Rock Salt/Halite (NaCl, $B1$) Structure: AB_cF8_225_a_b-001

This structure originally had the label `AB_cF8_225_a_b`. Calls to that address will be redirected here.

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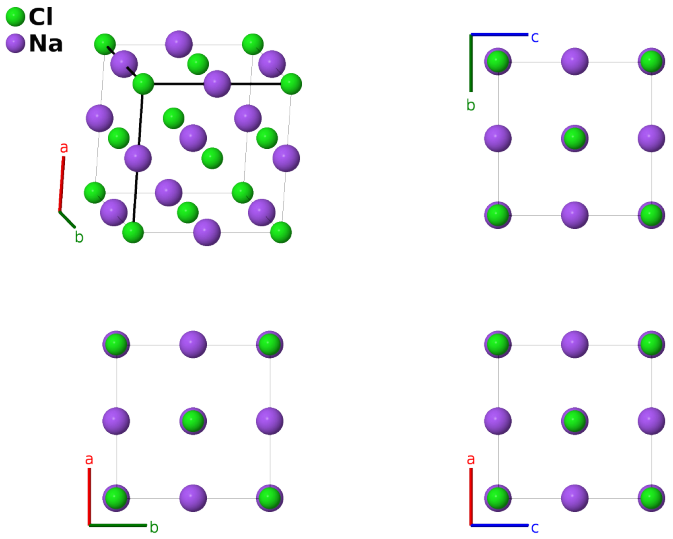
https://aflow.org/p/Q53X

https://aflow.org/p/AB_cF8_225_a_b-001



Prototype	NaCl
AFLOW prototype label	AB_cF8_225_a_b-001
***Strukturbericht* designation**	$B1$
Mineral name	halite
ICSD	240598
Pearson symbol	cF8
Space group number	225
Space group symbol	$Fm\bar{3}m$
AFLOW prototype command	`aflow --proto=AB_cF8_225_a_b-001 --params=`a

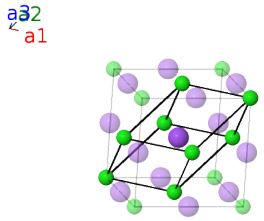
Other compounds with this structure

AgCl, AmO, BaO, BaPo, BaS, BaSe, BaTe, CaO, CaPo, CaS, CaSe, CdO, CeAs, CeBi, CeN, CeP, CeS, CeSb, CeSe, CeTe, CoO, CrN, DyAs, DyBi, DyN, DyP, DyS, DySb, DySe, DyTe, ErAs, ErBi, ErN, ErP, ErS, ErSb, ErSe, ErTe, EuN, EuO, EuS, EuSe, EuTe, GdAs, GdN, GdSb, GdSe, GdTe, HfB, HfC, HfN, HoAs, HoBi, HoN, HoP, HoS, HoSb, HoSe, HoTe, KBr, LaAs, LaBi, LaN, LaP, LaS, LaSb, LaTe, LiCl, LiF, LiH, LuN, LuS, LuSb, MgO, MgS, MgSe, MnO, MnS, MnSe, MnTe, NU, NaBr, NaF, NaH, NbO, NdAs, NdBi, NdN, NdP, NdS, NdTe, NiO, NpC, NpN, NpO, PaO, PbPo, PbS, PbSe, PbTe, PdH, PrAs, PrBi, PrN, PrP, PrS, PrSb, PrSe, PuAs, PuB, PuBi, PuC, PuN, PuO, PuP, PuS, PuTe, RbF, RbH, ScAs, ScBi, ScC, ScN, ScP, ScSb, SmAs, SmN, SmO, SmP, SmS, SmSe, SmTe, SmTm, SnAs, SnSb, SnSe, SrO, SrS, SrTe, TaC, TaO, TbAs, TbBi, TbN, TbP,

TbS, TbSb, TbSe, TbTe, ThAs, ThC, ThGe, ThN, ThSb, TiC, Tin, TiO, TmAs, TmBi, TmN, TmP, TmSb, TmSe, TmTe, UAs, UBi, UC, UO, UP, US, USb, USe, UTe, VO, YAs, YBi, YN, YP, YS, YSb, YSe, YTe, YbAs, YbN, YbO, YbP, YbS, YbSb, YbSe, YbTe, ZnSe, ZrB, ZrC, ZrN, ZrO, ZrS

Face-centered Cubic primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(4a)	Cl I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(4b)	Na I

References

[1] D. Walker, P. K. Verma, L. M. D. Cranswick, R. L. Jones, S. M. Clark, and S. Buhre, *Halite-sylvite thermoelasticity*, Am. Mineral. **89**, 204–210 (2004).

Found in

[1] R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).