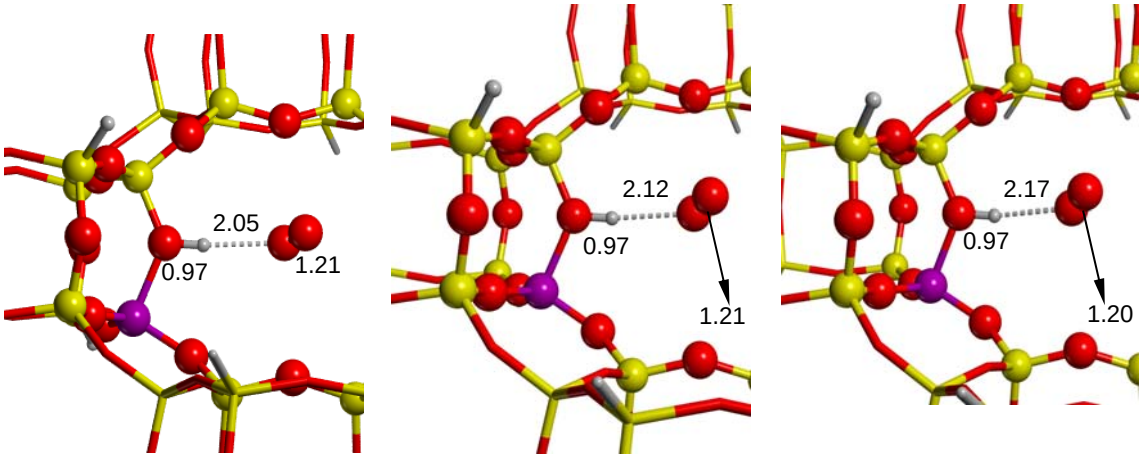
Table S1. $^3O_2$ adsorption energies (in kJ mol^{-1}) in H12T:48T using different basis sets. The total adsorption energy (E_{ads}) has been decomposed in two terms: the interaction energy (E_{int}) and dispersion (D)

	E_{ads}[b]	E_{INT}[b]	D[b]
$^3O_2$-H12T:48T/BSA[a]	-16.7	+1.3	-18.0
$^3O_2$-H12T:48T/BSA-D[a]	-18.3	+1.5	-19.8
$^3O_2$-H12T:48T/BSB[a]	-14.8	+0.8	-15.6
$^3O_2$-H12T:48T/BSC[a]	-14.8	+0.4	-15.2

[a] See computational details section for model description.

[b] See equation 1 to 3 and computational details section for partitioning scheme definition.



$^3O_2$-**H12T:48T**/BSA $^3O_2$-**H12T:48T**/BSB $^3O_2$-**H12T:48T**/BSC

Figure S1. Local view of the B3LYP/BSA:MNDO, B3LYP/BSB: MNDO and B3LYP/BSC:MNDO optimized $^3O_2$-H12T:48T adsorbed structures. Distances in Å.

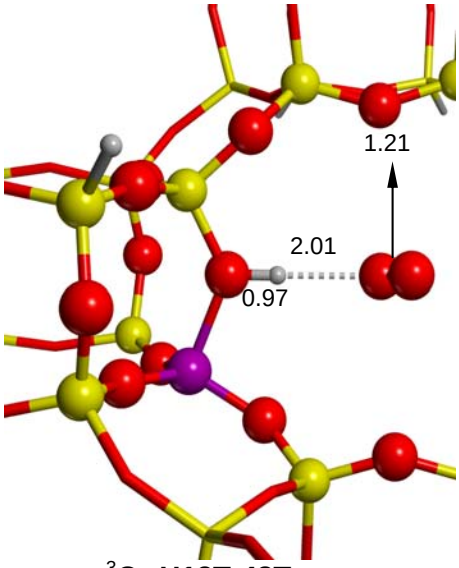
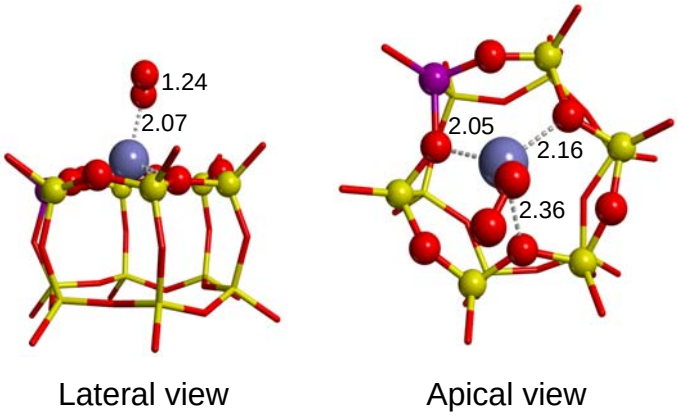


Figure S2. Local view of the B3LYP-D:MNDO optimized $^3O_2$-H12T:48T adsorbed structures. Distances in Å.



η^1-$^3O_2$-**CuCHA(I)**

Figure S3. Local view of η^1-O_2-CuCHA optimized ^{3} structures. Distances in Å.

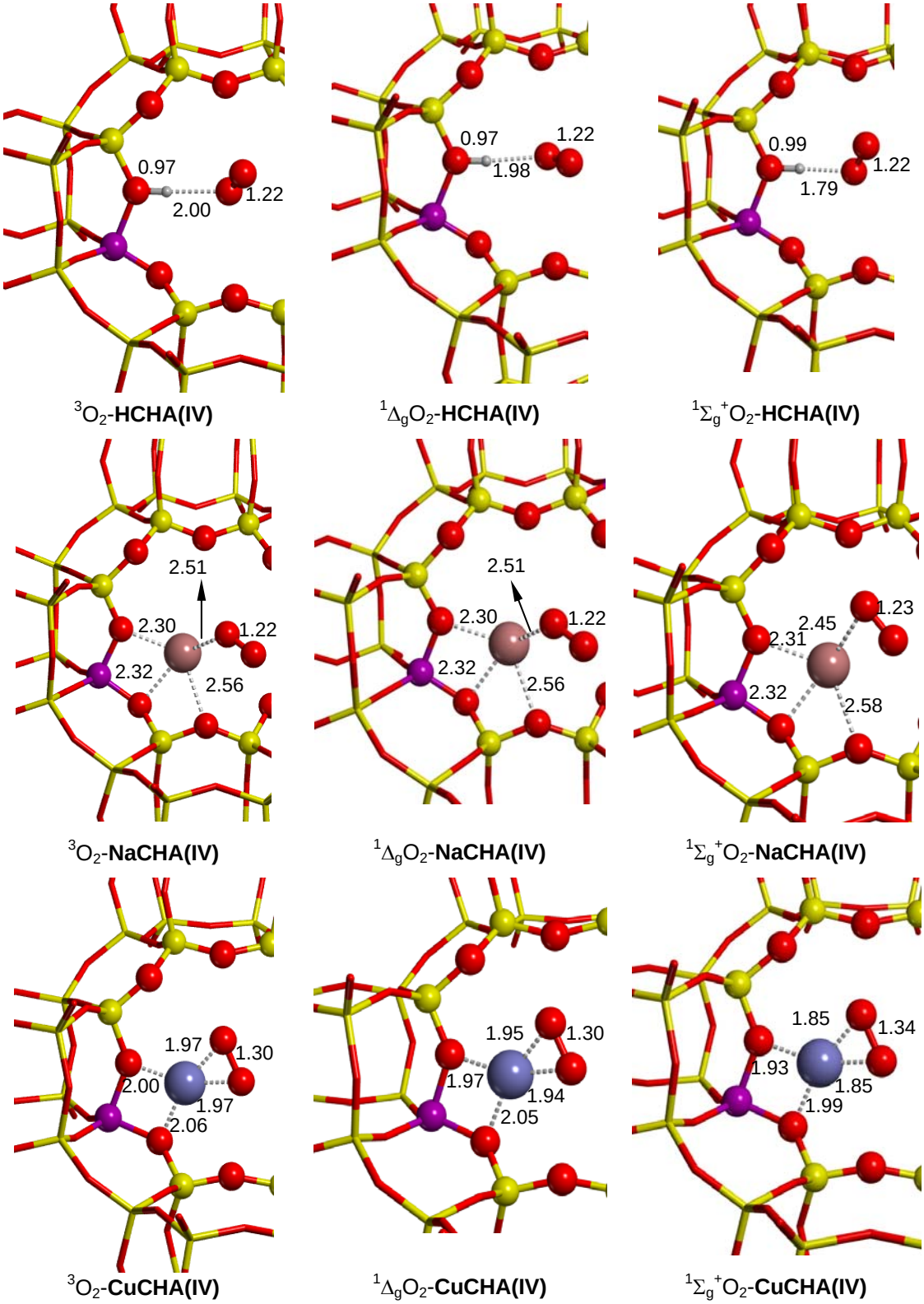


Figure S4. Local view of the optimized $^1\Delta_g$ and $^1\Sigma_g^+$ O_2-MCHA adsorbed structures (M= H^+, Na^+ or Cu^+). Distances in Å.