IS THERE A HYDROGEN BOND RADIUS?

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Pauling defined covalent radii, ionic radii and metallic radii for several atoms which were useful in estimating interatomic distances within a molecule/metal.[a]. Similarly van der Waals radius was defined to estimate the inter-molecular distances in crystals. Hydrogen bonding interactions have been known for more than eight decades now. However, accurate geometrical determination of hydrogen bonded complexes could be done in the last 3 decades only, beginning with the classical study on $(HF)_2$ by Klemperer and coworkers.[b] With the advent of pulsed nozzle Fourier transform microwave spectrometer[c] a wealth of experimental data has now become available. By evaluating ! the available structural data, we defined hydrogen bond radii for the hydrogen halides, such as HF, HCl, HBr and HCN recently.[d] An empirical correlation between the hydrogen bond radius and the dipole moment of the HX was also found. In this talk, we extend the analysis to H_2O and HCCH complexes to define hydrogen bond radius for OH (0.78 +/- 0.07 Å) and CH (1.09+/-0.05 Å) groups. The value for CH group is very close to the van der Waals radius for H atom as expected from the dipole moment correlation. Is hydrogen bond radius real? A critical evaluation of the data and our analysis will be given during the talk.

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[c] T. J. Balle and W. H. Flygare *Rev. Sci. Instrumen.* **52**, 33 (1981).
[d] P. K. Mandal and E. Arunan *J. Chem. Phys.* **114**, 3880 (2001).