

MODEL INTERMOLECULAR POTENTIALS FOR HCN-HF

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Models of the intermolecular potential energy surface in HCN--HF are reported. These studies of the HCN--HF hydrogen bonded dimer are based on the recent rovibrational analyses of far infrared and near infrared gas phase spectra recorded using FTIR spectroscopy. Aspects of the molecular dynamics associated with the low frequency intermolecular bending molecular dynamics are shown to be fully consistent with the Buckingham-Fowler electrostatic-hard sphere model of this hydrogen bond.