ROTATIONAL SPECTRUM OF PROPARGYL ALCOHOL DIMER

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Propargyl alcohol is a molecule of interest to astrophysics as well as combustion studies. Rotational-tunneling spectra of propargyl alcohol monomer is well known and shows that the molecule exists in gauche form[a b]. Recently we reported microwave spectra of Ar...propargyl alcohol complex[c]. Propargyl alcochol exists in gauche form in the complex as well. In this study we have recorded pure rotational spectra of propargyl alcohol dimer between 4-13 GHz range.A total of 47 transitions, 24 a-type, 16 b-type and 7 c-type, have been observed and fitted with semi rigid rotor asymmetric top hamiltonian. The fitted rotational constants are: A = 2321.83323(47) MHz, B = 1150.47726(24) MHz and C = 1124.89000(20) MHz. The standard deviation for the fit is 2.5 kHz. The experimental rotational constants are very close to the structure predicted by ab-initio calculations in which two gauche-propargyl alcohol moieties are in three point contact stabilized by O-H...O, O-H...pi and C-H...pi interactions. Few transitions for duterated isotopologues of the dimer have also been observed and search for the remaining transitions is in progress. Details will be presented in the talk.

[a] E. Hirota,J. Mol. Spectrosc. 26 (1968) 335-350.
[b] J.C. Pearson, B.J. Drouin, J. Mol. Spectrosc. 234 (2005) 149-156.
[c] D. Mani, E. Arunan, ChemPhysChem 14 (2013) 754-763.