

PLATON(V-311206)-Run for: a in C222

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Crystal Data

Input Cell (Lattice Type: C)		Temp = 296K	Reduced Cell (Acta Cryst.(1976), A32, 297-298)	
a = 6.840(3) Angstrom	alpha = 90 Degree		a = 4.207	alpha = 108.09 V = 301.2
b = 20.936(10)	beta = 90		b = 6.840	beta = 90.00
c = 4.2067(17)	gamma = 90		c = 11.013	gamma = 90.00
V = 602.4(5) Cubic-Angstrom	d(100) = 6.8401 Angstrom		Niggli Values	
	d(010) = 20.9364		17.696	46.787 121.280
Lambda(MoKa) = 0.71073 Angstrom	d(001) = 4.2067		-23.393	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) (6.84000 0 0) (X) , (X) (0.14620 0 0) (X0) Orthogonal Axes A0, B0 and C0
 (Y0) = (0 20.93600 0)*(Y) , (Y) = (0 0.04776 0)*(Y0) are defined as:
 (Z0) (0 0 4.20670) (Z) , (Z) (0 0 0.23772) (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 C222 No: 21, Laue: mmm [Hall: C 2 2]

Lattice Type oC, Acentric, Orthorhombic, Order 8(4) [Schoenflies: D2^6]

CHIRAL - See P.G. Jones, Acta Cryst. (1986), A42, 57.

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

1	X ,	Y ,	Z
2	- X ,	- Y ,	Z
3	X ,	- Y ,	- Z
4	- X ,	Y ,	- Z
5	1/2 + X ,	1/2 + Y ,	Z
6	1/2 - X ,	1/2 - Y ,	Z
7	1/2 + X ,	1/2 - Y ,	- Z
8	1/2 - X ,	1/2 + Y ,	- 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]

:: Excluded Disorder Atoms From ADDSYM Analysis:

Ge6A Ge7A Zn4A Zn5A

- Number of Excluded Disordered Input Atoms = 4

- Number of Input Atoms Included in Search 3 (Unitcell 5)

- Density based on Input Atom Set = 6.841 g.cm-3 - Vol / Non-H atom = 23.4 Ang+3

- The Structure Implies the Following Symmetry Elements Subject to the Criteria:

Criteria: 1.00 Deg (Metric), 0.25 Ang (Rot.), 0.25 Ang (Inv), 0.25 Ang (Transl)

Symm.	Input	Reduced	(Ang)		(Deg)	(%)	(Ang)					Input	Cell	
Elem	Cell_Row	Cell_Row	d	Typ	Dot	Angle	Fit	MaxDev.				x	y	z
m *	[0 0 1]	[1 0 0]	4.21	2	1	0.00	100	0.002	through			0	0	0
							La3A	-La3A						
m *	[0 1 0]	[0 1 2]	20.94	2	2	0.00	100	0.002	through			0	0	0
							La3A	-La3A						
m *	[1 0 0]	[0-1 0]	6.84	2	2	0.00	100	0.002	through			0	0	0
							La3A	-La3A						
-1 *	=====						100	0.002	at			0	0	0
							La3A	-La3A						

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 0 -1)	(1 0 0)	Det(T)
(0 -1 -2) X	(-1 0 0)	(0 -1 0)	=
(1 0 0)	(1/2 1/2 0)	(0 0 -1)	1.000

Cell Lattice	a	b	c	Alpha	Beta	Gamma	Volume	CrystalSystem	Laue
Input oC	6.840	20.936	4.207	90.00	90.00	90.00	602	Orthorhombic	mmm
Reduced P	4.207	6.840	11.013	108.09	90.00	90.00	301		
Convent oC	6.840	20.936	4.207	90.00	90.00	90.00	602	Orthorhombic	mmm

Conventional, New or Pseudo Symmetry

Space Group Cmmm No: 65, Laue: mmm [Hall: -C 2 2]

Lattice Type oC, Centric, Orthorhombic, Order 16(4) [Schoenflies: D2h¹⁹]

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

1	X ,	Y ,	Z
2	- X ,	- Y ,	Z
3	X ,	- Y ,	- Z
4	- X ,	Y ,	- Z
5	- X ,	- Y ,	- Z
6	X ,	Y ,	- Z
7	- X ,	Y ,	Z
8	X ,	- Y ,	Z
9	1/2 + X ,	1/2 + Y ,	Z
10	1/2 - X ,	1/2 - Y ,	Z
11	1/2 + X ,	1/2 - Y ,	- Z
12	1/2 - X ,	1/2 + Y ,	- Z
13	1/2 - X ,	1/2 - Y ,	- Z
14	1/2 + X ,	1/2 + Y ,	- Z
15	1/2 - X ,	1/2 + Y ,	Z
16	1/2 + X ,	1/2 - Y ,	Z

:: Origin Shifted to: 0.0000, 0.0000, 0.0000 after Transformation

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::
::      ( 1.0000 0.0000 0.0000) ( 0.0000)
:: R/t for Coordinates ( 0.0000 -1.0000 0.0000) ( 0.0000)
::      ( 0.0000 0.0000 -1.0000) ( 0.0000)
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:: * Symmetry Elements Preceded by an Asterisk are New and Indicate
:: Missed/Pseudosymmetry. Proposed Inversion or (Glide) Planes do NOT Apply
:: for Chiral Molecules.
:: Note: Glide Plane Codes are with Reference to the Input Cell !!
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P! a in C222 oC=>oC 0.0 0 0 0.000 0.00 0.500 100% Cmmm

:: An SPF-style file is written to be used for the cell transformation.