THEORETICAL AND EXPERIMENTAL STUDY OF THE ROVIBRATIONAL SPECTRA OF CO_2-(*para*-H_2)-He TRIMERS

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Clusters of *p*-H_2 had been predicted to exhibit superfluid behavior twenty years ago,[a] but direct observation of this phenomenon was elusive until our recent work[b] combining experimental measurments and theoretical simulations of the non-classical rotational inertia and superfluid response of *p*-H_2 clusters doped with CO_2. However, the size-dependent superfluid response of those clusters reached a maxmum at $N = 12$, and the clusters become frozen at larger N. It is therefore interesting to examine the effect of adding helium atoms to a pure *p*-H_2 shell around a CO_2 chromophore, and to investigate their effect on the superfluid response of CO_2-(*p*-H_2)$_N$ for $N > 12$. This will help us understand the role of helium as a 'second solvent' species, and help explain experiments that had been presented as evidence of superfluidity of doped hydrogen clusters embedded in helium nanodroplets.[c] Exact quantum calculation of infrared and microwave spectra for dopant molecules attached to two pure He atoms or two pure *p*-H_2 molecules, respectively, have been reported by Wang and co-workers and by Li *et al*.[d] To date, however, no such calculations have been reported for mixed *p*-H_2/He solvent species. The present paper therefore extends such work to the case of one *p*-H_2 and one He atom attached to one CO_2 dopant molecule. Three-dimensional *p*-H_2 and helium densities in the body-fixed frame are presented, and compared with those for the analogous CO_2–$(He)_2$ and CO_2–$(p\text{-}H_2)_2$ trimers.

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