Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

The Effect of Counter-Ions on the Far-Infrared Spectra of Tris(triphenylphosphinegold)oxonium Dimer Salts

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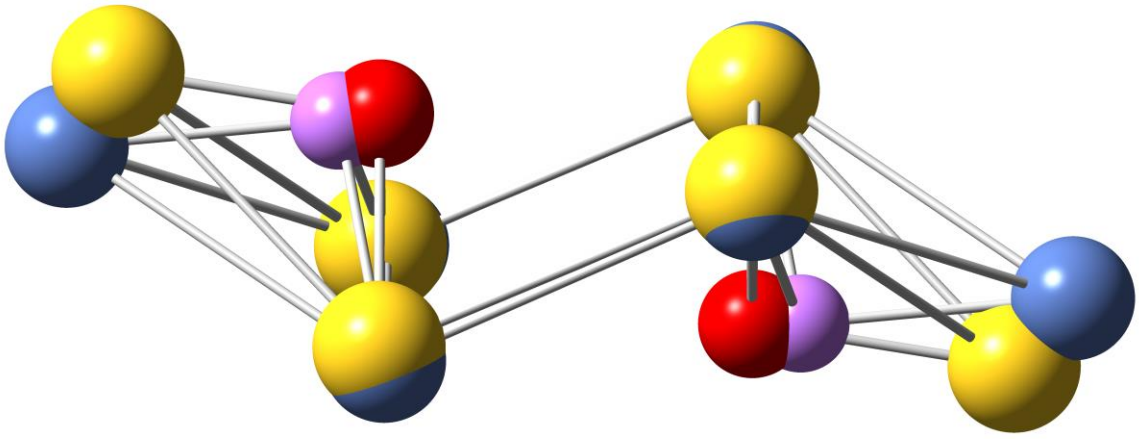

Figure S1: Comparison between X-ray crystallographic structure of the Au_6O_2 core before optimization (gold in yellow, oxygen in red) and after optimization (gold in blue, oxygen in pink).

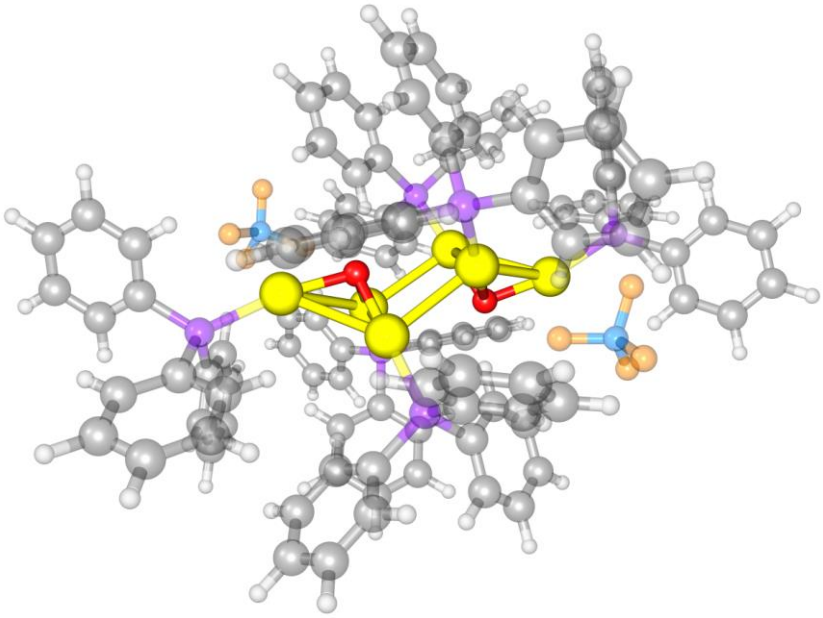

Figure S2: Structure of $[[(Ph_3PAu)_3O]BF_4]_2$, with PPh_3 ligands and counter-ions made transparent for clarity. Gold atoms are shown in yellow, oxygen in red, phosphorus in purple, boron in blue, fluorine in orange, carbon in dark grey and hydrogen in light grey.

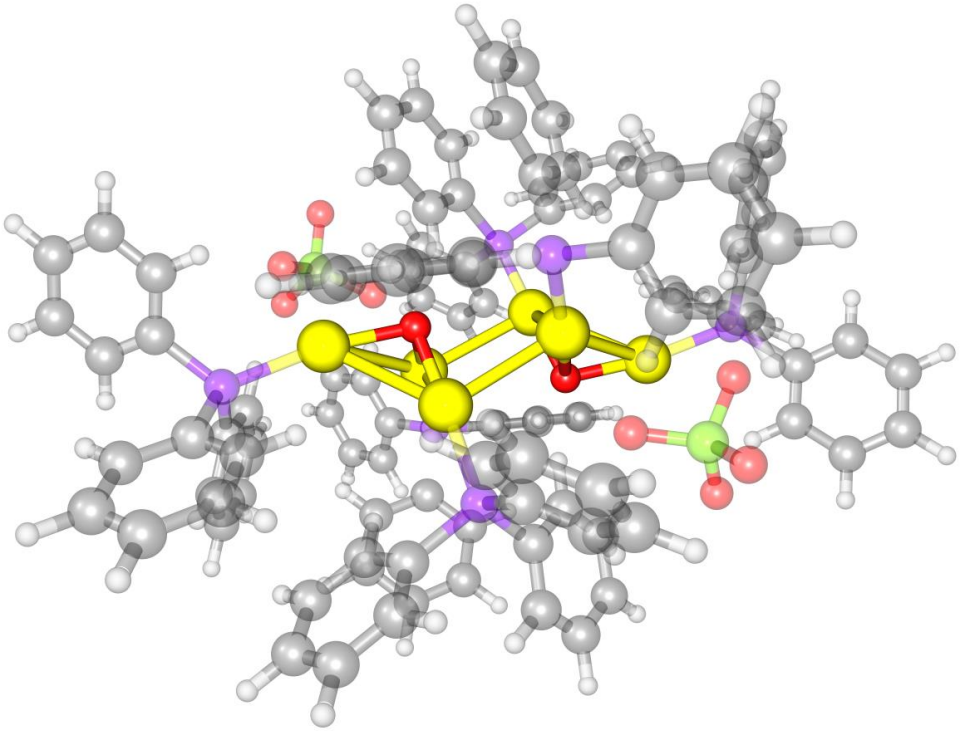

Figure S3: Structure of $[[(Ph_3PAu)_3O]MnO_4]_2$, with PPh_3 ligands and counter-ions made transparent for clarity. Gold atoms are shown in yellow, oxygen in red, phosphorus in purple, manganese in green, carbon in dark grey and hydrogen in light grey.

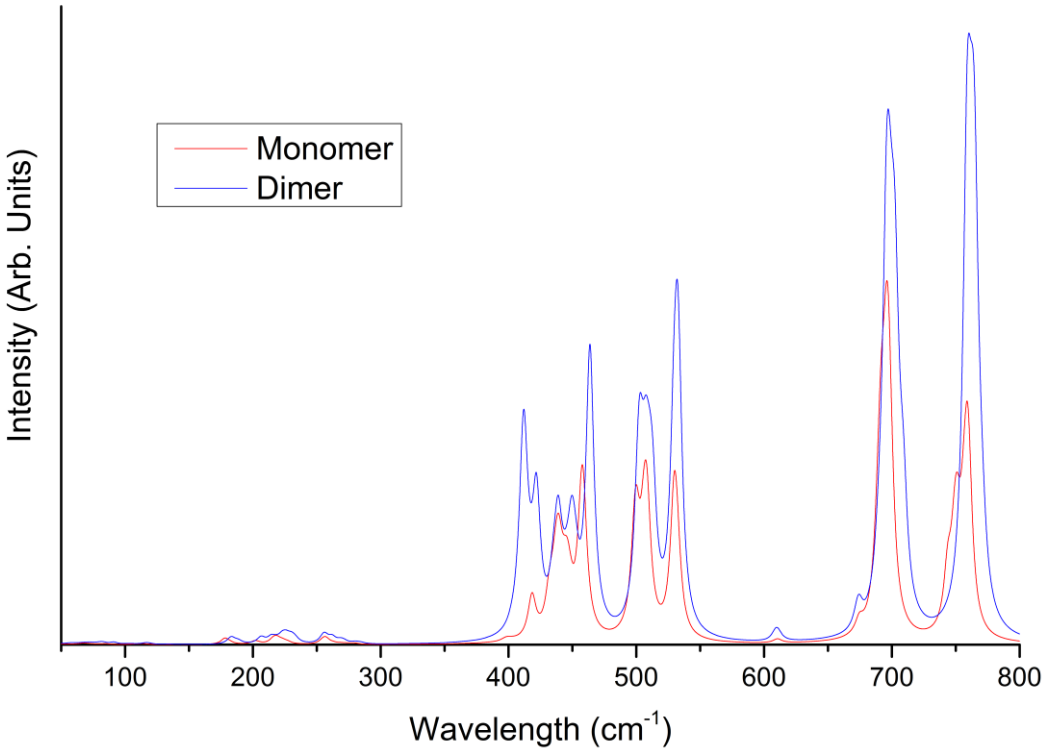

Figure S4: Comparison between the theoretical infra-red spectra of the $[(PPh_3Au)_3O]^-$ monomer, red, and the dimer of this species, blue.