Supporting Information

A computational study of the effect of the metal organic framework environment on the release of chemically stored nitric oxide

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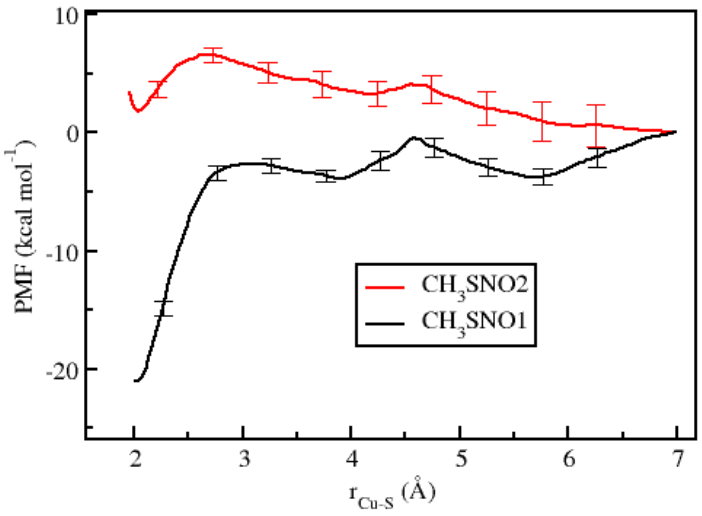
Table S1. Energies (relative to isomer III) and S-N distance of the various isomers, reactant and products (shown in Fig. 4 of the paper) at the B3LYP-D, M06, MP2 and CCSD(T) level of theory using a mixed basis set (LANLDZ for copper and 6-311G(d,p) for the other atoms). For the CCSD(T) energies, the CCSD optimized structures were used.

Cluster	CCSD(T) ΔE (kcal/mol)	MP2 ΔE (kcal/mol)	B3LYP-D2 ΔE ΔE (kcal/mol)	M06 ΔE ΔE(kcal/mol)
Reactant (I)	39.4	44.0	53.1	50.6
Product (II)	25.0	31.6	29.2	33.1
Isomer (III)	0.0	0.0	0.0	0.0
Isomer (IV)	7.2	11.6	9.7	9.2

Cluster	CCSD r_{S-N}(Å)	MP2 r_{S-N}(Å)	B3LYP-D2 r_{S-N}(Å)	M06 r_{S-N}(Å)
Reactant (I)	1.83	1.84	1.90	1.85
Product (II)	N/A	N/A	N/A	N/A
Isomer (III)	2.12	2.26	2.22	2.18
Isomer (IV)	1.69	1.66	1.69	1.68

Additional canonical simulations (NVT ensemble) were performed at a temperature of 300 K using a Nose-Hoover thermostat for the CH_3SNO case.[1-3] The box length was 26 Å. All bond lengths were constrained using the LINCS algorithm,[4] allowing a 2 fs time step in the simulation.

Figure S1. Free energy profiles of bringing CH_3SNO1 and the subsequently CH_3SNO2 to the same catalytic Cu(I) ion of MOF suspended in in ethanol solution in the NVT ensemble. Error bars were obtained by block averaging.



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