PROBING HYDROGEN, LITHIUM AND CHLORINE BONDING USING MICROWAVE SPECTROSCOPY AND THEORETICAL TOOLS

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In this talk, I will be focusing on a few topics that concern molecular interactions, which may be written as X-A•••Y where A carries a partial positive charge with respect to X and Y has a region of electron density that interacts with the electron deficient A = H, Li, or Cl.

1. Microwave spectroscopy of C_6H_6•••C_2H_4 and CH_4•••H_2S complexes. Experimental structures of these complexes indicate the structures of these complexes to be very intriguing. I will discuss microwave spectrum, ab initio and Atoms in Molecules theoretical results on these two complexes.[1] These are cases in which A = H, X = C/S and Y = C atom or π cloud
2. Shift in IR stretching frequency of X-A. I will present theoretical results which clearly show that X-H stretching frequency can be used as a measure of hydrogen bond strength in most cases.[2] This can not be extended to cases where A = Li or Cl. This will highlight the danger in extrapolating knowledge gained by studies on hydrogen bonding to lithium/chlorine bonded systems.[3]
3. Is binding energy a good criterion for hydrogen bond? I will show that binding energy is not meaningful to define a hydrogen bond and differentiate it from van der Waals interaction (energy along A•••Y stretching coordinate). What appears more crucial is energy along torsional/bending coordinates in which A undergoes bending motion.[4]
4. Electron density at bond critical points. I will discuss results from a comprehensive study on electron density at bond critical points for H/Cl/Li bonded complexes.[5] Can electron density topology offer a unifying picture for molecular interactions?

References

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3. A. C. Legon, *Phys. Chem. Chem. Phys.* **12**, 7736 (2010).
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5. Abhishek Shahi and E. Arunan, to be published.