ROTATIONAL SPECTRUM OF Ar...PROPARGYL ALCOHOL COMPLEX

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Pure rotational spectrum for Ar...Propargyl alcohol complex has been observed and fitted. Fitted rotational constants for the complex are : A=4346.17307(90) MHz, B=1617.15317(19)MHz and C= 1245.42065(15) MHz. These rotational constants are very close to the ab-initio rotational constants for the geometry, in which propargyl alcohol exists in gauche conformation and Ar interacts with both, the hydroxyl group and the acetylenic group of propargyl alcohol. Rotational spectrum of deuterated isotopologue (-OD) of the complex further confirms the existence of the above mentioned geometry. In previous studies tunneling frequency corresponding to -OH tunneling motion in propargyl alocohol monomer was determined to be 652.4 GHz and for -OD tunneling motion in mono-deuterated species, it was 213.5 GHz[a,b]. In Ar...Propargyl alcohol complex also, a-type and c-dipole transitions show tunneling splitting. In the parent complex, for a-type transitions, tunneling splitting was 10 KHz and for c-type transitions (c-dipole of the complex is in the same direction as in propargyl alcohol monomer, and it is antisymmetric with respect to OH tunneling motion in both monomer and the complex), it was 2.59 MHz. In deuterated complex (OD) splitting was not resolvable for a-type transitions while for c-type it reduces to 900 KHz. Search for C-13 isotopologues is in progress. Moreover, propargyl alcohol offers several possibilities for H-bonding and we are planning to study its complexes with water in near future. Results 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.