1? ? 1?* ultraviolet absorption bands and electronic charge transfers in singlet excited states of sulfur aromatic heterocycles

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Indoline-2-thione (BC), benzimidazole-2-thione (BN), benzoxazole-2-thione (BO), and benzothiazole-2-thione (BS) define an interesting series of aromatic compounds containing a NCS synthonic unit in a heterocyclic ring of five centers, substituted by atomic centers of the type C, N, O, or S, where the main electronic absorption bands are localized in the spectral range of ultraviolet A or B. The first two singlet electronic transitions of this series, 1S0 ? 1S1(n,?*) and 1S0 ? 1S2(?,?*) determine the main spectroscopic characteristic of these compounds in order to be used as potential photochemical actinometers of solar ultraviolet radiation. Furthermore, the second electronic transition, localized in the 270-360 nm ultraviolet spectral range, presents a hipsochromic spectral shift as function of the electronic nature of the heteroatomic centers in the heterocyclic ring. In order to determine a spectroscopic assignment of the main absorption bands in aqueous solution and analyze the eff