EFFECTIVE MOMENTS OF INERTIA OF LINEAR MOLECULES EMBEDDED IN ^{4}He CLUSTERS.

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In recent times, rotationally resolved infrared spectra of several linear molecules (HCN[a], HCCH[b], OCS[c], HCCCN[d]) embedded in ^{4}He clusters have been measured by us and by other groups. From such spectra, effective moments of inertia (I_{eff}) can be calculated that are consistently larger (up to a factor of 3, depending on the molecule) than the corresponding gas phase values. While the trend can be explained by a simple hydrodynamic model (a solid ellipsoid rotating in a non viscous, incompressible fluid[e]), quantitative predictions need to take into account the effect of the increased helium density around the guest molecule. We have calculated the density profiles of He clusters doped with the above molecules, using the density-functional approach[f], and we find that the agreement between measured and calculated values of I_{eff} is significantly improved.

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