Structural Features of a Sulfur-Containing Group 4 Metalla[11]-crown-4 Derivative

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Treatment of the ligand system (o-C₆H₄OH)–S–CH₂–CH₂–S–(o-C₆H₄–OH) (**2a**) with TiCl₄ gave the metalla-crown ether derivative [(–S–CH₂–CH₂–S–)(o-C₆H₄O)₂]TiCl₂ (**5a**). Complex **5a** was characterized by an X-ray crystal structure analysis. It showed a pseudo-octahedral structure with both sulfur atoms being *cis*-coordinated to the metal center. The chloride ligands are also *cis*positioned, whereas the remaining two Ti–oxygen bonds are *trans* to each other to complete the distorted octahedral coordination geometry. The reaction of **2a** with ZrCl₄ gave the analogous complex **5c**. The related ligand system (o-C₆H₄OH)–O–CH₂–CH₂–O–(o-C₆H₄OH) (**2b**) was doubly deprotonated by treatment with butyl lithium and then reacted with TiCl₄ to yield the complex [(–O– CH₂–CH₂–O–)(o-C₆H₄O)₂]TiCl₂ (**5b**).

Key words: Titanium Phenoxide Complexes, Internal Coordination, Thioether Chelate Ligands