

PROTON DONOR/ACCEPTOR PROPENSITIES OF AMMONIA: ROTATIONAL STUDIES OF ITS MOLECULAR COMPLEXES WITH ORGANIC MOLECULES

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We studied the rotational spectra of the adducts of ammonia with several organic molecules, namely *tert*-butanol,^a glycidol,^b ethyl alcohol, anisol and 1,4-difluorobenzene. The adducts with glycidol and ethanol have been observed for both conformers of the substrate molecule. Based on the rotational and ¹⁴N quadrupole coupling constants of the various complexes, we found a considerably different behaviour of ammonia, with respect to water, in its proton donor/acceptor double role. In the interaction with the three alcohol molecules, NH₃ acts as a proton acceptor and the OH groups as a proton donor. However, in the case of glycidol-NH₃, a secondary N-H...O interaction occurs between ammonia and the ether oxygen. This interaction generates a sizable V_3 barrier to the internal rotation of the NH₃ moiety, while NH₃ undergoes a free rotation in *tert*-butanol-NH₃ and in ethanol-NH₃. As to the anisole-NH₃ and 1,4-difluorobenzene-NH₃ complexes, the NH₃ group explicit its double proton donor/acceptor role, although through two weak ($C_{Me}-H \cdots N$ and $N-H \cdots \pi$) H-bonds. There is, however, an important difference between the two complexes, because in the first one NH₃ lies out of the aromatic plane, while in the second one it is in the plane of the aromatic ring.

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