Appendix A1

Name and formula

Reference code:	01-070-3038
Mineral name:	Copper
Compound name:	Copper
Empirical formula:	Cu
Chemical formula:	Cu

Crystallographic parameters

Crystal system:	Cubic
Space group:	Fm-3m
Space group number:	225
a (Å):	3.6250
b (Å):	3.6250
c (Å):	3.6250
Alpha (°):	90.0000
Beta (°):	90.0000
Gamma (°):	90.0000
Calculated density (g/cm^3):	8.86
Measured density (g/cm^3):	8.93
Volume of cell (10^6 pm^3):	47.63
Z:	4.00
RIR:	8.87

Subfiles and quality

Subfiles:	Alloy, metal or intermetalic ICSD Pattern Inorganic Mineral
Quality:	Calculated (C)

Comments

Creation Date:	1/1/1970
Modification Date:	1/1/1970
ICSD Collection Code:	053246
Test from ICSD:	REF Current Science
Test from ICSD:	REF Acta Crystallographica A (24,1968-38,1982)
Test from ICSD:	ACACB 25 (1969) 676-682
Test from ICSD:	CLAS m-3m (Hermann-Mauguin) - Oh (Schoenflies)
Test from ICSD:	PRS cF4
Test from ICSD:	ANX N
Test from ICSD:	WYCK a

Calculated Pattern Original Remarks: REM M Cell from 2nd reference: 3.61491 at RT, 3.61536 at 308. Calculated Pattern Original Remarks: REM 3.61638 at 328 K. Calculated Pattern Original Remarks: REM M PDF 00-004-0836. Test from ICSD: No R value given in the paper. (Code 51). Test from ICSD: At least one temperature factor missing in the paper. (C. Additional Patterns: See PDF 01-085-1326. Accurate evaluation of lattice parameters of alpha-brasses.

References

Primary reference: *Calculated from ICSD using POWD-12++*
Structure: Srinavasa-Rao, S., Anantharaman, T.R., *Curr. Sci.*, **32**, 262, (1963)

Peak list

No.	h	k	l	d [A]	2Theta[deg]	I [%]
1	1	1	1	2.09289	43.192	100.0
2	2	0	0	1.81250	50.300	42.7
3	2	2	0	1.28163	73.888	17.2
4	3	1	1	1.09298	89.622	15.7

Structure

No.	Name	Elem.	X	Y	Z	Biso	sof	Wyck.
1	CU1	Cu	0.00000	0.00000	0.00000	0.5000	1.0000	4a

Stick Pattern