

HCN IN CLUSTERS OF HELIUM-4: THEORETICAL MODELS FOR SPECTRAL LINESHAPES

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We present an adiabatic formulation of rotational coupling for linear molecules in clusters of ^4He . The model is combined with the Path Integral Monte Carlo (PIMC) method to calculate finite temperature spectra incorporating the heterogeneous broadening that arises from spatial delocalization of the dopant within the cluster. The full anisotropic molecule-helium interaction and all quantum exchange effects in ^4He are included in the calculation. Preliminary results of microscopic PIMC calculations using this spectral model are presented for HCN in $^4\text{He}_N$. Comparisons with experimental spectra and with spectra generated from a long-range continuum model are also presented.