

Core-modified hexaphyrin: synthesis and characterization of 31,34-disilahexaphyrinoid.

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Streszczenie

Condensation of 16-silatripyrrane with pentafluorobenzaldehyde under catalytic conditions followed by DDQ oxidation leads to 31,34-disilahexaphyrinoid--a four times reduced derivative of 31,34-disilahexaphyrin which contains two built-in silole units flanked by four tetrahedrally hybridized meso carbons. In the preferred folded macrocyclic conformation the silole rings remain perpendicular to each other. The steric hindrance of bulky substituents at silicon atoms and β -positions of siloles prevented aromatization. Only one meso diastereomer (5S, 15S, 20R, 30R) has been isolated and subsequently identified by 1D and 2D NMR techniques. The density functional theory (DFT) has been applied to model the molecular structure of 31,34-disilahexaphyrinoid consistent with constraints imposed by NOE experiments. The total energies calculated at the B3LYP/6-31G**//B3LYP/6-31G** level for four feasible meso diastereomers clearly demonstrated the energetic preference for the meso diastereomer (5S, 15S, 20R, 30R).

Adres publiczny

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