

Dy<sub>3</sub>SOF<sub>5</sub>*hP*20(176) *P*6<sub>3</sub>/*m* – h<sup>3</sup>d**Dy<sub>3</sub>OSF<sub>5</sub>** [1]

Structural features: Infinite columns of base-linked Dy[S<sub>2</sub>(F,O)<sub>2</sub>F<sub>2</sub>][(F,O)<sub>2</sub>F] tricapped trigonal prisms share atoms to form a 3D-framework with propeller-like prism columns and channels of hexagonal cross-section parallel to [001].

Grossholz H., Schleid T. (2002) [1]

Dy<sub>3</sub>F<sub>5</sub>OS*a* = 0.94258, *c* = 0.36812 nm, *c/a* = 0.391, *V* = 0.2832 nm<sup>3</sup>, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
M1	6 <i>h</i>	<i>m</i> ..	0.0468	0.4298	<sup>1</sup> / <sub>4</sub>		tetrahedron Dy <sub>4</sub>
F2	6 <i>h</i>	<i>m</i> ..	0.2667	0.1539	<sup>1</sup> / <sub>4</sub>		non-coplanar triangle Dy <sub>3</sub>
Dy3	6 <i>h</i>	<i>m</i> ..	0.29218	0.41126	<sup>1</sup> / <sub>4</sub>		tricapped trigonal prism F <sub>7</sub> S <sub>2</sub>
S4	2 <i>d</i>	-6..	<sup>2</sup> / <sub>3</sub>	<sup>1</sup> / <sub>3</sub>	<sup>1</sup> / <sub>4</sub>		trigonal prism Dy <sub>6</sub>

M1 = 0.667F + 0.333O

Transformation from published data: *y*,*x*,*-z*; origin shift 0 0 <sup>1</sup>/<sub>2</sub>

Experimental: single crystal, diffractometer, X-rays, wR = 0.022

Remarks: We assigned an approximate value to the F/O ratio of site M1 based on the nominal composition.

References: [1] Grossholz H., Schleid T. (2002), Z. Anorg. Allg. Chem. 628, 1012-1016.