Accurate vertical and adiabatic ionization potentials for some benzaldehydes using hybrid DFT, multilevel G3B3, and MP2 methods

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Abstract

DFT , MP2 and G3B3 methods were used to compute the adiabatic and vertical ionization potential for some benzaldehydes. The computed results were compared with the experimental data. Validation of the methods were performed using several error metrics and statistical analysis. Results of G3B3 and DFT method showed an excellent agreement with experimental ones. Substitution effect was also studied. Geometrical structure changes of the examined benzaldehydes upon ionization were followed and analyzed.

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