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An LCAO-MO-SCF Investigation on Nickel(II) Dithiocomplexes Containing the $[NiS_4]$ Chromophore

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The electronic properties of some complexes containing the planar $[NiS_4]$ chromophore are investigated by an LCAO-MO-SCF method. The calculations involve an extensive use of the Mulliken-type approximations and some point charge approximations. A satisfactory interpretation of the electronic structure of the molecules and consistent assignments of the electronic absorption spectra are obtained. The different ability to form adducts with nitrogen donor bases is fully rationalised.

Die elektronischen Eigenschaften einiger den planaren Chromophor $[NiS_4]$ enthaltenden Komplexe werden nach einer LCAO-MO-SCF-Methode untersucht. Die Berechnungen erfordern weitgehenden Gebrauch von Mulliken-Näherungen und einigen Punktladungs-Näherungen. Man erhält eine befriedigende Deutung der Molekülstrukturen und konsistente Zuordnungen der elektronischen Absorptionsspektra. Die verschiedene Fähigkeit zur Addukt-bildung mit Stickstoff-Donorbasen wird völlig verständlich gemacht.

1. Introduction

During the last few years, there has been an enormous upsurge of interest in the chemistry of transition metal complexes with sulphur donors. This interest has manifested itself in the general area of novel complex synthesis, of molecular structure, and in the field of biological inorganic chemistry. Nickel forms a wide variety of complexes with bidentate sulphur ligands, which, although containing the same planar $[NiS_4]$ chromophore, have different properties. For example, the ability to form adducts with nitrogen donor bases out of the molecular plane varies noticeably. There have been several important