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 $CO_2$–($p$-$H_2$)$_2$ trimers.

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