CsCl ($B2$) Structure: AB_cP2_221_a_b-002

This structure originally had the label `AB_cP2_221_b_a`. Calls to that address will be redirected here.

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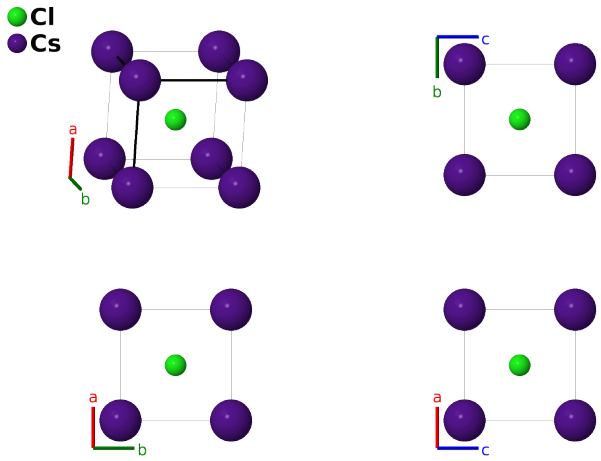
https://aflow.org/p/QM6B

https://aflow.org/p/AB_cP2_221_a_b-002



Prototype	ClCs
AFLOW prototype label	AB_cP2_221_a_b-002
***Strukturbericht* designation**	$B2$
ICSD	622367
Pearson symbol	cP2
Space group number	221
Space group symbol	$Pm\bar{3}m$
AFLOW prototype command	`aflow --proto=AB_cP2_221_a_b-002 --params=`a

Other compounds with this structure

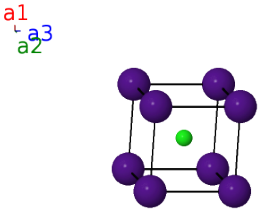
AgCd, AgCe, AgDy, AgGd, AgHo, AgLa, AgLi, AgLu, AgMg, AgNd, AgSc, AgSm, AgTb, AgTm, AgZn, AlCe, AlCo, AlDy, AlFe, AlIr, AlLu, AlMg, AlNd, AlNi, AlOs, AlPd (H.T.), AlRe, AlRh, AlRu, AuCd, AuCs, AuDy, AuGd, AuHRb, AuHo, AuLa, AuLi, AuLu, AuMg, AuMn (H.T.), AuNd, AuPr, AuSc, AuSm, AuTb, AuTi (H.T.), AuTm, AuY, AuZn, BaCd, BaHg, BeNi, BePd, BiTl, CaCd, CaHg, CaIn, CaTl, CdCe, CdGd, CdLa, CdPr, CdSc, CdSm, CdSr, CdY, CeHg, CeMg, CeZn, CoFe, CoGa, CoHf, CoSc, CoTi, CoZr, CuDy, CuEr, CuGd, CuSc, CuSm, CuTb, CuTm, CuY, DyIn, DyMg, DyTl, DyZn, ErMg, ErZn, FeRh, FeTi, FeV, GaIr, GaNi, GaRu, GdHg, GdIn, GdMg, GdRh, GdTl, GdZn, HfRu, HfTc, HgLa, HgLi, HgMg, HgMn, HgPr, HgSc, HgSr, HgY, HoIr, HoMg, HoRh, HoZn, InNi, InPd, IrMn, IrSc, IrTm, LuMg, LuPd, LuRh, MgNd, MgPd, MgPr, MgRh, MgSm, MgTb, MgTm, MgV, NdTl, NdZn, NiSc, NiTi, NiZn (H.T.), OsTl, OsV, OsZr, PdSc, PdSm, PdZn, PtSc, PuRu, ReTi, RhSc, RhSi, RhSm, RhTb, RhTi, RhTm, RhZr, ScZn, SmZn, SrTl, TaTc, TbZn, TcTi, TcV, TeTh, TiZn, TlY, TmZn, YZn

- The atoms are on the sites of a body-centered cubic lattice.

- We extrapolated the lattice constants of (Ganesan, 1986) to 0K. The ICSD entry uses their lattice constant at 298K.

Simple Cubic primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = a\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	Cl I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(1b)	Cs I

References

[1] V. Ganesan and K. S. Girirajan, *Lattice parameter and thermal expansion of CsCl and CsBr by x-ray powder diffraction. I. Thermal expansion of CsCl from room temperature to 90° K*, Paramana – Journal of Physics **27**, 469–474 (1986), doi:10.1007/BF02846872.