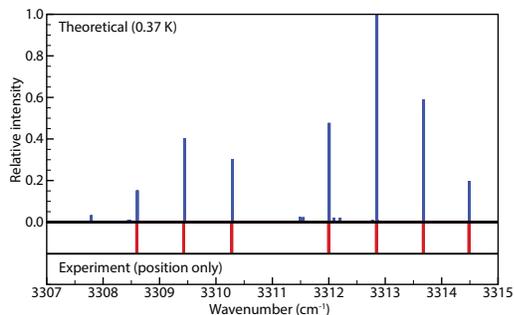# HIGH-ACCURATE INTERMOLECULAR POTENTIAL ENERGY SURFACE OF $HCN - H_2$ COMPLEX WITH INTRAMOLECULAR VIBRATIONAL MODE OF HCN INCLUDED

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Hydrogen is one of the most abundant interstellar species. Observation of rotational and vibrational spectra of H_2 containing complexes is of great importance because they are possible candidates for radio-astronomical detection. CO, HCN, HCCH are as isoelectronic molecules of N_2, each with a strong triple bond. It had been a big challenge to predict reliable theoretical rovibrational spectra of complexes including such species because the higher order electron correlation energy plays a non-negligible role in improving the accuracy. However, recent works on $CO - H_2$[a] have shown that it is possible to reproduce the experimental spectra quantitatively. In this work, we calculate a five-dimension potential energy surface (PES) of $HCN - H_2$ complex which explicitly include the intramolecular asymmetric stretching vibrational mode($C - H, Q_3$) coordinate at CCSD(T)/aug-cc-pVQZ+$3s3p2d1f1g$ level, corrected with electron correlation energy from the triple and quadruple excitation. Vibrational average over intramolecular vibration mode is made with HCN monomer at ground and the first excited vibrational states respectively, and the averaged data are fitted to two four-dimension Morse/Long-Range (MLR) potential energy functions. Based on the MLR PESs, for the first time, we calculated the spectra of $HCN - para H_2$ and $HCN - ortho H_2$. The results for $HCN - ortho H_2$ are in good agreement with the published experimental data[b] with root-mean-square-difference (RMSD) only 0.01cm^{-1}, which validates the accuracy of the PESs.

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[a]*J. Chem. Phys.*, **139**, 164315 (2013); *Science*, **336**, 1147 (2012).

[b]*J. Chem. Phys.*, **115**, 5137 (2001).