

COMPOUND-MODEL MORPHED POTENTIAL FOR THE HYDROGEN BOND HCN-HF

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A five-dimensional compound-model morphed potential has been generated for the prototype hydrogen-bonded dimer HCN-HF. The potential includes the intermolecular degree of freedom and the HF stretching vibration. Five morphing parameters only are optimized correcting for inadequacies in the underlying *ab initio* potentials. The morphing transformation utilized a rotationally resolved spectroscopic database composed of microwave and infrared spectroscopic information. Band origin fundamental vibrational frequencies in HCN-HF are fitted to an average absolute error of 0.006 cm^{-1} . The calculated value of the ground state dissociation energy, $D_0 = 1969 \text{ cm}^{-1}$ is in excellent agreement with the experimental value of $1970(10) \text{ cm}^{-1}$ [Oudejans and Miller, *Chem. Phys.* 239 (1998) 345]. Limitations of the morphing methodology and its potential applications will be discussed.