# Crystal structure of lutetium disilicate, $Lu_2Si_2O_7$

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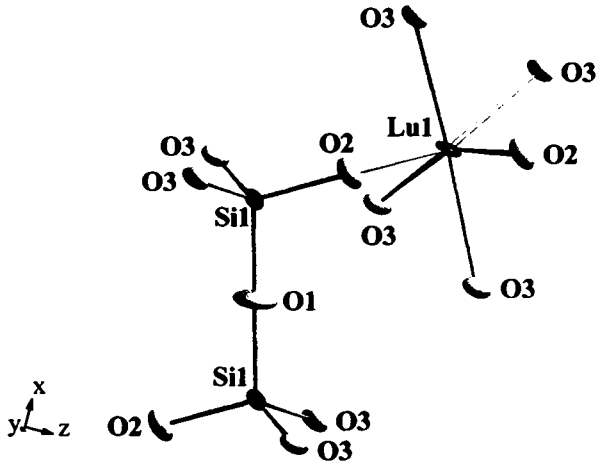


**Abstract**

$Lu_2O_7Si_2$, monoclinic, $C12/m1$ (No. 12), $a = 6.762(2)$ Å, $b = 8.835(3)$ Å, $c = 4.711(2)$ Å, $\beta = 101.99(4)°$, $V = 275.3$ Å$^3$, $Z = 2$, $R_{gt}(F) = 0.019$, $wR_{ref}(F^2) = 0.045$, $T = 293$ K.

**Source of material**

In attempt to prepare $Lu^{3+}$-$\beta$"-alumina by ion exchange reaction of $Na^+$-$\beta$"-$Al_2O_3$ with $LuCl_3$ in a quartz tube under argon atmosphere we obtained crystals of $Lu_2Si_2O_7$. Lutetium disilicate was grown as colourless rod-like crystals from the $LuCl_3$ melt (Aldrich 99.99%) via reaction with $SiO_2$ of the tube after heating at 1223 K for 23 hours.

**Discussion**

$Lu_2Si_2O_7$ isotypically to thortveitite, as already derived from powder investigations and film methods on single crystals [1]. The crystal structure parameters (e.g. atomic sites, displacement parameters and distances) have been determined and refined on single crystals for the first time. The Si—O distances vary from 161 to 163 pm, the Lu—O distances range from 220 to 226 pm. The Si–O–Si angle of 180° in the $Si_2O_7$ group is forced by the centre of symmetry. If there was a deviation of this angle, the thermal displacement ellipsoid should be larger. The terminal oxygen atoms of the disilicate group show a staggered confirmation (cf. figure).

**Table 1.** Data collection and handling.

| | |
|---|---|
| Crystal: | colorless rod-like, size 0.026 × 0.056 × 0.185 mm |
| Wavelength: | Mo $K_\alpha$ radiation (0.71073 Å) |
| $\mu$: | 180.34 cm$^{-1}$ |
| Diffractometer, scan mode: | Stoe IPDS, 240 exposures, $\Delta\varphi = 1.2°$ |
| $2\theta_{max}$: | 56.1° |
| $N(hkl)_{measured}$, $N(hkl)_{unique}$: | 2823, 331 |
| Criterion for $I_{obs}$, $N(hkl)_{gt}$: | $I_{obs} > 2\,\sigma(I_{obs})$, 311 |
| $N(param)_{refined}$: | 32 |
| Programs: | SHELXS-97 [2], SHELXL-97 [3] |

**References**

1. Felsche, J.: Polymorphism and crystal data of the rare-earth disilicates of the type $RE_2Si_2O_7$. J. Less-Common Met. **21** (1970) 1-14.
2. Sheldrick, G. M.: SHELXS-97, a program for the solution of crystal structures. University of Göttingen, Germany 1997.
3. Sheldrick, G. M.: SHELXL-97, a program for crystal structure refinement. University of Göttingen, Germany 1997.

**Table 2.** Atomic coordinates and displacement parameters (in Å$^2$).

| Atom | Site | $x$ | $y$ | $z$ | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{12}$ | $U_{13}$ | $U_{23}$ |
|---|---|---|---|---|---|---|---|---|---|---|
| Lu(1) | 4*h* | 1/2 | 0.80718(4) | 0 | 0.0011(2) | 0.0041(2) | 0.0064(3) | 0 | 0.0003(1) | 0 |
| Si(1) | 4*i* | 0.7196(3) | 1/2 | 0.4121(6) | 0.003(1) | 0.005(1) | 0.004(1) | 0 | -0.0005(8) | 0 |
| O(1) | 2*c* | 1/2 | 1/2 | 1/2 | 0.004(2) | 0.024(5) | 0.017(6) | 0 | 0.005(4) | 0 |
| O(2) | 4*i* | 0.8832(9) | 1/2 | 0.716(2) | 0.005(3) | 0.007(3) | 0.007(3) | 0 | -0.002(2) | 0 |
| O(3) | 8*j* | 0.7367(6) | 0.6510(5) | 0.220(1) | 0.003(2) | 0.006(2) | 0.007(3) | 0.001(2) | 0.000(2) | 0.003(2) |

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