shown in Fig. 1. The packing of molecules in the unit cell is shown in Fig. 2. The C_3S_8 molecule includes a seven-membered non-planar ring having a chair conformation. There are three planar fragments in the molecule: (i) dmit fragment C_3S_5; (ii) atoms S(4), S(5), S(7) and S(8), and (iii) atoms S(5), S(6) and S(7). Corresponding dihedral angles are 68.6° between (i) and (ii), 71.6° between (ii) and (iii), and 3.1° between (i) and (iii). According to molecular-mechanics calculations, the observed conformation of the C_3S_8 molecule is the most stable of all possible conformations for seven-membered cycles containing two C and five S atoms. The observed bond distances and angles are usual for sulfur-containing cyclic compounds and do not depend on their conformations (Steudel, Pickardt & Steudel, 1978; Steudel & Schuster, 1978).

The crystal structure of the title compound may be considered as composed of columns of C_3S_8 molecules along the crystallographic [100] direction. The closest intermolecular S⋯S distances are shorter than the sum of the van der Waals radii for S atoms (3.68 Å); S(2)⋯S(1) $(1 - x, -y, -z)$ 3.567 (2), S(2)⋯S(2) $(1 - x, -y, -z + 1)$ 3.406 (2), S(4)⋯S(2) $(x - 1, y, z)$ 3.488 (2), S(5)⋯S(1) $(x, y + 1, z)$ 3.359 (2), S(6)⋯S(1) $(x - 1, y + 1, z)$ 3.367 (2), S(7)⋯S(6) $(-x, 1 - y, -z)$ 3.510 (3), S(7)⋯S(7) $(1 - x, 1 - y, -z)$ 3.398 (3), S(8)⋯S(3) $(x - 1, y, z)$ 3.556 (2) Å.

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SHORT-FORMAT PAPERS

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Structure of the Laser Host Material LiYF₄

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Abstract. Lithium yttrium tetrafluoride, LiYF₄, M_r = 171.8, tetragonal, $I4_1/a$, $a = 5.164 (1)$, $c = 10.741 (2)$ Å, $V = 286.5 (1)$ Å³, $Z = 4$, $D_x = 3.99$ g cm⁻³, $\lambda(Mo K\alpha) = 0.7107$ Å, $\mu = 204$ cm⁻¹, $F(000) = 312$, $T = 295$ K, $R = 0.015$ for 156 unique observed $[F > 4\sigma(F)]$ reflections. The scheelite (CaWO₄) structure is confirmed. Lithium is located at a $\bar{4}$ site with four equidistant fluoride ions. Yttrium is in an eightfold coordination typical for rare-earth ions.

Experimental. Light-green crystals of the title compound were obtained from an equimolar mixture of LiF and YF₃. Since interest in this material is based on solid-state laser applications this mixture also contained 2% wt of PrF₃. The dried powders were heated in a platinum crucible in an inert atmosphere furnace (Ar) to 1123 K (melting point 1083 K) and allowed to cool slowly over 6 h. The solidified mass was broken up and a suitable crystal obtained.

Selected crystal *ca* 0.04 × 0.04 × 0.07 mm. Siemens *R3m/V* diffractometer, θ–2θ scan. Total scan range, 1.2° plus $K\alpha$ separation. Scan speed, 2.0 to 15° min⁻¹ in θ. Background stationary crystal and counter beginning and end of scan, each 25% of total scan time. Graphite-monochromated Mo $K\alpha$

Table 1. *Positional parameters* ($\times 10^4$) *and equivalent isotropic thermal parameters* ($\mathring{A}^2 \times 10^2$) *for* $LiYF_4$

U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
Y	0	2500	$\frac{5}{8}$	10 (1)
Li	0	2500	$\frac{1}{8}$	20 (2)
F	2183 (2)	5855 (2)	5437 (1)	17 (1)

Table 2. *Bond distances* ($\mathring{A}$) *and angles* (°) *in* $LiYF_4$

Y—F	2.244 (1) (×4)	Li—F	1.898 (1) (×4)
Y—F	2.297 (1) (×4)		
F—Li—F	102.2 (1) (×4)	125.2 (1) (×2)	
F—Y—F	98.7 (1) (×4)	128.5 (1) (×4)	
	134.2 (1) (×2)	75.8 (1) (×2)	
	75.1 (1) (×4)	69.8 (1) (×4)	
	150.7 (1) (×4)	74.5 (1) (×4)	

radiation. Unit cell from 22 reflections, $9 < 2\theta < 30°$. Absorption correction, semi-empirical ψ-scan correction, minimum/maximum transmission 0.093/0.016. $\mathrm{Sin}\theta/\lambda$ max. $= 0.69\ \mathring{A}^{-1}$. Index range, $-6 < h < 6$, $-6 < k < 6$, $-13 < l < 13$, 2648 reflections measured to yield 171 unique reflections, of which 156 observed with $F > 4\sigma(F)$, merge $R_I = 0.024$. Standard reflection 101 measured every 50 reflections, no significant variation. Least-squares minimized $\sum w(\Delta F)^2$ with $w = [\sigma^2(F) + 0.0002F^2]^{-1}$, $\sigma^2(F)$ based on counting statistics. All structure solution, refinement and graphics software from the *SHELXTL-Plus* package (Sheldrick, 1990). Structure solved by direct methods. Extinction correction $\chi = 0.0021$ (4) where $F^* = F[1 + 0.0002\chi F^2/\mathrm{sin}(2\theta)]^{-1/4}$. Scale factor, extinction parameter, positional parameters for F and anisotropic thermal parameters for Li, Y and F were refined (16 parameters). Final $R = 0.013$, $wR = 0.015$, $S = 0.94$. Largest $\Delta/\sigma = 0.001$. Final ΔF Fourier synthesis $-0.31 < \Delta\rho < 0.29\ \mathrm{e\ }\mathring{A}^{-3}$. Scattering factors f, f', f'' from *International Tables for X-ray Crystallography* (1974, Vol. IV). Final parameters are given in Table 1. Bond lengths and angles are given in Table 2. A view of the fluoride coordination around lithium and yttrium can be seen in Figs. 1 and 2, respectively.

Related literature. For references on the optical properties of rare-earth-doped $LiYF_4$ see Chicklis, Naiman, Folweiler, Gabbe, Jenssen & Linz (1971); Agladze & Popova, (1985); Erickson (1985); Harmer,

* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 71166 (3 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: HH0619]
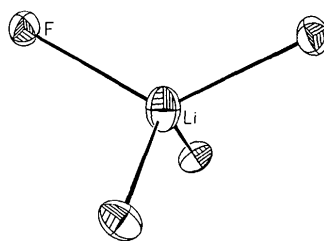

Fig. 1. Drawing of the environment around lithium with thermal ellipsoids shown at the 50% probability level.
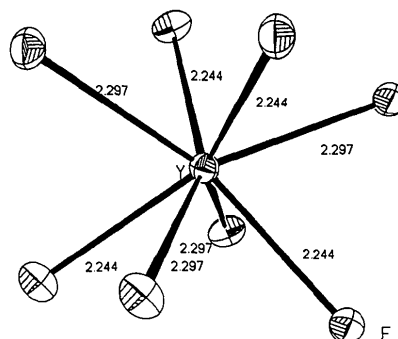

Fig. 2. Drawing of the environment around yttrium with thermal ellipsoids shown at the 50% probability level.

Linz & Gabbe (1969); Ivanova, Morozov, Petrova, Podkolzina & Feofilov (1975); Shand (1969); Jenssen, Linz, Leavitt, Morrison & Wortman (1975), and references therein. For synthesis and previous structural studies see Thoma, Weaver, Friedman, Insley, Harris & Yakel (1961); Blanchfield & Saunders (1979); Keller & Schmutz (1965).

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