Crystal structure of lithium magnesium chloride, $\text{Li}_{1.7}\text{Mg}_{1.15}\text{Cl}_4$

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Source of material: Single crystals of $\text{Li}_{1.7}\text{Mg}_{1.15}\text{Cl}_4$ were grown from the melt at a cooling rate of 5K/h (see ref. 1).

The nonstoichiometric compound $\text{Li}_{1.7}\text{Mg}_{1.15}\text{Cl}_4$ crystallizes in the inverse spinel type. Hence, the assumption that in the case of lithium deficient spinel type chlorides the phase transition to the likewise cubic Li_2MnBr_4 *cF56*-type NaCl superstructure occurs below ambient temperature (see ref. 2) has not been confirmed.

$\text{Cl}_4\text{Li}_{1.70}\text{Mg}_{1.15}$, cubic, $Fd\bar{3}m$ (No. 227), $a = 10.417(1) \text{ \AA}$, $V = 1130.4 \text{ \AA}^3$, $Z = 8$, $R(F) = 0.016$, $R_w(F) = 0.013$.

Table 1. Parameters used for the X-ray data collection

Crystal:	colorless, irregular crystal, size 0.26 x 0.22 x 0.18 mm
Wavelength:	Mo $K\alpha$ radiation (0.71069 Å)
μ :	20.56 cm^{-1}
Diffractometer:	Enraf-Nonius CAD4
Scan mode:	$\omega/2\theta$
$T_{\text{measurement}}$:	293 K
$2\theta_{\text{max}}$:	80°
$N(hkl)_{\text{unique}}$:	200
Criterion for I_o :	$I_o > 2 \sigma(I_o)$
$N(\text{param})_{\text{refined}}$:	10
Program:	SDP

Table 2. Final atomic coordinates and displacement parameters (in $\text{\AA}^2$)

Atom	Site	Occ.	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Li(1)	8a	0.850	1/8	1/8	1/8	0.032(2)	U_{11}	U_{11}	0	0	0
Mg	16d	0.575	1/2	1/2	1/2	0.0187(2)	U_{11}	U_{11}	-0.0022(3)	U_{12}	U_{12}
Li(2)	16d	0.425	1/2	1/2	1/2	0.0187	U_{11}	U_{11}	-0.0022	U_{12}	U_{12}
Cl	32e		0.25723(2)	x	x	0.01830(5)	U_{11}	U_{11}	-0.00144(7)	U_{12}	U_{12}

References

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