

Thiaporphyrin with an inverted thiophene ring - DFT studies.

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Streszczenie

The structure and electronic energy have been investigated applying the density functional theory (DFT) for two idealized 2-thia-21-carbaporphyrin, (SCP)H and (3H-SCP), 2-thia-21-carbaporphyrin anion (SCP)⁻ and 21-thiaporphyrin (SP)H. The analysis of calculated total electronic energies, using the B3LYP/6-31-G* approach, demonstrates that the energy difference between 21-thiaporphyrin and its inverted isomer equals 10.34 kcal/mol [(SCP)H] and 52.08 kcal/mol [(3H-SCP)]. In contrast to 21-thiaporphyrin the thiophene fragments in (SCP)H and SCP⁻ present a geometry resembling that one of an isolated thiophene molecule.

Adres publiczny

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<http://link.springer.com>