06. CHARGE, SPIN AND MOMENTUM DENSITIES

06.2–31 EXPERIMENTAL CHARGE DENSITY STUDY OF
(CH₃SO₂)₃C²⁺ By T. 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 2₁/n, a=5.527(2), b=5.709(1), c=8.042(2)°, β=100.89(3)°, and Z=2. The crystals are a four membered S-C-S-C ring with the center of the ring at T. Using all the observed reflections below sinθ/λ < 0.65°, the structure was refined to R=0.020. Distances and angles are: S-C 1.8096(6); S-O 1.4353(5); C-S-C 104.84(3)°; O-S-O 118.84(3)°. 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 Å), There is 0.57 e/Å³ in the S-C bond but polarized toward sulfur atom. S₂O 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 BENZYL/ENCYCLOPENTADIENE TRANSITION-METAL COMPLEXES. 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 Cp₅Cr(C₅H₅)₂, I, and Cp₅Fe(C₅H₅)n, II, by ab initio methods at the double-ζ valence level (6-31G*, V.R. Saunders 1976). The deformation densities are compared with each other and with those determined by experiment, (X-X) (X-N).

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

The deformation density distribution (X-Y, and X-N for I, 104°K) in the two iso-electronic, paramagnetic 17e-transition metal complexes, C₅H₅Fe(C₅H₅)₂(I) and C₅H₅Mo(C₅H₅)₂(II), are compared.

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 (MoKα) and 3013 (AgKα) measurements of the x-ray structure amplitudes of the cubic BN (a = 3.6153(2) Å; F43m) were carried out up to a maximum 2θ = 156°, 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, Rw = 0.0202 (set I) and R = 0.0203, Rw = 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-Y 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