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 $\mathrm{cm}^{-1}$is in excellent agreement with the experimental value of 1970(10) cm^{-1}[Oudejans and Miller, Chem. Phys. 239 (1998) 345]. Limitations of the morphing methodology and its potential applications will be discussed.