y	Input Cell z
c	[0 1 0]	[1 0 0]		13.67	2 1	0.00	100		0	through	0	1/4 0
										Glide =	0	0 1/2
-1							100		0	at	0	0 0

T.R.A.N.S.F.O.R.M.A.T.I.O.N M.A.T.R.I.X for CELL and HKL DATA

Reduced->Convent	Input->Reduced	T = Input->Convent:	a' = T a
(0 1 0)	(0 -1 0)	(1 0 0)	Det(T)
(-1 0 0)	X (1 0 0)	= (0 1 0)	=
(0 0 1)	(0 0 1)	(0 0 1)	1.000

Cell Lattice	a	b	c	Alpha	Beta	Gamma	Volume	CrystalSystem	Laue
Input mP	18.701	13.666	23.540	90.00	101.46	90.00	5896	Monoclinic	2/m
Reduced P	13.666	18.701	23.540	101.46	90.00	90.00	5896		
Convent mP	18.701	13.666	23.540	90.00	101.46	90.00	5896	Monoclinic	2/m

:: *** No Obvious Extra Crystallographic Symmetry was Detected ***

:: Note: Rerun in EQUAL Atom Type Mode for more Checks