Computational and experimental investigation of the release of nitric oxide from s-nitrosothiols, mediated through metal organic framework catalysis events

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Abstract: Nitric oxide is a biologically active species with a number of biomedical applications including vasodilation, as a neurotransmitter, in anti-angina medication etc. Biocompatible storage and delivery of nitric oxide is an active area of research. The use of a copper based metal organic framework as a storage vehicle and catalyst (copper sites of the MOF) in the controlled and sustained release of chemically stored nitric oxide (NO) from S-nitrosocysteine has been shown to occur both computationally and experimentally. Previous computational studies by our group on HKUST-1 concluded that modifications in the R-group of s-nitrosothiols and/or organic linkers of MOFs could lead to a method capable of modulating nitric oxide release. The desire to investigate larger RSNOs (R=cysteine, N-Acetyl-D,L-Penicillamine or glutathione) due to our hypothesis that larger R-groups slow down nitric oxide release, necessitated the probing of larger copper based MOFs capable of acting as drug delivery and storage vehicles. Due to its desirable copper centers and more extensive frameworks, MOF-143 and PCN-6', both analogs of HKUST-1 were chosen to further explore the effect of the MOF environment on nitric oxide release with several biologically relevant RSNOs. In order to investigate this phenomenon computationally, a combination of gas phase *ab initio* studies and condensed phase classical molecular dynamics simulations are utilized to study the effect of the complex MOF environment on the RSNO species and the catalytic reaction. Experimental probing of this system was done via chemiluminescence. The ultimate goal of this research is to determine how the substitution of R-groups in the RSNO species and organic linkers within the MOF affect catalytic properties and compare to previously studied s-nitrosothiol/MOF systems. Information pertaining to how varying MOF environments affects potential drug delivery will give tremendous insight on successful MOF candidates to study as pharmaceutical agents.