Structural consequences of proton transfer in some selected complexes of phenol derivatives with trimethylamine.

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Streszczenie

General tendencies in structure modifications resulting from proton transfer in complexes of six selected phenols with trimethylamine are established on the basis of DFT B3LYP/6-31G(d,p) calculations with complete optimization of the structure for a given OH distance. It was found that various parameters linearly depend on C–O distance (*d*(CO)). Separate correlation lines are obtained for the complexes of different phenols. Values *d*(CO) depend on substitution and are proportional to pK_a. The O–H distance does not depend on pK_a in free phenols, but is strongly sensitive, while is engaged into hydrogen bond.

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