

# Quantumchemical Investigation of Borabenzene Adduct with Pyridine

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**Abstract**—Atomic charges and structural parameters of borabenzene, pyridine and their adduct in free state, in liquid argon and in tetrahydrofuran are calculated by the quantum-chemical method B3LYP/6-311G(3d5f7,p) & PCM. Mutual polarization of the adduct and medium results in small increase in boron–nitrogen interatomic distance and dihedral angle between the aromatic heterocycles. Calculated dipole moment of the adduct (7.17 D) is by 4.55 D over than the sum of dipole moments of the free components. Internal rotation barriers are not high: 1 kcal mol<sup>-1</sup> (0° and 180°) and 4 kcal mol<sup>-1</sup> (90°). The borabenzene–pyridine bonding energy (46 kcal mol<sup>-1</sup>) is higher than that with dinitrogen (19 kcal mol<sup>-1</sup>) and xenon atom (6 kcal mol<sup>-1</sup>). The B–N bond length in the little stable adduct with dinitrogen is by 0.08 Å shorter than in the stable adduct with pyridine. The Lewis acid properties inherent in borabenzene are transferred on the π-electron system of pyridine fragment in the adduct. The electron transfer wavelength from borabenzene to pyridine fragment in argon matrix is by 109 nm higher than in tetrahydrofuran, as calculated by CIS CNDO/S method.

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