$Rb_3Mn_2Cl_7$ Structure: A7B2C3_tI24_139_aeg_e_be-001

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https://aflow.org/prototype-encyclopedia/7JA2

https://aflow.org/prototype-encyclopedia/A7B2C3_tI24_139_aeg_e_be-001

Prototype	$Cl_7Mn_2Rb_3$
AFLOW prototype label	A7B2C3_tI24_139_aeg_e_be-001
ICSD	9491
CCDC	1594478
Pearson symbol	tI24
Space group number	139
Space group symbol	$I4/mmm$
AFLOW prototype command	`aflow --proto=A7B2C3_tI24_139_aeg_e_be-001 --params=`$a, c/a, z_3, z_4, z_5, z_6$

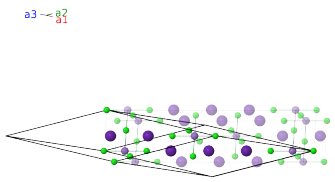
Other compounds with this structure

$Cs_3Ca_2Cl_7$, $Cs_3Mg_2Cl_7$, $K_3Mn_2Cl_7$, $Rb_3Mn_2Br_7$

- Quaternary compounds with this structure are listed under the $Sr_3Sc_2O_5Cl_2$ prototype. The ICSD list some, but not all, of those structures under the $Rb_3Mn_2Cl_7$ structure type.

Body-centered Tetragonal primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	Cl I

$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(2b)	Rb I
$\mathbf{B_3}$	=	$z_3\,\mathbf{a}_1 + z_3\,\mathbf{a}_2$	=	$cz_3\,\hat{\mathbf{z}}$	(4e)	Cl II
$\mathbf{B_4}$	=	$-z_3\,\mathbf{a}_1 - z_3\,\mathbf{a}_2$	=	$-cz_3\,\hat{\mathbf{z}}$	(4e)	Cl II
$\mathbf{B_5}$	=	$z_4\,\mathbf{a}_1 + z_4\,\mathbf{a}_2$	=	$cz_4\,\hat{\mathbf{z}}$	(4e)	Mn I
$\mathbf{B_6}$	=	$-z_4\,\mathbf{a}_1 - z_4\,\mathbf{a}_2$	=	$-cz_4\,\hat{\mathbf{z}}$	(4e)	Mn I
$\mathbf{B_7}$	=	$z_5\,\mathbf{a}_1 + z_5\,\mathbf{a}_2$	=	$cz_5\,\hat{\mathbf{z}}$	(4e)	Rb II
$\mathbf{B_8}$	=	$-z_5\,\mathbf{a}_1 - z_5\,\mathbf{a}_2$	=	$-cz_5\,\hat{\mathbf{z}}$	(4e)	Rb II
$\mathbf{B_9}$	=	$\left(z_6 + \frac{1}{2}\right)\,\mathbf{a}_1 + z_6\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8g)	Cl III
$\mathbf{B_{10}}$	=	$z_6\,\mathbf{a}_1 + \left(z_6 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + cz_6\,\hat{\mathbf{z}}$	(8g)	Cl III
$\mathbf{B_{11}}$	=	$-\left(z_6 - \frac{1}{2}\right)\,\mathbf{a}_1 - z_6\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(8g)	Cl III
$\mathbf{B_{12}}$	=	$-z_6\,\mathbf{a}_1 - \left(z_6 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - cz_6\,\hat{\mathbf{z}}$	(8g)	Cl III

References

[1] M. Amit, A. Horowitz, and J. Makovsky, *Crystal Structure of Rb_2CoCl_4 and $Rb_3Mn_2Cl_7$*, Israel J. Chem. **10**, 715–719 (1972), doi:10.1002/ijch.197200070.

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Cl
Mn
Rb