

Supporting Information

Effect of chemical structure of S-nitrosothiols on nitric oxide release mediated by the copper sites of a metal organic framework based environment

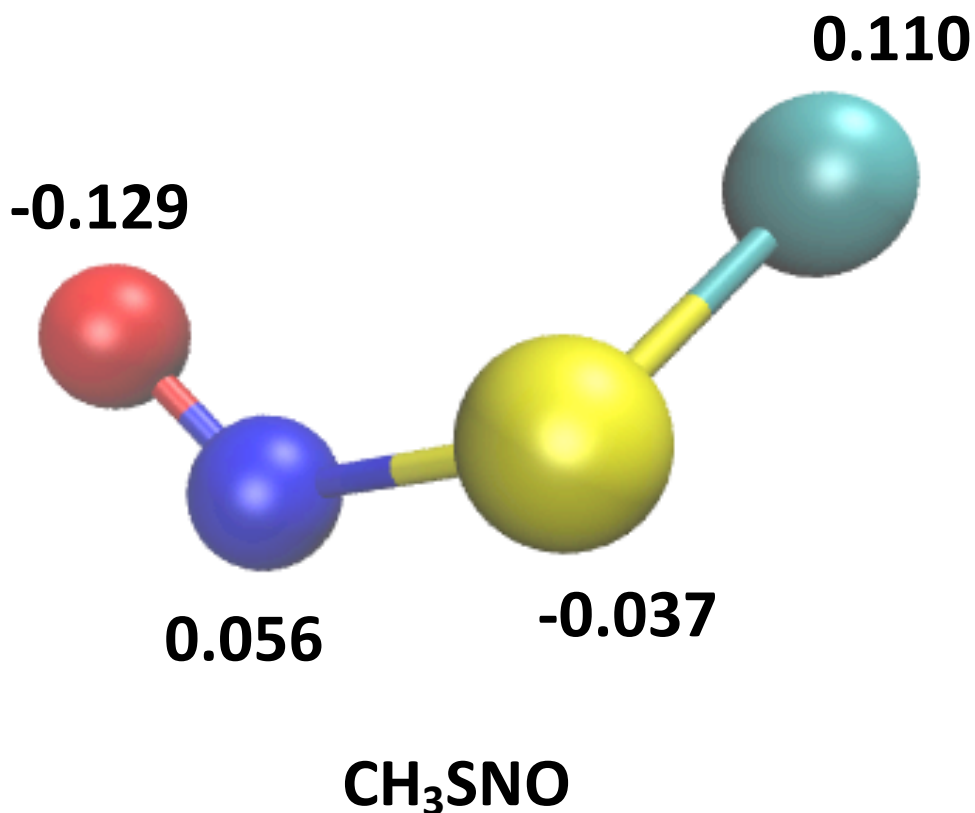
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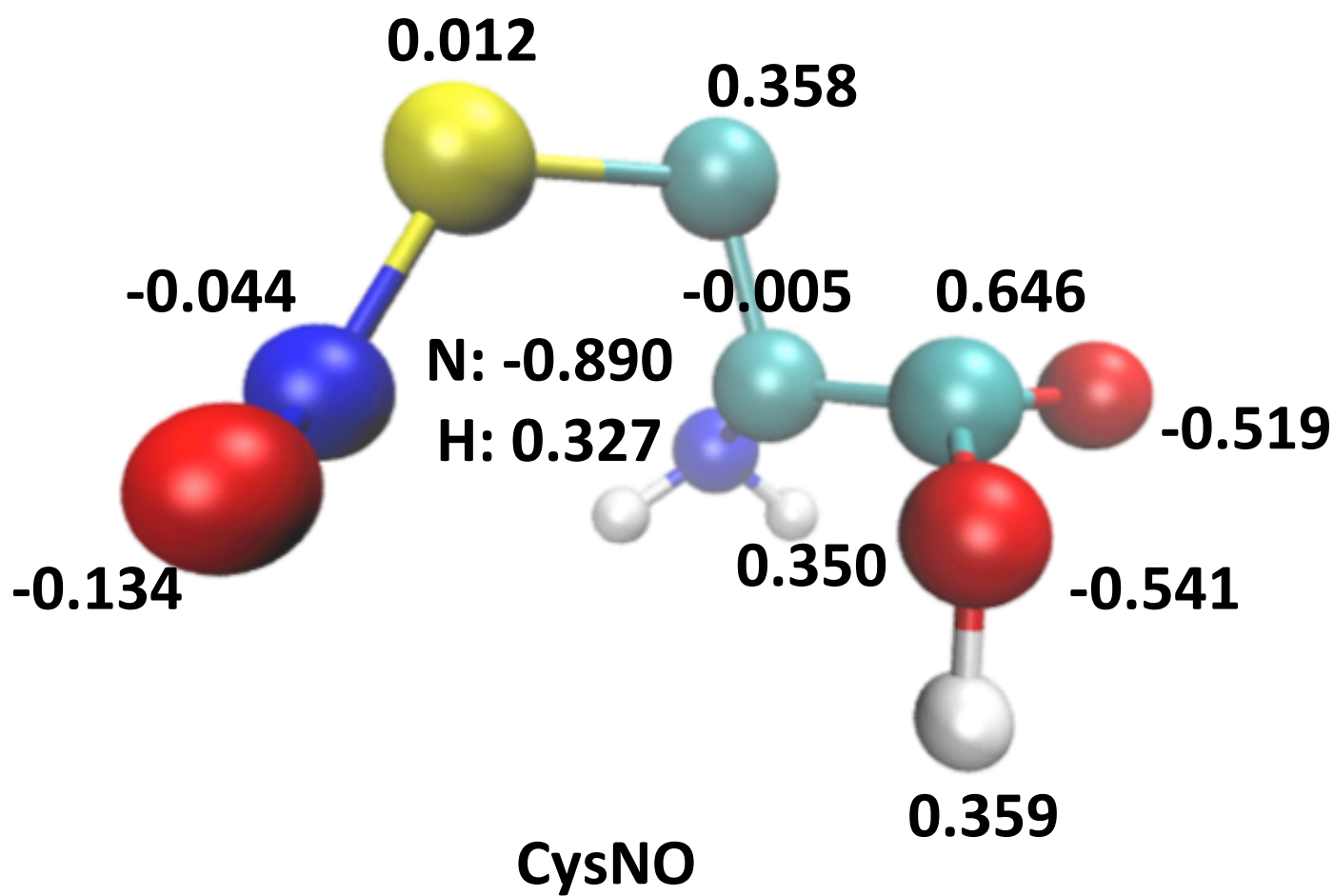
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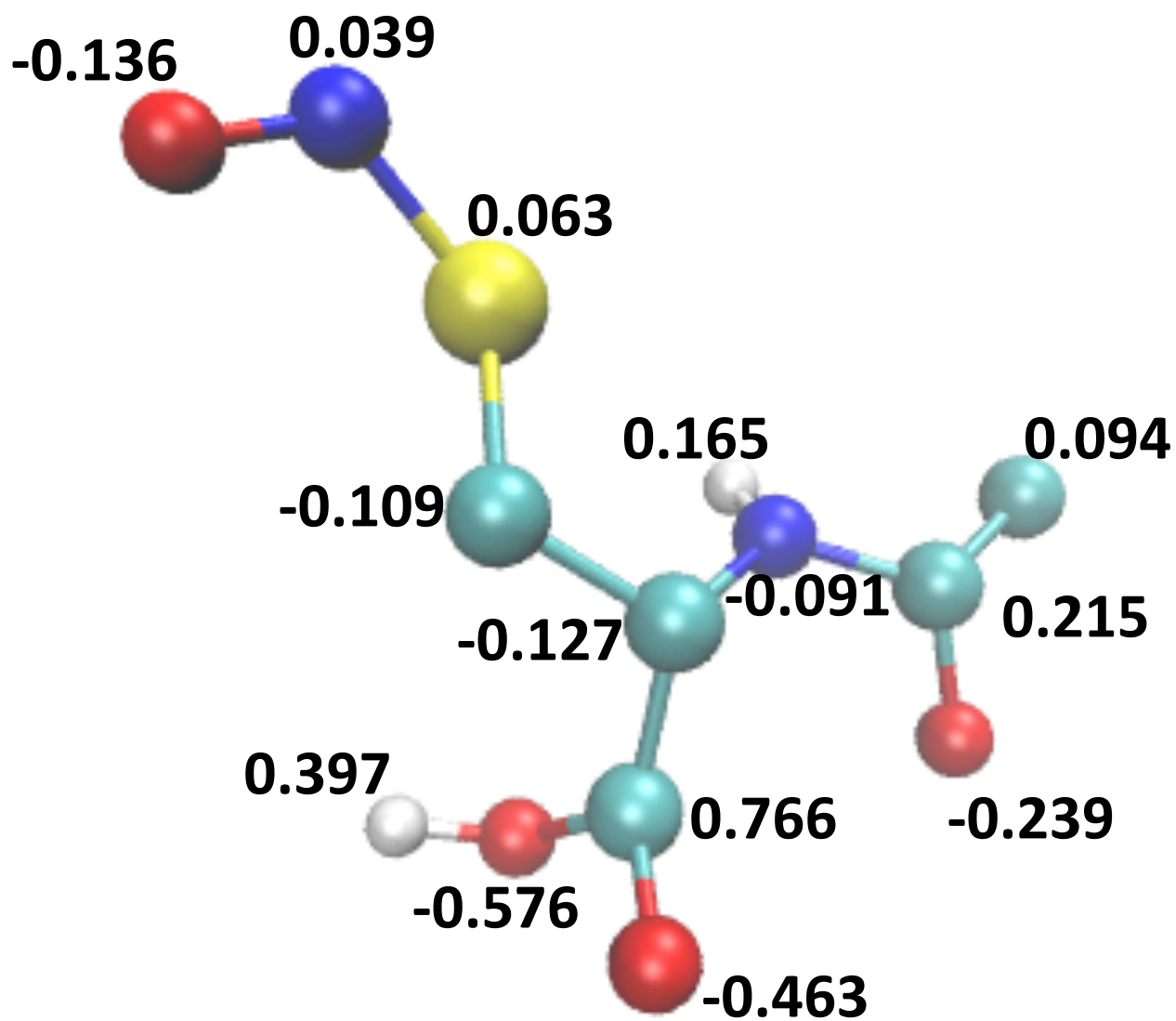
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Partial charges

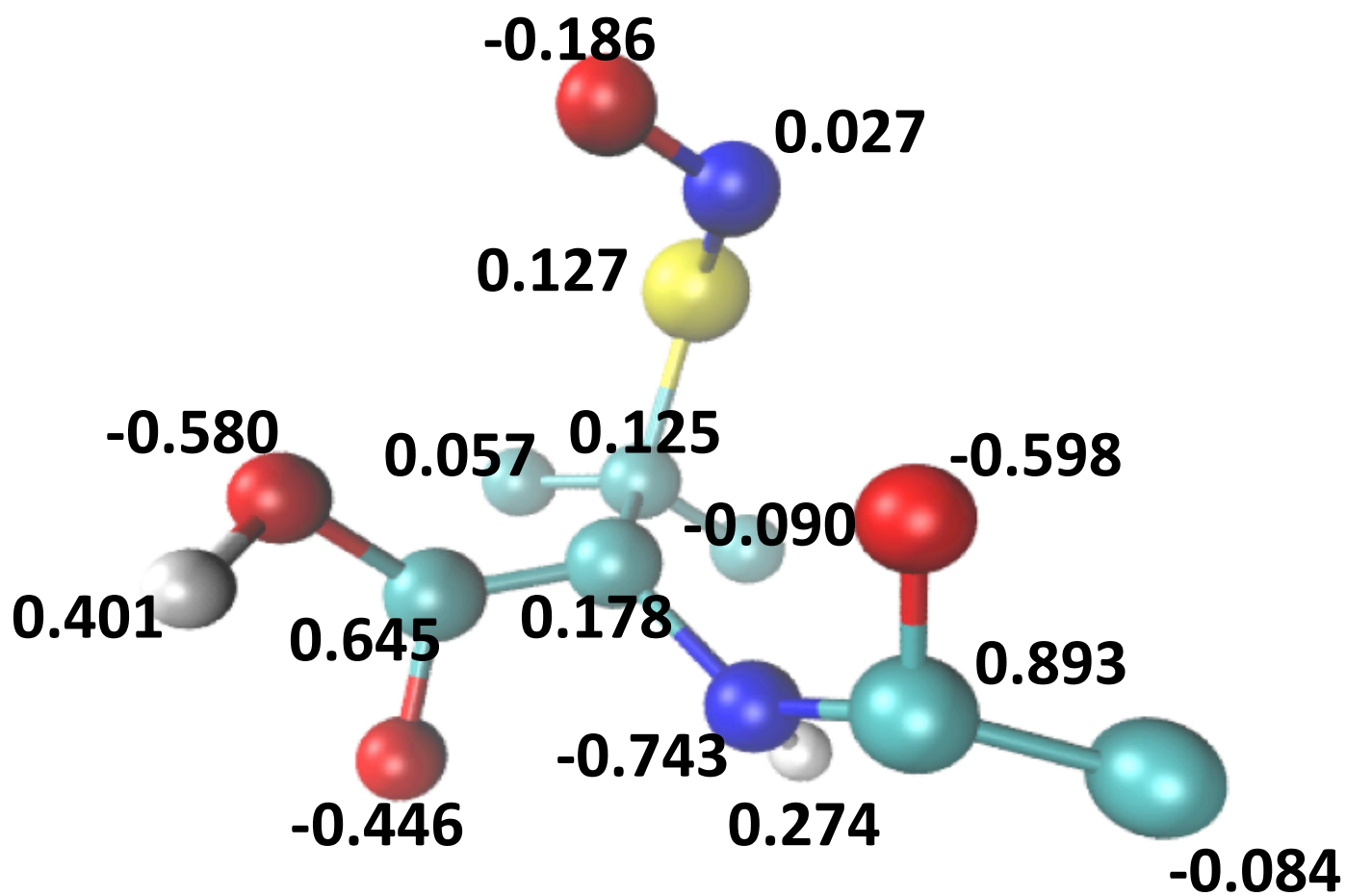
S1. The representative monomer clusters along with the partial charges (electron/elementary charge) for CH₃SNO, CysNO, SNAC, SNAP, GSNO and ethanol. Atomic representation is as follows: carbon (cyan), oxygen (red), hydrogen (white), sulfur (yellow) and nitrogen (dark blue).



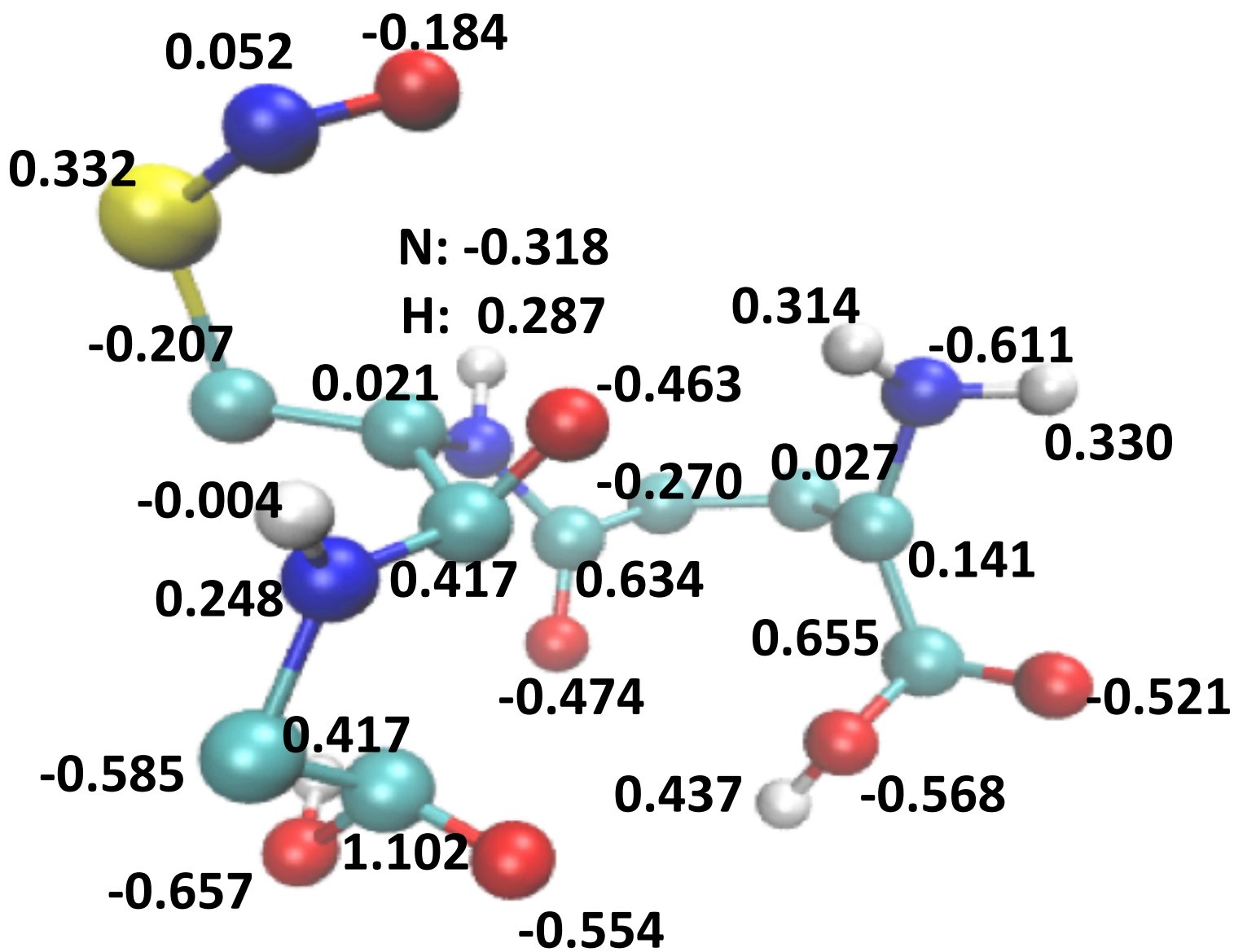




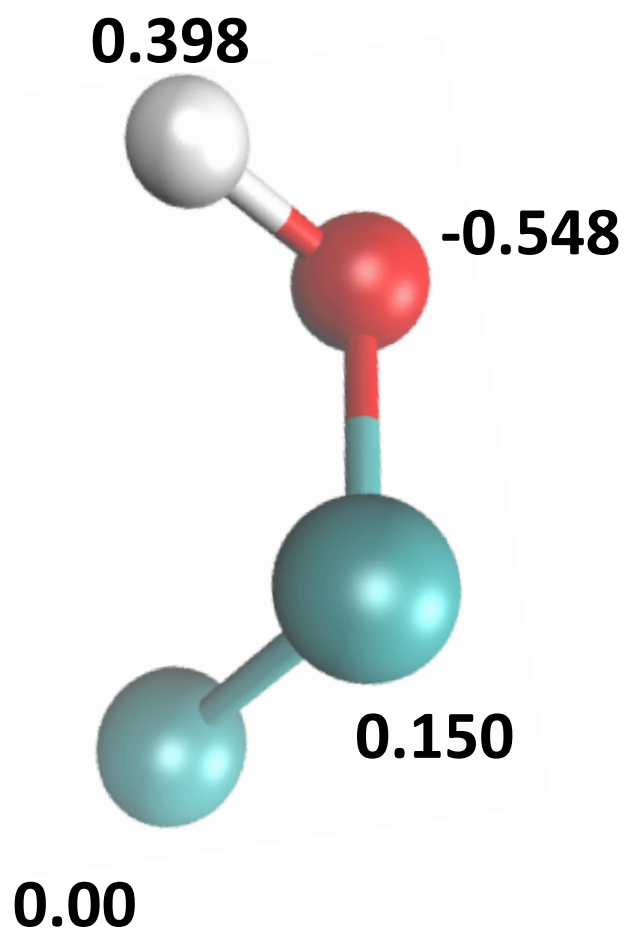
SNAC



SNAP



GSNO



Ethanol