Supplementary Information

While the decreased binding energy of site 1 could be due to the shorter O-O distance (despite almost no increase in the hydrogen bond length), this analysis does not hold for sites 2-4. Thus, distortion of bonds besides the hydroxyl and hydrogen bonds must be considered. Figure SI 1 shows that each proton site's hydrogen-bond length is closely correlated with the distance between the two oxygen involved in hydroxyl and hydrogen bonds with the proton.

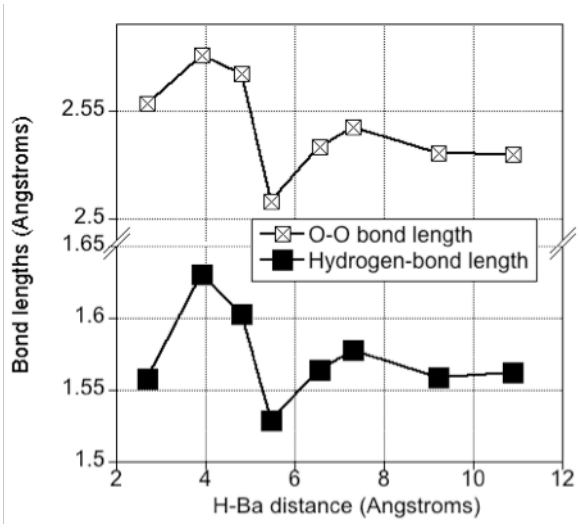

Figure SI 1: The O-O bond length correlates well with the hydrogen-bond length, except for site 1. The proton draws the two closest oxygen towards itself, decreasing the hydrogen bond and the O-O distance.

Table SI 1: The proton stabilization and environment, as described by the hydroxyl and hydrogen bond lengths and the hydroxyl-oxygen hydrogen-oxygen bond lengths (O-O), are given for each site. The effect of the proton on the average Ba-O bond length is given in the last column. The last row (0) gives bond lengths without the Ba-dopant and the average La-O bonds.

H+ site	ΔEnergy (eV)	Hydroxyl bond	Hydrogen bond	O-O bond
1	-0.202	1.035	1.558	2.553
2	0.049	1.025	1.630	2.576
3	0.003	1.027	1.603	2.567
4	-0.042	1.041	1.528	2.508
5	-0.016	1.034	1.564	2.533
6	0.015	1.030	1.577	2.542
7	-0.010	1.035	1.559	2.530
8	0	1.033	1.562	2.529
0		1.03	1.56	2.5