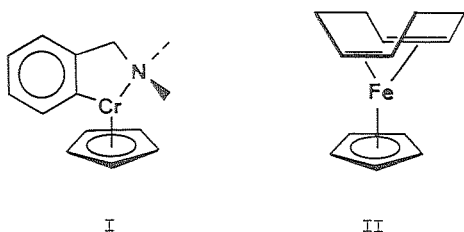


06.2-31 EXPERIMENTAL CHARGE DENSITY STUDY OF $(\text{CH}_2\text{SO}_2)_2$. By Y. Wang, C.T. Kao, C.J. Tsai, L.W. Guo; Dept. of Chem., National Taiwan University. J.W. Bats, Univ. of Frankfurt.

Single crystal of 1,3-dithietane-1,1,3,3-tetraoxide was studied by x-ray diffraction at 300°K and 104°K . It crystallized in monoclinic $P 2_1/n$. $a=5.527(2)$, $b=5.709(1)$, $c=8.042(2)\text{\AA}$, $\beta=100.89(3)^\circ$ and $Z=2$. The crystals are a four membered S-C-S-C ring with the center of the ring at $\bar{1}$. Using all the observed reflections below $\sin\theta/\lambda$ 0.66\AA^{-1} , the structure was refined to $R=0.020$. Distances and angles are : S-C $1.8058(8)$, $1.8096(6)\text{\AA}$; S-O $1.4353(5)$, $1.4376(6)\text{\AA}$; C-S-C $88.37(3)^\circ$; O-S-O $118.84(3)^\circ$. A charge density study was performed on 104°K data. The X-X deformation map of the 4-membered ring showed significant amount of density around sulfur atom but nothing significant between the two sulfur atoms (non-bonding distance 2.593\AA). There is 0.57 e/\AA^3 in the S-C bond but polarized toward sulfur atom. SO_2 plane is perpendicular to the 4-membered ring (88.6°). The density of S-O bond is at the center of the bond.

06.2-32 AB INITIO THEORETICAL CALCULATIONS OF THE ELECTRON DEFORMATION DENSITY FOR BENZYLAMINECYCLOPENTADIENYLCHROMIUM AND CYCLOOCTADIENECYCLOPENTADIENYLIRON. A COMPARISON OF THEORY WITH EXPERIMENT. By R. Goddard, MPI für Kohlenforschung, D-4330 Mülheim-Ruhr, FRG.

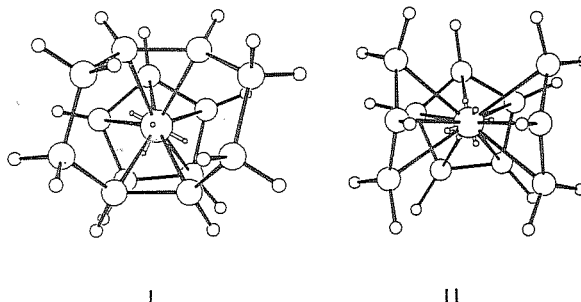
This paper describes the results of the calculation of the static electron deformation density distribution for $\text{C}_5\text{H}_5\text{Cr}(\text{C}_{12}\text{H}_{13}\text{N})$, I, and $\text{C}_5\text{H}_5\text{Fe}(\text{C}_8\text{H}_{13})$, II, by *ab initio* methods at the double- ζ level (AIMOL, V.R. Saunders 1976). The deformation densities are compared with each other and with those determined by experiment, (X-X) (X-N).



The distribution of the charge around the metals is discussed in terms of the electron count on the metal (the oxidation state), the nature of the ligands and their geometrical arrangement. An explanation for the stability of these unsaturated complexes (I, $14e^-$; II, $17e^-$) is suggested. A general approach for predicting the positions of the maxima about a transition metal based on simple ligand field theory is proposed and developed for more complicated systems.

06.2-33 THE ELECTRON DENSITY DISTRIBUTION IN TWO ISO-ELECTRONIC CYCLOPENTADIENYL-TRANSITION-METAL COMPLEXES. By C. Krüger, R. Goddard, and J. Allibon*, MPI für Kohlenforschung, D-4330 Mülheim-Ruhr, FRG and *Institut Laue-Langevin, F-38042-Grenoble, France.

The deformation density distribution (X-X, and X-N for I, 100 K) in the two isoelectronic, paramagnetic $17e^-$ -transition metal complexes, $\text{C}_5\text{H}_5\text{Fe}(\text{C}_8\text{H}_{12})$ (I) and $\text{C}_5\text{H}_5\text{Mo}(\text{C}_3\text{H}_5)_2$ (II), are compared.



Both compounds show an octahedral electron density distribution about the metal. The orientation of the octahedra with respect to the ligands is similar in the two complexes, but there are significant differences (see figures).

The spacial arrangement of the electron density around the metals appears to have stereochemical consequences and provides an explanation for the observed chemical behaviour of these and similar compounds.

06.2-34 A CHARGE DENSITY STUDY OF THE CUBIC FORM OF BORON NITRIDE. By B. Josten, A. Kirfel and G. Will, Mineralogisches Institut der Universität Bonn, Lehrstuhl für Mineralogie und Kristallographie, Poppelsdorfer Schloß, D-5300 Bonn, FRG.

$1253(\text{MoK}\alpha)$ and $3013(\text{AgK}\alpha)$ measurements of the X-ray structure amplitudes of the cubic BN ($a = 3.6153(2)\text{\AA}$; $F\bar{4}3m$) were carried out up to a maximum $2\theta = 156^\circ$, resulting in sets I and II of 41 and 76 observed unique reflections respectively. The conventional refinements of the spherical-atom model yielded agreement factors $R = 0.0156$, $R_w = 0.0202$ (set I) and $R = 0.0203$, $R_w = 0.0239$ (set II). The isotropic temperature factors of B and N and the respective scale factors were determined from high-order refinements and used for ensuing calculations of $X-X^{\text{HO}}$ difference density-, valence density- and deformation potential distributions in the (110) and (111) planes.

Further studies of the charge density distribution in BN were based on two models, both leading to significantly improved least-squares fits to the data: a) the "bond model" with a