C_{60}-PIPERAZINE ADDUCT, $C_{60}N_2C_4H_8$: INFLUENCE OF THE FULLERENE ON THE PROTON AFFINITY AND VIBRATIONAL PROPERTIES OF THE PIPERAZINE MOIETY.

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The C_{60} aminoderivatives obtained via functionalization of fullerene with biologically-active fragments are of great interest due to their possible medical applications. In this respect, an understanding of the fullerene addition effect on the properties of an active center is important for the perspectives of such compounds utilization.

We have studied C_{60}-piperazine adduct (1, 2) (**C_{60}P**) as a model molecule for a series of the aminoderivatives, employing quantum-chemical calculations at the Hartree-Fock and a DFT (in the form of PBE (3) functional) levels of a theory.

The first and the second proton affinities of **C_{60}P** molecule have been calculated as energy difference between protonated and initial forms. The values were compared to those obtained for piperazine molecule itself, both in the chair and boat conformations, thus revealing the influence of the structural as well as electronic effects as in the case of fulleropyrrolidines (4).

IR spectra of **C_{60}P** were measured experimentally and compared to the spectra simulated at HF/6-31G* and PBE/TZ2P levels of theory (Fig. 2). HF approximation, after the uniform scaling of the calculated frequencies, was found to predict the wavenumbers and peak intensities of the vibrations with the preferential piperazine contribution much better than the DFT approach, while the latter provided more realistic description of the fullerene modes. Besides the spectra assignment, comparison of the piperazine vibrations in the adduct and in the different conformations of a free molecule was performed.

Figure 1. Molecular structure of C_{60}-piperazine adduct.

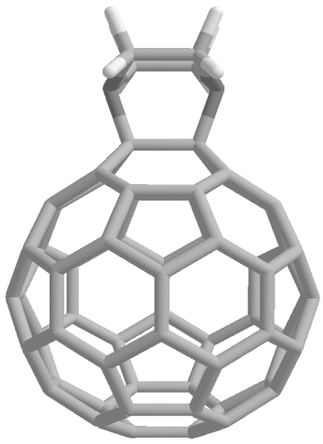
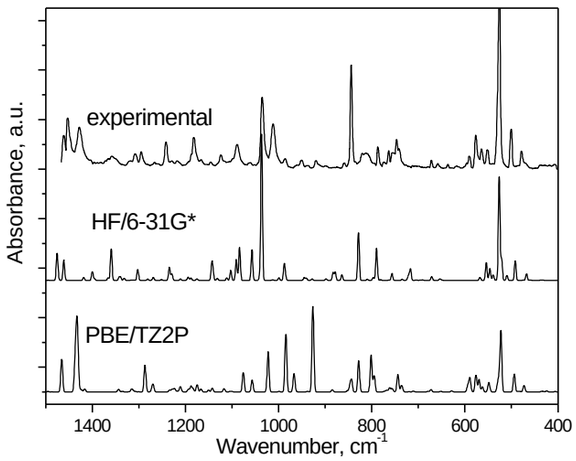


Figure 2. Experimental and simulated IR spectra of **C_{60}P**.



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