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

Daniela Gerlach\(^a\), Andreas W. Ehlers\(^b\), Koop Lammertasma\(^b\), and Jörg Wagler\(^a\)

\(^a\) Institut für Anorganische Chemie, Technische Universität Bergakademie Freiberg, Leipziger Straße 29, 09596 Freiberg, Germany
\(^b\) Department of Chemistry, Faculty of Sciences, Vrije Universiteit Amsterdam, De Boelelaan 1083, 1081 HV Amsterdam, The Netherlands

Reprint requests to Dr. Jörg Wagler. Fax: (+49) 3731 39 4058.
E-mail: joerg.wagler@chemie.tu-freiberg.de

Z. Naturforsch. 2009, 64b, 1571–1579; received September 14, 2009

Dedicated to Professor Hubert Schmidbaur on the occasion of his 75th birthday

The tridentate \((ONN')\)-chelator properties of the pyrrole-2-\((o\)-hydroxyphenyl)carbaldimine dianion \((L_2^-)\) were explored for the neutral penta-coordinate dionorganicosilicon complexes \(LSiRR'\) \((R,R' = \text{Ph, Ph; Ph, Me; Ph, }t\text{Bu})\) where the ligand \(L\) occupies the ax-eq-ax sites in a distorted trigonal-bipyramidal arrangement arround 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 \(\pi-\pi^*\) transitions from the \(N-o\)-oxyphenylimine towards the imine moiety.

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