| $Gd_3[SeO_3]_4F$ | *hP*40 | (186) $P6_3mc$ – $dc^4b^2$ |
|---|---|---|

**$Gd_3(SeO_3)_4F$** [1]
Structural features: :$SeO_3$ ψ-tetrahedra and $FGd_3$ triangular clusters.

Wickleder M.S., Göhausen I. (2000) [1]
$FGd_3O_{12}Se_4$
$a$ = 1.0443, $c$ = 0.69432 nm, $c/a$ = 0.665, $V$ = 0.6558 $nm^3$, $Z$ = 2

| site | Wyck. | sym. | $x$ | $y$ | $z$ | occ. | atomic environment |
|---|---|---|---|---|---|---|---|
| O1 | 12*d* | 1 | 0.4156 | 0.0826 | 0.2418 | | single atom Se |
| O2 | 6*c* | .*m*. | 0.1818 | 0.8182 | 0.0465 | | single atom Se |
| O3 | 6*c* | .*m*. | 0.4172 | 0.5828 | 0.3706 | | single atom Se |
| Gd4 | 6*c* | .*m*. | 0.46266 | 0.53734 | 0.0473 | | tricapped trigonal prism $O_8F$ |
| Se5 | 6*c* | .*m*. | 0.84513 | 0.15487 | 0.3136 | | non-coplanar triangle $O_3$ |
| F6 | 2*b* | 3*m*. | $^1/_3$ | $^2/_3$ | 0.0 | | non-coplanar triangle $Gd_3$ |
| Se7 | 2*b* | 3*m*. | $^1/_3$ | $^2/_3$ | 0.48 | | non-coplanar triangle $O_3$ |

Transformation from published data: -*x*,-*y*,-*z*; origin shift 0 0 0.0383
Experimental: single crystal, diffractometer, X-rays, R = 0.027, T = 293 K

Remarks: In table 1 of [1] the *y*-coordinate of former site Gd is misprinted as -*x* instead of *x*/2 (checked on interatomic distances); the cell volume is misprinted as 0.0558 $nm^3$ instead of 0.6558 $nm^3$.

References: [1] Wickleder M.S., Göhausen I. (2000), Z. Anorg. Allg. Chem. 626, 1725-1727.