

Table S1. Cartesian coordinates/ Å of all atoms in the H₄SiO₄.28H₂O (D₄SiO₄.28D₂O) minima discussed in this work.

Atom	x	y	z
Si	-0.121008	-0.052497	0.932765
O	-0.393294	0.475367	2.469547
O	-1.566069	-0.338398	0.157087
O	0.713756	1.115531	0.133938
O	0.761794	-1.448443	1.105504
H/D	-1.479598	-0.516108	-0.823623
H/D	0.900867	-2.122675	0.373478
H/D	0.185918	1.658057	-0.522616
H/D	-0.786249	-0.148821	3.145039
H/D	-4.333563	-1.448772	-2.604266
O	-3.709222	-2.160852	-2.847964
H/D	-2.834176	-1.720503	-2.861793
H/D	-1.314152	-2.113359	3.866919
O	-1.277075	-1.239235	4.337933
H/D	-2.157351	-1.096769	4.717902
H/D	-5.589971	-0.333315	-0.12954
O	-5.469431	-0.342032	0.841769
H/D	-4.94471	-1.152344	1.039071
H/D	1.106473	-2.997718	-3.863273
O	1.054849	-2.474128	-3.049072
H/D	1.676394	-1.680052	-3.156205
H/D	-1.651194	2.571007	-1.617996
O	-0.66898	2.603588	-1.648798
H/D	-0.386522	3.587164	-1.505454
H/D	0.146401	4.54808	1.732921
O	-0.564197	5.156809	1.445105
H/D	-1.415371	4.760783	1.730084
H/D	-2.836904	-1.620987	0.72461
O	-3.422778	-2.275937	1.156723
H/D	-3.585665	-2.976344	0.448536
H/D	-0.14052	1.885015	-3.04697
O	0.11019	1.215237	-3.750406
H/D	-0.03754	1.634141	-4.611921
O	0.0644	5.034236	-1.229981
H/D	1.053707	5.042768	-1.15681
H/D	-0.247079	5.229101	-0.308216

O	-1.254622	-3.28944	2.536321
H/D	-2.092474	-3.010052	2.079407
H/D	-0.533648	-2.845104	2.050483
O	-3.603505	1.566001	1.006444
H/D	-4.379493	0.931643	1.063899
H/D	-2.829869	0.978449	0.891573
O	2.469253	-0.279523	-3.247611
H/D	2.965428	-0.024356	-2.432714
H/D	1.781104	0.402786	-3.402689
O	-1.186209	-0.911478	-2.494558
H/D	-0.488218	-1.589162	-2.663351
H/D	-0.894313	-0.142406	-3.039477
O	-1.112707	-5.082559	0.040804
H/D	-1.201015	-4.893045	0.993006
H/D	-0.29523	-4.612502	-0.226994
O	-5.270511	0.169475	-2.016257
H/D	-6.035412	0.373189	-2.576028
H/D	-4.708026	0.980321	-2.005011
O	-3.567185	2.402966	-1.535914
H/D	-3.639684	2.219019	-0.554617
H/D	-3.909138	3.302101	-1.66692
O	1.197866	-3.474187	-0.531338
H/D	1.252584	-3.234906	-1.489235
H/D	2.068675	-3.865844	-0.270178
O	-3.632823	-4.065609	-0.7864
H/D	-3.648871	-3.527416	-1.612599
H/D	-2.759011	-4.51183	-0.725438
O	3.325435	-0.523877	1.713726
H/D	2.455859	-0.958745	1.549359
H/D	3.133105	0.12108	2.431678
O	5.139042	-2.501485	1.571819
H/D	5.718559	-2.600503	2.342658
H/D	4.516981	-1.745269	1.767506
O	3.62207	-4.487949	0.299151
H/D	3.584397	-5.333643	0.770345
H/D	4.174123	-3.881477	0.843547
O	-3.06732	4.035454	2.177444
H/D	-3.385034	4.151693	3.084267
H/D	-3.29105	3.115491	1.912923
O	1.691488	3.37521	1.662345
H/D	2.030535	2.964158	2.479694
H/D	1.400439	2.610716	1.121442
O	4.028195	0.357379	-1.021651

H/D	3.649778	0.261369	-0.122526
H/D	4.824261	-0.230105	-1.022638
O	2.077265	1.238476	3.554366
H/D	2.138354	1.201941	4.521107
H/D	1.14583	1.001862	3.32206
O	2.732972	4.835038	-0.578434
H/D	2.593676	4.447591	0.308569
H/D	3.410933	4.266051	-1.004674
O	6.136548	-1.437413	-0.837682
H/D	5.92579	-1.916147	-0.005968
H/D	6.194129	-2.110169	-1.532646
O	4.653958	3.038374	-1.615811
H/D	4.463305	2.094803	-1.407924
H/D	4.922338	3.062268	-2.545678