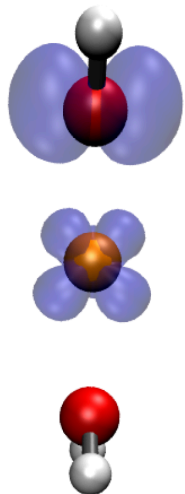
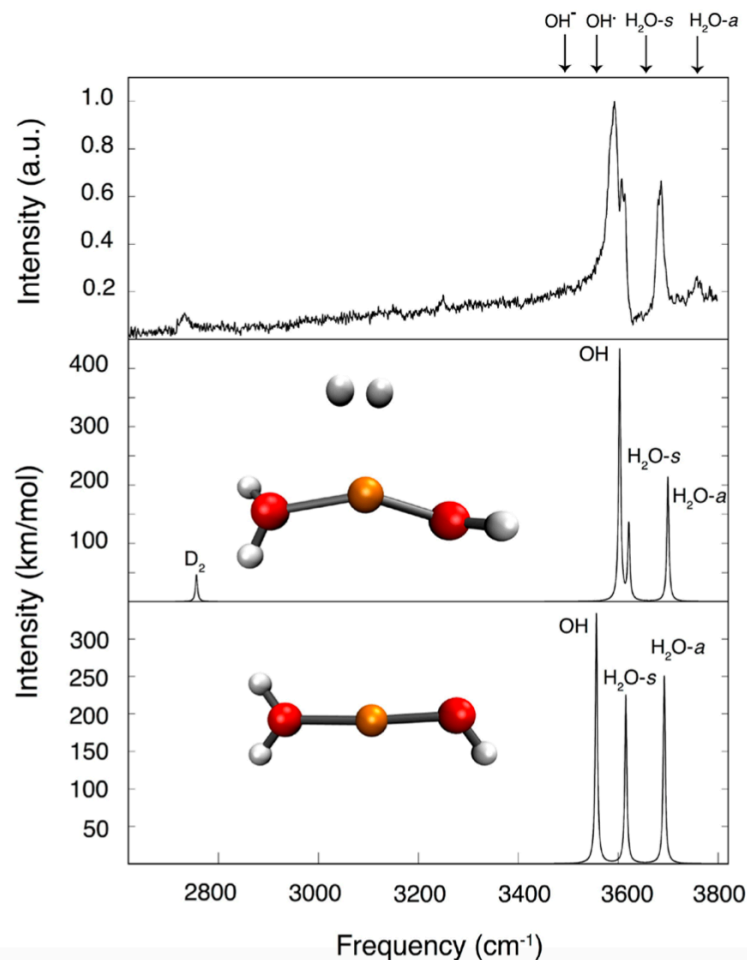


# P5707: ELECTRONIC STRUCTURE AND VIBRATIONAL SIGNATURES OF THE DELOCALIZED RADICAL IN HYDRATED CLUSTERS OF COPPER ("II") HYDROXIDE, $\text{CuOH}^+(\text{H}_2\text{O})_{0-2}$

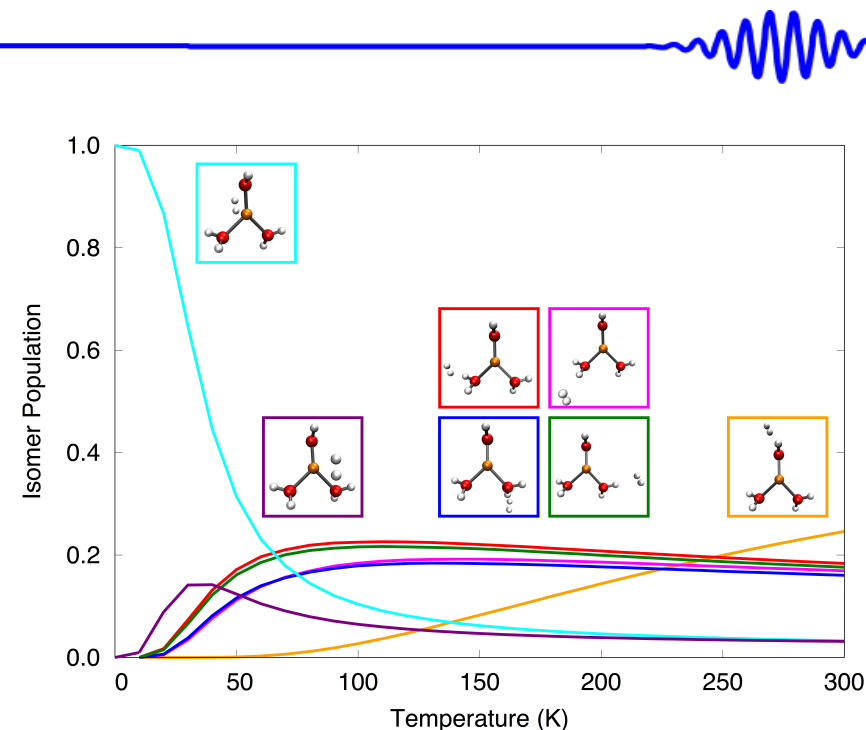
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- Delocalized radical for  $\text{CuOH}^+(\text{H}_2\text{O})_{0-2}$
- Some degree of multireference character



- $\text{D}_2$  tag distorts equilibrium geometry  $\text{CuOH}^+(\text{H}_2\text{O})$



- Tag degenerately binds to copper and water  $\text{CuOH}^+(\text{H}_2\text{O})_2$
- Experimental agreement with
  - EOM-IP-CCSD/cc-pVTZ
  - Correct tag location
  - Thermal weighted spectrum