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Crystal structure of dirubidium lithium dysprosium(III) hexabromide, $Rb_2LiDyBr_6$

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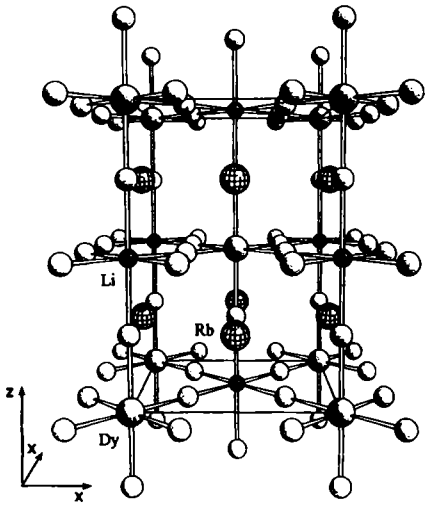
Received June 27, 1996, transferred to 2nd update of database ICSD in 1997, CSD-No. 402536



$Br_6DyLiRb_2$, tetragonal, *I4/mmm* (No. 139), a =7.699(5) Å, c =11.032(6) Å, V =653.9 Å^3, Z =2, $R(F)$ =0.099, $R_w(F^2)$ =0.241.

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

Crystal:	colorless, irregular, size 0.05 x 0.1 x 0.05 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	306.90 cm^{-1}
Diffractometer:	Siemens-Stoe
Scan mode:	profile fitted ω/2θ
$T_{measurement}$:	293 K
$2\theta_{max}$:	45.84°
$N(hkl)_{unique}$:	159
Criterion for I_o:	$I_o > 2\,\sigma(I_o)$
$N(param)_{refined}$:	14
Program:	SHELXL-93

Source of material: $Rb_2LiDyBr_6$ crystallizes from a melt of RbBr, LiBr and $DyBr_3$ (molar ratio 2:1:1) by slow cooling from 873 K to room temperature in a sealed silica tube under strict exclusion of oxygen and moisture.
$Rb_2LiDyBr_6$ crystallizes in a tetragonally distorted variant of the elpasolite type of structure (see refs. 1-3). As a consequence of the distortion, the coordination number of Rb^+ is reduced from 12 to 4+8. Li^+ and Dy^{3+} remain octahedrally coordinated.

Table 2. Final atomic coordinates and displacement parameters (in Å^2)

Atom	Site	x	y	z	U_{iso}
Li(1)	2*b*	0	0	1/2	0.07(3)

Table 3. Final atomic coordinates and displacement parameters (in Å^2)

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Dy(1)	2*a*	0	0	0	0.020(2)	U_{11}	0.022(3)	0	0	0
Br(1)	4*e*	0	0	0.250(1)	0.130(9)	U_{11}	0.030(6)	0	0	0
Br(2)	8*h*	0.251(1)	x	0	0.16(1)	U_{11}	0.14(1)	–0.13(1)	0	0
Rb(1)	4*d*	0	1/2	1/4	0.086(6)	U_{11}	0.062(7)	0	0	0

Acknowledgments. We thank the Deutsche Forschungsgemeinschaft, Bonn, the Fonds der Chemischen Industrie, Frankfurt/Main, and the Herbert-Quandt-Stiftung der VARTA AG, Bad Homburg, for support.

References

1. Morss, L. R.: Crystal structure of dipotassium sodium fluoroaluminate (elpasolite). J. Inorg. Nucl. Chem. **36** (1974) 3876-3878.
2. Meyer, G.: The Synthesis and Structures of Complex Rare-Earth Halides. Prog. Solid State Ch. **14** (1982) 141-220.
3. Bührer, W.; Güdel, H. U.: Soft rotary mode and structural phase transition in the rare-earth bromo-elpasolites $Cs_2NaREBr_6$. J. Phys. C Solid State **20** (1987) 3809-3821.

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