TRIDENTATE BINDING STRUCTURE OF Cu-(2,2′:6′,2″-TERPYRIDINE)

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In the gas phase, four low energy isomers of 2,2′:6′,2″-terpyridine are predicted in the energy range of 12 kcal mol^{-1} by density functional theory calculations. These isomers include trans-trans, trans-gauche, gauche-gauche (C_2), and gauche-gauche (C_s) configurations, with the trans-trans form being the most stable. Copper coordination induces ring rotations so that the metal binds with three nitrogen atoms of the ligand and two five-membered rings are formed by the Cu tridentate binding. The complex has C_{2v} symmetry in the neutral form and C_s symmetry in the ion. This complex is produced by laser vaporization molecular beam techniques, and the molecular structure is determined with pulsed field ionization zero electron kinetic energy photoelectron spectroscopy in combination with theoretical calculations.