

$\text{Ca}_{2.725}[\text{GeO}_4](\text{O}_{0.45}\text{F}_{0.55})$ $hP28$ $(186) P6_3mc - c^3b^4a$ $\text{Ca}_{3-x}\text{GeO}_4(\text{O}_{1-2x}\text{F}_{2x})$ [1]

Structural features: Single GeO_4 tetrahedra (2-fold orientational disorder) and infinite columns of face-linked $(\text{F},\text{O})\text{Ca}_6$ octahedra (partial vacancies ignored); Ge forms a Mg-type (h.c.p.) sublattice.

Nishi F., Takéuchi Y. (1984) [1]

 $\text{Ca}_{2.72}\text{F}_{0.55}\text{GeO}_{4.45}$ $a = 0.7223$, $c = 0.5681$ nm, $c/a = 0.787$, $V = 0.2567$ nm³, $Z = 2$

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|------|-------|------|---------------|---------------|--------|-------|--------------------|
| O1 | 6c | .m. | 0.2 | 0.8 | 0.165 | 0.62 | |
| O2 | 6c | .m. | 0.2 | 0.8 | 0.3154 | 0.38 | |
| Ca3 | 6c | .m. | 0.8442 | 0.1558 | 0.2326 | 0.908 | |
| Ge4 | 2b | 3m. | $\frac{1}{3}$ | $\frac{2}{3}$ | 0.211 | 0.38 | |
| Ge5 | 2b | 3m. | $\frac{1}{3}$ | $\frac{2}{3}$ | 0.269 | 0.62 | |
| O6 | 2b | 3m. | $\frac{1}{3}$ | $\frac{2}{3}$ | 0.5806 | 0.62 | colinear GeO |
| O7 | 2b | 3m. | $\frac{1}{3}$ | $\frac{2}{3}$ | 0.8998 | 0.38 | colinear GeO |
| M8 | 2a | 3m. | 0 | 0 | 0.0 | | |

 $\text{M8} = 0.55\text{F} + 0.45\text{O}$

Transformation from published data: origin shift 0 0 0.761

Experimental: single crystal, diffractometer, X-rays, $wR = 0.048$, $T = 298$ K

Remarks: Short interatomic distances for partly occupied site(s).

References: [1] Nishi F., Takéuchi Y. (1984), Acta Crystallogr. C 40, 730-733.