# Vibrational analysis of Ni(II) complex with 4,12-ditolyl-16,24-diphenyl-3-thiaporphyrin (SDTDPPNi(II)Cl) and its isotopic labeled ($^{61}$Ni(II), -$d_6$, and -$d_{10}$) derivatives.

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Streszczenie

This work presents complete vibrational analysis of a chloride complex of Ni(II) 4,12-ditolyl-16,24-diphenyl-3-thiaporphyrin (SDTDPPNi(II)Cl) and its isotopic derivatives ($^{61}$Ni(II), -$d_6$, and -$d_{10}$). Five-coordinate SDTDPPNi(II)Cl, SDTDPP$^{61}$Ni(II)Cl, (SDTDPP-$d_6$)Ni(II)Cl, and (SDTDPP-$d_{10}$)Ni(II)Cl were investigated by FT-IR, RR, and UV-vis methods. Geometry optimization and vibrational frequencies were calculated for STPPNi(II)Cl model molecule and its isotopically labeled analogues using Gaussian'03. Also, charge distributions (GAPT) and geometrical aromaticity indexes (Bird's $I_5$ and HOMA) were calculated.

Adres publiczny

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