

First principle simulation of vibrationally resolved $A^2B_1 \leftarrow X^2A_1$ electronic transition of phenyl radical

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Streszczenie

The $A^2B_1 \leftarrow X^2A_1$ electronic transition of phenyl radical has been studied by a recently introduced procedure to compute vibrationally resolved electronic spectra from first principles. Structural and vibrational properties have been obtained with the B3LYP/TD-B3LYP//N07D model, designed for computational studies of free radicals. The Franck–Condon Herzberg–Teller (FC-HT) spectra computed taking into account changes in structures, normal modes, and vibrational frequencies between both electronic states closely resemble their experimental counterpart. It is shown that full-dimensional vibronic models are necessary to reproduce correctly the spectrum shape and should be fully exploited prior to analyze the possible role of nonadiabatic effects.

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