Entry # 96-900-8815

Phase classification

Name	Brass
Formula	CuZn
I/Ic	16.820000
Sample Name	9008814
Quality	C (calculated)

References

Publication

Bibliography	Wyckoff R. W. G., "Second edition. Interscience Publishers, New York, New YorkNote: CsCl structure, cesium chloride structure", Crystal Structures **1**, 85-237 (1963).

Origin of data

Source of entry	COD (Crystallography Open Database)
Link to orig. entry	9008814

Crystal structure

Crystallographic data

Space group	P m -3 m (221)
Crystal system	cubic
Cell parameters	a= 2.94500 Å

Atom coordinates

Element	Oxid.	*x*	*y*	*z*	Bi	Focc
Cu		0.000	0.000	0.000	1.000000	1.000000
Zn		0.500	0.500	0.500	1.000000	1.000000

Diffraction data

Diffraction lines

d [Å]	Int.	h	k	l	Mult.
2.9450	0.3	1	0	0	6
2.0824	1000.0	1	0	1	12
1.7003	0.1	1	1	1	8
1.4725	136.4	2	0	0	6
1.3170	0.2	2	0	1	24
1.2023	233.2	2	1	1	24
1.0412	68.8	2	0	2	12

Experimental

Physical Properties

Calc. density	8.38200 g/cm³

Entry # 96-210-2764

Phase classification

Name	
Formula	Si
I/Ic	4.970000
Sample Name	2102763
Quality	C (calculated)

References

Publication

Bibliography	Wu Hui, Hartman Michael R., Udovic Terrence J., Rush John J., Zhou Wei, Bowman Jr Robert C., Vajo John J., "Structure of the novel ternary hydrides Li~4~*Tt*~2~D (*Tt*= Si and Ge)", Acta Crystallographica Section B **63(1)**, 63-68 (2007).

Origin of data

Source of entry	COD (Crystallography Open Database)
Link to orig. entry	2102763

Crystal structure

Crystallographic data

Space group	F d -3 m (227)
Crystal system	cubic
Cell parameters	a= 5.42712 Å
Z	8

Atom coordinates

Element	Oxid.	*x*	*y*	*z*	Bi	Focc
Si		0.125	0.125	0.125	0.568000	1.000000

Diffraction data

Diffraction lines

d [Å]	Int.	h	k	l	Mult.
3.1333	1000.0	1	1	1	8
1.9188	639.2	2	0	2	12
1.6363	369.6	3	1	1	24
1.3568	94.3	4	0	0	6
1.2451	138.7	3	1	3	24
1.1078	189.2	4	2	2	24
1.0444	107.8	5	1	1	24
0.9594	69.7	4	0	4	12
0.9174	136.0	5	3	1	48
0.8581	145.7	6	0	2	24
0.8276	82.7	5	3	3	24
0.7833	104.9	4	4	4	8

Experimental

Physical Properties

Calc. density	2.33400 g/cm³

Entry # 96-153-9325

Phase classification

Name	Zn Se
Formula	SeZn
I/Ic	12.570000
Sample Name	1539324
Quality	C (calculated)

References

Publication

Bibliography	Shalimova K.V., Botnev A.F., Dmitriev V.A., Kognovitskaya N.Z., Starostin V.V., "Crystal structure of solid solutions on the Zn Se - Cd Se system", Soviet Physics, Crystallography (= Kristallografiya) **14**, 531-534 (1969).

Origin of data

Source of entry	COD (Crystallography Open Database)
Link to orig. entry	1539324

Crystal structure

Crystallographic data

Space group	F -4 3 m (216)
Crystal system	cubic
Cell parameters	a= 5.65000 Å
Z	4

Atom coordinates

Element	Oxid.	*x*	*y*	*z*	Bi	Focc
Se		0.000	0.000	0.000	1.000000	1.000000
Zn		0.250	0.250	0.250	1.000000	1.000000

Diffraction data

Diffraction lines

d [Å]	Int.	h	k	l	Mult.
3.2620	1000.0	1	1	1	8
2.8250	2.8	0	2	0	6
1.9976	678.5	2	0	2	12
1.7035	387.4	3	1	1	24
1.6310	0.8	2	2	2	8
1.4125	93.7	0	4	0	6
1.2962	133.4	3	1	3	24
1.2634	1.4	4	0	2	24
1.1533	168.3	2	4	2	24
1.0873	92.1	5	1	1	24
0.9988	54.0	4	0	4	12
0.9550	100.4	5	1	3	48
0.9417	1.3	0	6	0	6
0.8933	95.1	6	0	2	24
0.8616	49.7	3	5	3	24
0.8518	1.2	6	2	2	24
0.8155	39.9	4	4	4	8
0.7912	166.3	7	1	1	24
0.7835	2.6	6	0	4	24

Experimental

Physical Properties

Calc. density	5.31600 g/cm³

Entry # 96-901-3402

Phase classification

Name	
Mineral Name	Galena
Formula	PbS
I/Ic	18.770000
Sample Name	9013401
Quality	C (calculated)

References

Publication

Bibliography	Noda Y., Masumoto K., Ohba S., Saito Y., Toriumi K., Iwata Y., Shibuya I., "Temperature dependence of atomic thermal parameters of lead chalcogenides,PbS, PbSe and PbTe Locality: synthetic Sample: T = 150 K", Acta Crystallographica, Section C **43**, 1443-1445 (1987).

Origin of data

Source of entry	COD (Crystallography Open Database)
Link to orig. entry	9013401

Crystal structure

Crystallographic data

Space group	F m -3 m (225)
Crystal system	cubic
Cell parameters	a= 5.91810 Å
Cell meas. conditions	T= 150.0 K

Atom coordinates

Element	Oxid.	*x*	*y*	*z*	Bi	Focc
Pb		0.000	0.000	0.000	0.690000	1.000000
S		0.500	0.500	0.500	0.709000	1.000000

Diffraction data

Diffraction lines

d [Å]	Int.	h	k	l	Mult.
3.4168	977.5	1	1	1	8
2.9590	1000.0	2	0	0	6
2.0924	725.3	2	0	2	12
1.7844	476.1	3	1	1	24
1.7084	248.3	2	2	2	8
1.4795	112.2	4	0	0	6
1.3577	185.0	3	1	3	24
1.3233	300.4	4	0	2	24
1.2080	218.8	4	2	2	24
1.1389	136.1	5	1	1	24
1.0462	72.7	4	0	4	12
1.0003	150.8	5	3	1	48
0.9863	164.4	6	0	0	6
0.9357	126.8	6	0	2	24
0.9025	72.5	5	3	3	24
0.8922	130.1	6	2	2	24
0.8542	47.6	4	4	4	8
0.8287	184.0	7	1	1	24
0.8207	172.0	4	6	0	24
0.7908	514.7	6	4	2	48

Experimental

Physical Properties

Calc. density	7.66700 g/cm³

Entry # 96-901-1683

Phase classification

Name	
Mineral Name	Bromargyrite
Formula	AgBr
I/Ic	12.580000
Sample Name	9011682
Quality	C (calculated)

References

Publication

Bibliography	Hull S., Keen D. A., "Pressure-induced phase transitions in AgCl, AgBr, and AgILocality: syntheticSample: P = 0.0 GPa, Phase I", Physical Review B **59**, 750-761 (1999).

Origin of data

Source of entry	COD (Crystallography Open Database)
Link to orig. entry	9011682

Crystal structure

Crystallographic data

Space group	F m -3 m (225)
Crystal system	cubic
Cell parameters	a= 5.77210 Å

Atom coordinates

Element	Oxid.	*x*	*y*	*z*	Bi	Focc
Ag		0.500	0.500	0.500	6.299000	1.000000
Br		0.000	0.000	0.000	3.299000	1.000000

Diffraction data

Diffraction lines

d [Å]	Int.	h	k	l	Mult.
3.3325	31.5	1	1	1	8
2.8860	1000.0	2	0	0	6
2.0407	536.3	2	0	2	12
1.7404	0.5	3	1	1	24
1.6663	137.6	2	2	2	8
1.4430	47.4	4	0	0	6
1.3242	0.6	3	1	3	24
1.2907	97.9	4	0	2	24
1.1782	55.8	4	2	2	24
1.1108	1.4	5	1	1	24
1.0204	11.8	4	0	4	12
0.9757	2.3	5	3	1	48
0.9620	21.5	6	0	0	6
0.9126	13.5	6	0	2	24
0.8802	1.3	5	3	3	24
0.8702	11.5	6	2	2	24
0.8331	3.5	4	4	4	8
0.8083	3.5	7	1	1	24
0.8004	11.5	4	6	0	24

Experimental

Physical Properties

Calc. density	6.48500 g/cm³

Entry # 96-900-8800

Phase classification

Name	
Formula	AgMg
I/Ic	16.209999
Sample Name	9008799
Quality	C (calculated)

References

Publication

Bibliography	Wyckoff R. W. G., "Second edition. Interscience Publishers, New York, New YorkNote: CsCl structure, cesium chloride structure", Crystal Structures **1**, 85-237 (1963).

Origin of data

Source of entry	COD (Crystallography Open Database)
Link to orig. entry	9008799

Crystal structure

Crystallographic data

Space group	P m -3 m (221)
Crystal system	cubic
Cell parameters	a= 3.28000 Å

Atom coordinates

Element	Oxid.	*x*	*y*	*z*	Bi	Focc
Ag		0.000	0.000	0.000	1.000000	1.000000
Mg		0.500	0.500	0.500	1.000000	1.000000

Diffraction data

Diffraction lines

d [Å]	Int.	h	k	l	Mult.
3.2800	539.6	1	0	0	6
2.3193	1000.0	1	0	1	12
1.8937	132.2	1	1	1	8
1.6400	148.5	2	0	0	6
1.4669	150.9	2	0	1	24
1.3391	264.5	2	1	1	24
1.1597	75.1	2	0	2	12
1.0933	63.8	3	0	0	6
1.0372	104.9	3	0	1	24

Experimental

Physical Properties

Calc. density	6.22000 g/cm³

Entry # 96-900-8808

Phase classification

Name	
Formula	BeCu
I/Ic	8.790000
Sample Name	9008807
Quality	C (calculated)

References

Publication

Bibliography	Wyckoff R. W. G., "Second edition. Interscience Publishers, New York, New YorkNote: CsCl structure, cesium chloride structure", Crystal Structures **1**, 85-237 (1963).

Origin of data

Source of entry	COD (Crystallography Open Database)
Link to orig. entry	9008807

Crystal structure

Crystallographic data

Space group	P m -3 m (221)
Crystal system	cubic
Cell parameters	a= 2.69800 Å

Atom coordinates

Element	Oxid.	*x*	*y*	*z*	Bi	Focc
Be		0.000	0.000	0.000	1.000000	1.000000
Cu		0.500	0.500	0.500	1.000000	1.000000

Diffraction data

Diffraction lines

d [Å]	Int.	h	k	l	Mult.
2.6980	1000.0	1	0	0	6
1.9078	924.6	1	0	1	12
1.5577	201.7	1	1	1	8
1.3490	117.9	2	0	0	6
1.2066	203.4	2	0	1	24
1.1015	207.9	2	1	1	24

Experimental

Physical Properties

Calc. density	6.13500 g/cm³

Entry # 96-900-3138

Phase classification

Name	
Mineral Name	Sylvite
Formula	ClK
I/Ic	6.410000
Sample Name	9003137
Quality	C (calculated)

References

Publication

Bibliography	Walker D., Verma P. K., Cranswick L. M. D., Jones R. L., Clark S. M., Buhre S., "Halite-sylvite thermoelasticitySample: msl515037, T = 600 C, P = 0.0 kbar, cell volume = 270.14 ang**3", American Mineralogist **89**, 204-210 (2004).

Origin of data

Source of entry	COD (Crystallography Open Database)
Link to orig. entry	9003137

Crystal structure

Crystallographic data

Space group	F m -3 m (225)
Crystal system	cubic
Cell parameters	a= 6.46440 Å
Cell meas. conditions	T= 873.1 K

Atom coordinates

Element	Oxid.	*x*	*y*	*z*	Bi	Focc
K		0.000	0.000	0.000	1.000000	1.000000
Cl		0.500	0.500	0.500	1.000000	1.000000

Diffraction data

Diffraction lines

d [Å]	Int.	h	k	l	Mult.
3.7322	5.7	1	1	1	8
3.2322	1000.0	2	0	0	6
2.2855	654.0	2	0	2	12
1.9491	3.7	3	1	1	24
1.8661	205.6	2	2	2	8
1.6161	86.8	4	0	0	6
1.4830	1.0	3	1	3	24
1.4455	219.1	4	0	2	24
1.3195	150.6	4	2	2	24
1.2441	0.4	5	1	1	24
1.1428	43.7	4	0	4	12
1.0927	0.3	5	3	1	48
1.0774	90.8	6	0	0	6
1.0221	63.7	6	0	2	24
0.9858	0.1	5	3	3	24
0.9745	58.7	6	2	2	24
0.9331	18.9	4	4	4	8
0.9052	0.2	7	1	1	24
0.8965	57.1	4	6	0	24
0.8638	120.6	6	4	2	48
0.8416	0.3	7	3	1	48
0.8080	20.7	8	0	0	6
0.7898	0.2	7	3	3	24
0.7839	264.3	8	0	2	24

Experimental

Physical Properties

Calc. density	1.83300 g/cm³