$Ti_3Se_4[H_2O]_{0.75}$	*hP*20	(176) $P6_3/m$ – h^3d

$(H_2O)_{1.5}Ti_6Se_8$ [1]
Structural features: Units of three face-linked $TiSe_6$ octahedra share edges to form a 3D-framework; H_2O in channels of hexagonal cross-section parallel to [001] (partial disorder). Filled-up derivative of Nb_3Te_4.

Bensch W. et al. (1994) [1]
$H_{1.50}O_{0.75}Se_4Ti_3$
a = 0.986, c = 0.35822 nm, c/a = 0.363, V = 0.3016 nm^3, Z = 2

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Se1	6*h*	*m*..	0.0498	0.3504	$^1/_4$		trigonal bipyramid $(OH_2)Ti_4$
$(OH_2)2$	6*h*	*m*..	0.0806	0.004	$^1/_4$	0.25	non-colinear $(OH_2)_2$
Ti3	6*h*	*m*..	0.3588	0.4878	$^1/_4$		octahedron Se_6
Se4	2*d*	-6..	$^2/_3$	$^1/_3$	$^1/_4$		trigonal prism Ti_6

Transformation from published data: origin shift 0 0 $^1/_2$
Experimental: single crystal, diffractometer, X-rays, wR = 0.042, T = 295 K

Remarks: Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Bensch W., Koy J., Braun T., Hug P. (1994), Solid State Ionics 74, 141-148.