

Silicon(IV) Chelates of an (*ONN'*)-Tridentate Pyrrole-2-Carbaldimine Ligand: Syntheses, Structures and UV/Vis Properties

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The tridentate (*ONN'*)-chelator properties of the pyrrole-2-(*o*-hydroxyphenyl)carbaldimine dianion (L^{2-}) were explored for the neutral penta-coordinate diorganosilicon complexes $LSiRR'$ ($R, R' = Ph, Ph; Ph, Me; Ph, tBu$) where the ligand *L* occupies the *ax*-*eq*-*ax* sites in a distorted trigonal-bipyramidal arrangement around the silicon atom, and for the neutral hexa-coordinate L_2Si , that has a *mer*-coordination. Single-crystal X-ray diffraction analyses show an almost planar ligand backbone with a Si–N bond to the imine group that is shorter in hexa-coordinate L_2Si than in penta-coordinate $LSiRR'$. In sharp contrast to the almost colorless neutral ligand LH_2 , both complexes show pronounced UV/Vis absorptions in the red-brown region that originate from HOMO - LUMO and HOMO-1 - LUMO transitions, and that are due to intra-ligand π - π^* transitions from the *N*-*o*-oxyphenylimine towards the imine moiety.

Key words: Chelate, Time-dependent DFT, Hypercoordination, Pyrrole, Schiff Base, UV/Vis