DENSITY FUNCTIONAL THEORY STUDY ON MOLECULAR STRUCTURE AND VIBRATIONAL SPECTRA OF 4-AMINO-1-METHYLBENZENE

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We have discussed the applicability limits of HF, MP2 and DFT-B3LYP methods on 4-amino-1-methylbenzene in our previous work [1]. We have found the DFT-B3LYP method very promising for vibrational spectral analyses.
In this study, we extend DFT calculations with different basis sets for more appropriateness to exprimental results. The optimized molecular structures, vibrational frequencies and coresponding vibrational assigments of 4-amino-1-methylbenzene have been obtained from the DFT-B3LYP, DFT-B3PW91 and DFT-PBEPBE methods implementing the 6-311G+** and aug-ccPVQZ basis sets. Scale factors, which bring computational frequencies in closer agreement with the experimental data, have been calculated for predominant vibrational motions of the normal modes at each level considered. All observed harmonic IR and Raman bands of 4-amino-1-methylbenzene have been assigned in the frameworks of the calculations. The comparison of calculations with FT-IR and FT-Raman spectra of 4-amino-1-methylbenzene have been carried out.
We are planing to extend this work to the transition metal complexes in the form of MX2L2 [M: Transition metals e.g. Mn(II), Co(II) and Ni(II) . . . ; X : Halogens e.g Cl, Br, I, L: 4-amino-1-methylbenzene]

1. A. Altun, K. Golcuk, M. Kumru, ”Structure and vibrational spectra of p-methylaniline: Hartree-Fock, MP2 and density functional theory studies”, JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM 637: 155-169 OCT 3 2003