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Vibrational and Electronic Spectra of 9, 10-Dihydrobenzo (a) Pyren-7 (8H)-One and 7, 8, 9, 10-Tetrahydrobenzo (a) Pyrene: An Experimental and Computational Study [Abstract]

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Vibrational and Electronic Spectra of 9, 10-Dihydrobenzo (a) Pyren-7 (8H)-One and 7, 8, 9, 10-Tetrahydrobenzo (a) Pyrene: An Experimental and Computational Study [Abstract]

The molecular geometries, vibrational and UV-vis spectra of 9,10-dihydrobenzo(a)pyrene-7(8H)-one (9,10-H₂BaP) and 7,8,9,10-tetrahydrobenzo(a)pyrene (7,8,9,10-H₄BaP) were investigated using density functional theory (DFT-B3LYP), with the triple- ζ 6-311 + G(d,p) and Dunning's cc-pVTZ basis sets. From the comparison of infrared experimental and calculated infrared, and Raman data comprehensive assignments are made. The calculated infrared frequencies below 1800 cm⁻¹ are in good agreement with experimental data, with an average deviation of <4 cm⁻¹. Using the B3LYP/6-311 + G(d,p)//TD-B3LYP/6-311G(d,p) level of theory, transition energies, and oscillator strengths of the 30 lowest electronic absorption bands are assigned to π - π^* transitions, with good qualitative agreement between experimental and simulated absorption data. In addition, the HOMO-LUMO gaps and their chemical hardness were analyzed.