Table 2. Results of the geometry optimization of T-F0H8 models with different hydrogen configurations.

Configuration	*ΔE (kJ/mol)*	*a (Å)*	*b (Å)*	*c* (Å)	*V* (Å^3)
H1 - H1	20.09	4.70681	9.02970	8.62742	366.67
H1 - H2	0.00	4.78079	8.97916	8.49003	364.46
H2 - H2*	50.92	4.76698	8.92043	8.63186	367.06

Notes: data with asterisk (*) are related to a probable saddle point, not a local minima.

Table 3. B3LYP atomic fractional coordinates in the symmetric topaz structures (T-F0H8, T-F4H4 and T-F8H0).

		DFT – present work				Experimental data		
Model	**Atom**	**x/a**	**y/b**	**z/c**	**Atom**	**x/a**	**y/b**	**z/c**
T-F0H8[a]	Al1	0.9006	0.1377	0.0790	Al	0.9050	0.1321	0.0798
	Al2	0.4053	0.3720	0.9194				
	H1	0.0361	0.2284	0.8279				
	H2	0.4311	0.1732	0.0808	H1	0.4430	0.1990	0.0880
	O1	0.7912	0.5278	0.2487	O1	0.7104	0.0262	0.2500
	O2	0.4516	0.7577	0.2464	O2	0.4439	0.7561	0.2500
	O3	0.7915	0.0108	0.9053				
	O4	0.2826	0.4979	0.0939	O3	0.2100	0.9929	0.0943
	O5	0.9240	0.7470	0.0645	OH	0.5906	0.2507	0.0659
	O6	0.4087	0.7520	0.9341				
	Si1	0.4022	0.9413	0.2500	Si	0.4019	0.9405	0.2500
T-F4H4	Al1	0.9034	0.1308	0.0794				
	Al2	0.4106	0.3685	0.9180				
	F1	0.4003	0.7478	0.9401				
	H1	0.4989	0.2517	0.1625				
	O1	0.7945	0.5326	0.2520				
	O2	0.4474	0.7564	0.2492				
	O3	0.7926	0.0116	0.9054				
	O4	0.2878	0.4905	0.0929				
	O5	0.9028	0.7533	0.0631				
	Si1	0.4012	0.9413	0.2503				
T-F8H0[a]	Al1	0.9013	0.1297	0.0838	Al	0.9030	0.1309	0.0828
	F1	0.8972	0.7526	0.0512	F	0.5982	0.2525	0.0561
	O1	0.6989	0.0334	0.2500	O1	0.7034	0.0321	0.2500
	O2	0.4625	0.7554	0.2500	O2	0.4577	0.7560	0.2500
	O3	0.2067	0.9877	0.0933	O3	0.2102	0.9892	0.0924
	Si1	0.3951	0.9392	0.2500	Si	0.3972	0.9404	0.2500

Experimental data for $Al_2SiO_4(OH)_2$ and $Al_2SiO_4F_2$ are taken from Northrup et al. (1994)

Table 4. Calculated elastic parameters, bulk (K_0) and axial moduli ($K_0(a)$, $K_0(b)$ and $K_0(c)$), their first derivatives (K') and corresponding zero-pressure (V_0, a_0, b_0 and c_0) values.

	T-F0H8	**T-F2H6**	**T-F4H4**	**T-F6H2**	**T-F7H1**	**T-F8H0**	**XRD**
K_0 (GPa)	145(3)	163(3)	165(3)	151(3)	164(3)	168(3)	158(6)
K'	4.2(5)	3.4(4)	3.4(4)	3.6(5)	3.0(4)	3.0(4)	3.3(4)
V_0 (Å^3)	365.4(9)	360.8(8)	357.6(8)	357.2(9)	355.0(8)	354.0(8)	-
K_0 *(a)* (GPa)	165(3)	174(3)	152(3)	134(3)	144(3)	144(3)	146(5)
K′(a)	3.6(4)	3.0(4)	3.8(5)	3.9(5)	3.3(4)	3.4(4)	4.6(3)
a_0 (Å)	4.785(5)	4.748(3)	4.717(4)	4.714(6)	4.703(4)	4.700(6)	-
K_0 *(b)* (GPa)	201(4)	234(4)	251(4)	222(4)	229(4)	227(4)	220(4)
K′(b)	3.7(5)	2.4(5)	2.0(4)	2.9(5)	2.5(5)	2.5(4)	2.6(3)
b_0 (Å)	8.985(5)	8.963(5)	8.958(5)	8.919(6)	8.888(5)	8.863(7)	-
K_0 *(c)* (GPa)	100(3)	113(3)	125(4)	125(3)	141(3)	150(3)	132(4)
K′(c)	4.8(5)	4.1(5)	3.9(4)	3.7(4)	3.0(3)	2.9(4)	3.3(3)
c_0 (Å)	8.503(10)	8.481(9)	8.466(9)	8.499(10)	8.493(7)	8.498(10)	-

Notes: XRD values are from the experimental work of Gatta et al. (2014) – $Al_2SiO_4(OH)_{0.25}F_{1.75}$

Table 5. Bond lengths (Å), polyhedral volumes (Å^3) and bond angles (°) in the different topaz models at selected pressures.

	P1	P2	P3	P4	P5
T-F0H8					
Pressure (GPa)	0.7	7.0	18.9	34.3	52.5
< Al – O >	1.9167	1.8949	1.8660	1.8372	1.8077
< Al–(O,F)–Al>	138.9	136.7	133.9	131.6	129.6
< V (Al-octah) >	9.3068	9.0083	8.6160	8.2302	7.8436
< Si – O >	1.6660	1.6533	1.6359	1.6180	1.5998
< V (Si-tetrah) >	2.3672	2.3142	2.2429	2.1709	2.0995
< H – O >	0.9658	0.9668	0.9679	0.9695	0.9713
< H–O–Al>	105.7	105.8	105.9	105.9	105.9
T-F2H6					
Pressure (GPa)	1.1	6.9	19.0	34.0	51.5
< Al – O >	1.9027	1.8842	1.8563	1.8283	1.7997
< Al–(O,F)–Al>	143.5	140.6	136.5	133.0	130.4
< V (Al-octah) >	9.1086	8.8554	8.4831	8.1146	7.7435
< Si – O >	1.6613	1.6508	1.6334	1.6158	1.5978
< V (Si-tetrah) >	2.3476	2.3040	2.2324	2.1613	2.0897
< H – O >	0.9620	0.9642	0.9646	0.9651	0.9653
< H–O–Al>	108.7	108.0	108.3	108.7	108.9
T-F4H4					
Pressure (GPa)	1.1	9.2	22.1	37.8	52.2
< Al – (F,O) >	1.8964	1.8740	1.8464	1.8187	1.7907
< Al–(O,F)–Al >	142.5	139.7	136.3	133.4	131.1
< V (Al-octah) >	9.0066	8.7082	8.3466	7.9879	7.6313
< Si – O >	1.6622	1.6479	1.6303	1.6120	1.5940
< V (Si-tetrah) >	2.3527	2.2931	2.2205	2.1464	2.0754
< H – O >	0.9615	0.9615	0.9608	0.9583	0.9555
< H–O–Al>	109.6	110.8	112.3	113.6	114.6
T-F6H2					
Pressure (GPa)	1.1	6.9	19.0	34.0	51.5
< Al – O >	1.8867	1.8597	1.8368	1.8058	1.7848
< Al–(O,F)–Al>	147.1	143.1	139.6	135.0	132.2
< V (Al-octah) >	8.8565	8.5047	8.2122	7.8195	7.5558
< Si – O >	1.6609	1.6431	1.6278	1.6069	1.5930
< V (Si-tetrah) >	2.3479	2.2737	2.2104	2.1258	2.0700
< H – O >	0.9616	0.9611	0.9605	0.9589	0.9571
< H–O–Al>	109.3	110.7	112.0	113.6	114.4
T-F7H1					
Pressure (GPa)	1.1	6.9	19.0	34.0	51.5
< Al – O >	1.8799	1.8632	1.8364	1.8056	1.7849
< Al–(O,F)–Al>	147.7	145.1	140.8	135.9	133.1
< V (Al-octah) >	8.7630	8.5460	8.2043	7.8161	7.5571

< Si – O >	1.6557	1.6446	1.6269	1.6062	1.5927
< V (Si-tetrah) >	2.3270	2.2809	2.2083	2.1241	2.0698
< H – O >	0.9609	0.9607	0.9602	0.9582	0.9562
< H–O–Al>	110.8	111.7	113.1	114.7	115.4
T-F8H0					
Pressure (GPa)	1.2	9.4	22.1	37.1	50.6
<Al – (F,O)>	1.8758	1.8533	1.8270	1.7995	1.7764
< Al–(O,F)–Al >	148.6	145.3	141.1	137.9	133.7
< V (Al-octah) >	8.6941	8.4057	8.0755	7.7319	7.4505
<Si – O>	1.6587	1.6434	1.6250	1.6042	1.5896
< V (Si-tetrah) >	2.3402	2.2769	2.2015	2.1187	2.0594

Table 6. Calculated elastic constants (GPa), bulk (K), shear (μ) and Young's (E) moduli in GPa and mean shear and longitudinal wave velocities (v_s and v_l, respectively) in km/s at 0 GPa for the different topaz models.

SOEC Component	**T-F0H8**	**T-F2H6**	**T-F4H4**	**T-F6H2**	**T-F7H1**	**T-F8H0**	**Exp.**
C_{11}	302.30	285.07	259.50	267.36	269.04	270.31	278.5(5)
C_{12}	104.74	111.97	119.40	118.25	117.91	119.41	120.4(2)
C_{13}	78.32	75.543	79.27	78.14	79.71	81.01	80.6(1)
C_{22}	340.94	343.05	342.94	337.48	334.14	331.07	344.8(6)
C_{23}	77.04	79.19	79.86	80.55	80.49	81.21	80.3(1)
C_{33}	229.79	245.49	256.02	278.44	288.70	295.98	292.5(5)
C_{44}	102.69	103.76	104.59	104.16	103.78	103.47	108.6(8)
C_{55}	111.34	115.61	122.23	125.16	126.63	127.88	132.9(8)
C_{66}	123.90	126.16	127.47	127.04	126.86	126.32	130.3(8)
K_V	154.80	156.33	157.28	159.68	160.90	162.29	-
K_R	149.12	151.50	153.03	156.96	158.89	160.68	-
K_{VRH}	151.96	153.92	155.15	158.32	159.89	161.49	-
μ_V	108.45	109.56	109.52	111.69	112.37	112.58	-
μ_R	106.61	107.46	106.55	109.27	109.95	110.13	-
μ_{VRH}	107.53	108.51	108.03	110.48	111.16	111.36	-
E_{VRH}	261.02	263.59	263.05	268.90	270.74	271.64	-
v_s	5.73	5.71	5.66	5.69	5.69	5.69	-
v_p	9.73	9.71	9.67	9.71	9.73	9.74	-

Experimental data taken from the work of Haussuhl (1993) – $Al_2SiO_4F_2$.