Supporting Information

Effect of solvent nature on propylene glycol oxidation with *tert*-butyl hydroperoxide over metal-organic framework Cr-MIL-101

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Table S1. Bond lengths in isolated molecules and in those adsorbed on Cr sites of MOF model calculated at B3LYP/LANL2DZ/6-31G* level of theory.

Model	r(O-O) in TBHP, Å	r(C-O) in Solvent/TBHP, Å	r(O-H) in Solvent/TBHP, Å
methanol		1.419	0.969
tert-butanol		1.439	0.971
n-butanol		1.425	0.969
ethoxyethanol		1.422	0.968
ethyl acetate		1.212	-
butyl acetate		1.212	-
acetone		1.216	-
TBHP*	1,476	1.448	0,974
MOF+methanol		1.439	0,974
MOF+*tert*-butanol		1.464	0,975
MOF+n-butanol		1.447	0,974
MOF+ethoxyethanol		1.443	0,972
MOF+ethyl acetate		1.227	-
MOF+butyl acetate		1.229	-
MOF+acetone		1.231	-
MOF+TBHP	1.470	1.455	0.981
MOF+methanol+TBHP	1.464	1.432/1.455	0.992/0.991
MOF+*tert*-butanol+TBHP	1.468	1.471/1.444	0.972/0.981

* r(O-O) was fixed in calculation for the isolated gas phase TBHP. Experimental value was 1.473 Å [1].

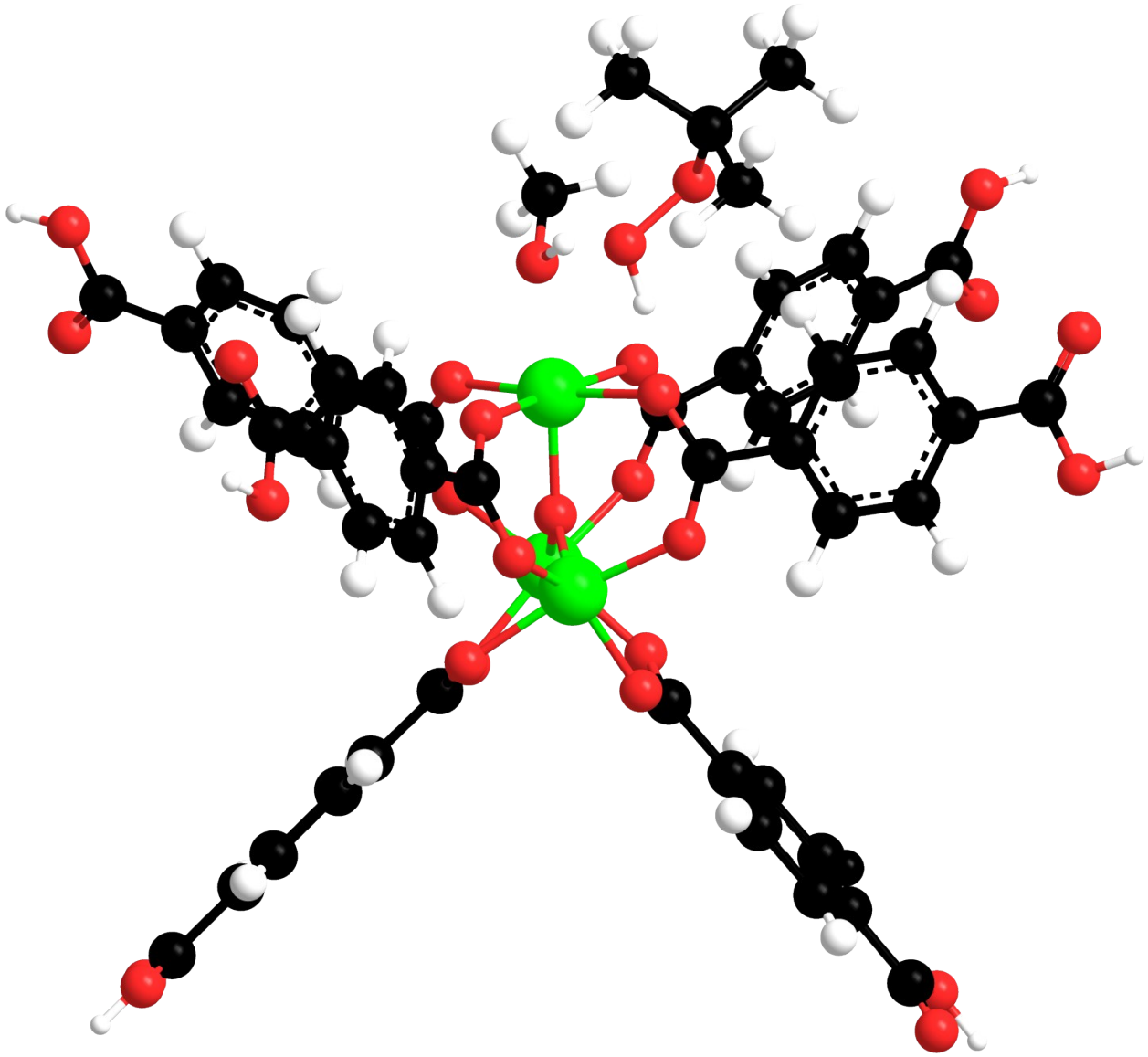

Figure S1. A model of methanol and TBHP binding with active site of Cr-MIL-101. Black, white, red, and green atoms correspond to carbon, hydrogen, oxygen, and chromium, respectively.

References

1. Kosnikov A.Yu., Antonovskii V.L., Lindeman S.V., Antipin M.Yu., Struchkov Yu.T., Turovskii N.A., Zyat'kov I.P. X-ray crystallographic and quantum-chemical investigation of tert-butyl hydroperoxide // Theoretical and Experimental Chemistry. – 1989. – Vol. 25. - Iss. 1. – P. 73 – 77.