| $Yb_2S_3$ | *hP*30 | (185) $P6_3cm$ – $c^3b^2a^2$ |
|---|---|---|

**$Yb_2S_3$ ε** [1], "sesquisulfide E"
Structural features: Close-packed S layers in distorted h stacking; Yb in octahedral voids (displaced from the octahedron centers). $YbS_6$ octahedra (of very different sizes) share faces, edges and vertices to form a 3D-framework.

Kuz'micheva G.M., Eliseev A.A. (1977) [1]
$S_3Yb_2$
$a$ = 0.6772, $c$ = 1.828 nm, $c/a$ = 2.699, $V$ = 0.7260 $nm^3$, $Z$ = 6

| site | Wyck. | sym. | $x$ | $y$ | $z$ | occ. | atomic environment |
|---|---|---|---|---|---|---|---|
| S1 | 6*c* | ..*m* | 0.3290 | 0 | 0.0871 | | 7-vertex polyhedron $Yb_4S_3$ |
| S2 | 6*c* | ..*m* | 0.3642 | 0 | 0.3762 | | square pyramid $Yb_5$ |
| S3 | 6*c* | ..*m* | 0.6700 | 0 | 0.2109 | | non-coplanar triangle $Yb_3$ |
| Yb4 | 4*b* | 3.. | $^1/_3$ | $^2/_3$ | 0.0000 | | octahedron $S_6$ |
| Yb5 | 4*b* | 3.. | $^1/_3$ | $^2/_3$ | 0.2517 | | octahedron $S_6$ |
| Yb6 | 2*a* | 3.*m* | 0 | 0 | 0.0000 | | 7-vertex polyhedron $S_6Yb$ |
| Yb7 | 2*a* | 3.*m* | 0 | 0 | 0.1667 | | 7-vertex polyhedron $S_6Yb$ |

Transformation from published data: -*x*,-*y*,-*z*
Experimental: single crystal, oscillation and precession photographs, X-rays, R = 0.103

Remarks: Short interatomic distances: d(Yb-S) = 0.238 nm. Preliminary data in [2]. Supersedes a report on $Yb_2S_3$ with α-$Al_2O_3$ type structure in [3], however, according to [4] true symmetry is effectively (167) R-3c (α-$Al_2O_3$ type) and the structure proposed in [1] is based on a wrong interpretation of twinning effects.

References: [1] Kuz'micheva G.M., Eliseev A.A. (1977), Russ. J. Inorg. Chem. 22, 497-499 (Zh. Neorg. Khim. 22, 897-900). [2] Eliseev A.A., Kuz'micheva G.M., Pisarev E.A., Borodulenko G.P., Grizik A.A. (1975), Russ. J. Inorg. Chem. 20, 657-659 (Zh. Neorg. Khim. 20, 1167-1170). [3] Flahaut J., Domange L., Pardo M.P. (1964), C. R. Hebd. Seances Acad. Sci. 258, 594-596. [4] Schleid T., Lissner F. (1996), Z. Naturforsch. B 51, 733-738.