$KTiO_2[OH]$	*hP*180	(178) $P6_122 - c^{11}b^6a^2$

$KTiO_2(OH)$ [1], perovskite 4H
Structural features: Close-packed $K(O,OH)_3$ layers in hc stacking; Ti in octahedral voids. Units of two face-linked $Ti(O_4[OH]_2)$ octahedra share vertices to form a 3D-framework. Deformation derivative of 4H-$BaMnO_3$.

Masaki N. et al. (2002) [1]
HKO_3Ti
$a = 0.98889$, $c = 2.8671$ nm, $c/a = 2.899$, $V = 2.4281$ nm^3, $Z = 36$

site	Wyck.	sym.	*x*	*y*	*z*	occ.	atomic environment
Ti1	12*c*	1	0.0018	0.3367	0.12117		octahedron $O_4(OH)_2$
O2	12*c*	1	0.003	0.5012	0.4183		non-colinear Ti_2
(OH)3	12*c*	1	0.1332	0.4619	0.16567		non-coplanar triangle Ti_2O
O4	12*c*	1	0.1673	0.3145	0.08357		non-colinear Ti_2
O5	12*c*	1	0.1995	0.1974	0.33793		non-coplanar triangle $Ti_2(OH)$
Ti6	12*c*	1	0.3214	0.3342	0.053		octahedron $O_4(OH)_2$
Ti7	12*c*	1	0.3313	0.0116	0.44927		octahedron $O_4(OH)_2$
K8	12*c*	1	0.3405	0.3333	0.4956		anticuboctahedron $O_8(OH)_4$
O9	12*c*	1	0.3574	0.1576	0.41673		single atom Ti
(OH)10	12*c*	1	0.4891	0.1443	0.50293		non-colinear Ti_2
(OH)11	12*c*	1	0.5095	0.3307	0.33743		non-colinear Ti_2
K12	6*b*	..2	0.0013	0.0026	$^1/_4$		cuboctahedron O_{12}
O13	6*b*	..2	0.1801	0.3602	$^1/_4$		non-colinear Ti_2
K14	6*b*	..2	0.3403	0.6806	$^1/_4$		cuboctahedron $O_6(OH)_6$
O15	6*b*	..2	0.5034	0.0069	$^1/_4$		non-colinear Ti_2
K16	6*b*	..2	0.6569	0.3139	$^1/_4$		cuboctahedron $O_6(OH)_6$
O17	6*b*	..2	0.8313	0.6626	$^1/_4$		non-colinear Ti_2
K18	6*a*	.2.	0.3301	0	0		anticuboctahedron $(OH)_4O_8$
O19	6*a*	.2.	0.8329	0	0		non-colinear Ti_2

Transformation from published data: origin shift 0 0 $^1/_2$
Experimental: powder, diffractometer, X-rays, $R_B = 0.076$

Remarks: When relevant, we changed the last digit of the atom coordinates to respect the symmetry conditions for special positions. The average structure was refined in space group (194) $P6_3/mmc$ with $^1/_6$ cell volume ($R_B = 0.067$). We assume that in table 5 of [1] the *z*-coordinate of former Ti1 is misprinted as 0.0955 instead of 0.0455 (better interatomic distances); the space group number is misprinted as 176 instead of 178. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Masaki N., Uchida S., Yamane H., Sato T. (2002), Chem. Mater. 14, 419-424.