PLATON(V-311206)-Run for: klat85 - SHELXL TIME: Nov 29 22:42:04 2011

Crystal Data

Input Cell (Lattice Type: P) - Temp = 200K

a =	14.371(6)	Angstrom	alpha =	90	Degree	a =	9.736	alpha =	103.77
b =	9.736(4)		beta =	109.716(18)		b =	14.371	beta =	90.00
c =	25.297(8)		gamma =	90		c =	24.519	gamma =	90.00
V =	3332(2)	Cubic-Angstrom	d(100) =	13.5285	Angstrom				
			d(010) =	9.7360					
Lambda(MoKa) =	0.71073	Angstrom	d(001) =	23.8140					

Reduced Cell (Acta Cryst.(1976),A32,297-298)

V = 3332.0

Niggli Values

94.790	206.526	601.175
-83.882	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)

$$\begin{pmatrix} XO \\ YO \\ ZO \end{pmatrix} = \begin{pmatrix} 14.37100 & 0 & -8.53415 \\ 0 & 9.73600 & 0 \\ 0 & 0 & 23.81400 \end{pmatrix} \begin{pmatrix} X \\ Y \\ Z \end{pmatrix} , \quad \begin{pmatrix} X \\ Y \\ Z \end{pmatrix} = \begin{pmatrix} 0.06958 & 0 & 0.02494 \\ 0 & 0.10271 & 0 \\ 0 & 0 & 0.04199 \end{pmatrix} \begin{pmatrix} XO \\ YO \\ ZO \end{pmatrix}$$

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

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   39 (Unitcell 156)
- Density based on Input Atom Set = 1.175 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_Row	Reduced Cell_Row	(Ang) d	Typ	Dot	(Deg) Angle	(%) Fit	(Ang) MaxDev.		Input Cell x	y	z
c	[0 1 0]	[1 0 0]	9.74	2	1	0.00	100	0	through	0	3/4	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 -1 -1)	(-1 0 -1)	(0 0 1)	1.000

Cell	Lattice	a	b	c	Alpha	Beta	Gamma	Volume	CrystalSystem	Laue
Input	mP	14.371	9.736	25.297	90.00	109.72	90.00	3332	Monoclinic	2/m
Reduced	P	9.736	14.371	24.519	103.77	90.00	90.00	3332		
Convent	mP	14.371	9.736	25.297	90.00	109.72	90.00	3332	Monoclinic	2/m

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

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