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HYDROGEN BOND POTENTIALS FOR HCN/HNC COMPLEXES

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Hydrogen bonding controls the properties of water and DNA, molecules of life, and has received enormous attention in the last century. Yet, it does not have a universally accepted potential due to its dependence on various physical and chemical forces, such as electrostatics, polarization, dispersion, exchange repulsion, and charge-transfer covalency. Recently, Shahi et al.1 and Hays et al.2 observed binding energy and collisional excitation properties for CN/HCN complexes and noted that HNC has stronger interaction than HCN, though both have nearly identical dipole moment. Theoretical estimates on charges indicated that the H in HNC has higher charge than that in HCN. This suggested that the HCN/HNC interaction could be charge-dipole and the potential could show r⁻2 dependence. We studied the potential energy surface of HCN/HNC complexes with different HB acceptors such as HF, HCN, HNC, C2H4, C2H2 and Ar. The first three acceptors have strong dipole moments, the next two have a quadrupole moment, and Ar is a spherical electron cloud. Depending on the acceptor, the interactions could vary as charge-dipole, charge-quadrupole and charge-induced dipole. The attractive part of the potential would then be expected to vary. This talk will summarize our results, which confirm that hydrogen bonding cannot be characterized as a specific physical force.

References:
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