Characterisation of new 26,28-diheterosapphyrins : 5,10,15,20-tetraphenyl-26,28-dioxasapphyrin and 5,10,15,20-tetraphenyl-26,28-dithiasapphyrin.

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Streszczenie

5,10,15,20-Tetraphenyl-26,28-dioxasapphyrin (O_2TPSH) and 5,10,15,20-tetraphenyl-26,28-dithiasapphyrin (S_2TPSH), heteroanalogues of 5,10,15,20-tetraphenylsapphyrin ($TPSH_3$) have been synthesised by condensation of the respective precursors, namely 2,5-bis(arylhydroxymethyl)furan or bis(arylhydroxymethyl)thiophene and pyrrole. 26,28-Dioxasapphyrin presents an unusual skeleton with an inverted pyrrole ring lying opposite to the bipyrrolic unit at each protonation stage. In contrast, the planar arrangement of the macrocycle has been determined for 26,28-dithiasapphyrin.The tautomeric equilibrium of S_2TPSH which involves the exchange of a proton between N-25 and N-29 has been found to be slow on the ^{1}H NMR timescale below 213 K. Activation parameters of tautomerization were determined by the line shape analysis: $\Delta H^{\ddagger} = 47.2 \pm 1.1$ kJ mol^{-1}, $\Delta S^{\ddagger} = 19.9 \pm 5.5$ J K^{-1} ($\Delta H^{\ddagger} = 10.9 \pm 0.3$ kcal mol^{-1}, $\Delta S^{\ddagger} = 4.6 \pm 1.4$ cal K^{-1}).

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