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Preference of hydrogen bond binding site in 1:1 chromone-methanol complexes in different electronic states

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The cluster formed by chromone and methanol serves as an excellent model for studying the various contributions to intermolecular interaction energy. The asymmetric ketone motif of chromone provides distinct hydrogen-bonding sites, enabling the differentiation between an "inside" and an "outside" isomer.

We present the delicate balance between these two competing arrangements, investigated by combining IR/R2PI and UV/IR/UV spectroscopy in a molecular beam, supported by quantum-chemical calculations. Upon electronic excitation, chromone undergoes efficient intersystem crossing into the triplet manifold, allowing studies on aromatic molecule–solvent complexes to be extended to a cluster in a triplet state. We show that in both electronic states, the "outside"isomer dominates experimentally, in agreement with simulations performed at the DFT, SAPT0, and DLPNO-CCSD(T) levels.

These findings raise the question of whether chromone derivatives could exhibit a change in binding site preference upon electronic excitation. To explore this, we screen a variety of chromone derivatives with functional groups at positions 2 and 6 of the chromone backbone. A detailed study using DFT simulations identifies three chromone derivatives that meet this criterion.

Keywords

Hydrogen bond: medium, State of the system: gas

This abstract is submitted for....

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