and 18-electron complexes, respectively. Crystal Be1o
fonnation refinement. all compounds studied that was
ment with the metals was observed in the deformation electron density maps for
A. radiation up to higher than any other of these bonds.
5tetral1edron around iron atom. the assumed local
symmetry of the different metal orbitals was observed that was in agree­
pany of the different metal orbitals.
In the maleate ligand the two carbonyl groups are linked by a
diffraction at a temperatme of
Asymmetry of the electron density distribution picture near the
lips was observed in the deformation electron density maps for
al compounds studied that was attributed to the different occu­
capacities of the 3d-metal orbitals. Numerical values of these occu­
capacities were estimated using a multipole refinement procedure.
In the series of the 16-, 17-, 18-electron complexes a gradual occu­
pacity of the different metal orbitals was observed that was in agree­
ment with the performed ab initio calculations and measured va­
or-phase electronic absorption spectra of the compounds studied.
It was found for Ti-complexes with the C₂H₂ and C₆H₆­
ligands that due to the different size of the ligand ring the energy
sequence of the molecular e₁, e₂, and e₃ orbitals has been changed,
and this effect is clearly seen in the deformation electron density maps.


Electron density distribution using single crystal X-ray dif­
fraction data was studied for the the similar π-complexes (η³-
C₅H₅)M(η²-C₇H₇) where M=Ti, V, and Cr. This series represents the
16-, 17- and 18-electron complexes, respectively. Crystal struc­
tures studied are isomorphic and compounds are isostructural
(space group Pmnă, Z=4, molecules in crystals have m-symmetry),
that allows to compare carefully their molecular geometry
and electron density distribution features caused mainly by the
different nature of the transition metal. All experimental data
were obtained at low temperatures (100-150K) with the “Siemens P3/
PC” diffractometer using Mo-radiation, for each crystal ca. 15000
reflections were collected, and R values were 0.025-0.031. Simversi­
lar crystal structure has the 17- electron complex (η²C₅H₅)Ti(η²-
C₇H₇) that was also studied (data collection at 293K because of the
phase transition, ca 9000 reflections, R=0.025). All complex­
es have the sandwich-like structure with the planar cyclic ligands
that are symmetrically bonded with the metal atoms. A typical
asymmetry of the electron density distribution picture near the
metals was observed in the deformation electron density maps for
all compounds studied that was attributed to the different occu­
capacities of the 3d-metal orbitals. Numerical values of these occu­
capacities were estimated using a multipole refinement procedure.
In the series of the 16-, 17-, 18-electron complexes a gradual occu­
pacity of the different metal orbitals was observed that was in agree­
ment with the performed ab initio calculations and measured va­
or-phase electronic absorption spectra of the compounds studied.
It was found for Ti-complexes with the C₂H₂ and C₆H₆­
ligands that due to the different size of the ligand ring the energy
sequence of the molecular e₁, e₂, and e₃ orbitals has been changed,
and this effect is clearly seen in the deformation electron density maps.

**PS09.01.17** ELECTRON DENSITY STUDIES ON TETRAAQUABIS (HYDROGENMALEATE)IRON(II), Isolda M. de C. Mendes & Nelson G. Fernandes. Department of Chemistry, Federal University of Minas Gerais, CP702-31270 901 Belo Horizonte, Brazil.

The non-spherical distribution of the valence electrons in a crys­
tal of Fe(C₇H₇O₄)₂H₂O was investigated according to the Hirshfeld deformation refinement, as part of a study of short hydrogen bonds in compounds of divalent transition metals with maleic acid.

X-ray data were collected on a Siemens four-circle diffractometer at 298 K, by the θ-2θ scan technique, using MoKα radiation up to sinθ/λ=1.20 Å⁻¹. For a P1 space group, 8131 reflections were measured which resulted in 6461 unique reflections (Rint= 0.0085), all of them were considered as observed in subsequent refinement, based on F² with applied extinction correction. For deformation refinement, 260 parameters, R=0.0299, wR=0.0277 against the conventional refinement, 126 parameters, R=0.0495, wR=0.0474.

In the maleate ligand the two carbonyl groups are linked by a short quasi-linear hydrogen bond with an O...O distance of 2.428(1) Å. The asymmetric crystallographic environment on this bond is revealed by the different O...H distances and electron density maxima of 1.09(2) Å and 0.2 eÅ⁻³ for the shorter and 1.35(2) Å and 0.1 eÅ⁻³ for the longer bond. Both maxima are at a distance of ~0.7 Å from the oxygen atoms. Density maps show that one of C...O bonds is significantly shorter and with an electron density maximum twice higher than any of other these bonds. Six oxygens atoms form a octahedron around iron atom, the assumed local symmetry is 4mmm.

In this case, the maps reveal an aspherical density distribution with maxima of ~0.2 eÅ⁻³ and ~0.3 eÅ⁻³ directed between the vertices of the octahedron.

**PS09.01.18** THE CHARGE DENSITY IN ADENOSINE AT 123K. H. W. Yang, J. R. Ruble, W. T. Klooster, S. K. Kampermann, B. M. Craven, Department of Crystallography, University of Pittsburgh, Pittsburgh, PA 15260.

New X-ray diffraction data for adenosine (C₅H₇N₅O₂) have been collected at high resolution (sinθ/λ < 1.34Å⁻¹) and reduced temperature (123K). The structure has been refined by least squares using Stewart’s rigid pseudopotom model. All nuclear positional and anisotropic m. s. displacement parameters were assigned fixed values from a previous neutron diffraction study at 123K (1). Thus the least squares refinement in­
volved only the scale factor, an isotropic extinction parameter, three X radial parameters (for C, N and O), and 356 pseudopotom electron popula­
tion parameters. The refinement, which was based on F² and included all 10,835 reflections, gave R(F)= 0.046 and Rcr(F)= 0.077 with good­
ness-of-fit = 1.64.

The total electronic charge density in the crystal ρ(r), has been mapped for pseudopotom as rest. Also the Laplacian of the charge density V²ρ(r) has been analysed at the (3,-1) bond critical points (2). At the bond critical points, ρ(r) is consistently greater in the adenine base than in the ribose sugar. Thus C4-C5 and C5-C6 in adenine ring system have ρ(r) = 2.05(7), 2.02(7)eÅ⁻³, whereas C1'-C2' and C2'-C3' in the ribose ring have ρ(r) = 1.78(6), 1.67(5)eÅ⁻³. Also, the Hessian matrix at the bond critical points indicates considerable double bond character for C4-
C5 and C9-C6 (ie 0.43, 0.43) whereas this is lacking for C1'-C2' and C2'-C3' (ie 0.09, 0.12). The Lapacian at all H-bond critical points is positive, indicating a lack of covalent bonding. There is a week H bond, C2-H2...O2.

Work supported by a grant GM-39513 from NIH.


**PS09.01.19** EXPERIMENTAL CHARGE DENSITY OF DL-SERINE AND L-SERINE. J. Buschmann, T. Koritsanszky, M. Ramun, P. Luger, Institute for Crystallography, Free University of Berlin, Germany.

Full topological analyses 1/1 of the electron density of the racemic and the enantiomeric form of serine will be presented. This investigation is part of a project where the electronic properties of amino acids are to be determined, using Bader’s approach 1/1, from the experimental density calculated with the multipole program package XD 2/.

Reflection intensity data were collected up to a limit of (sinθ/λ) = 1.18Å⁻¹ on a Siemens 4-circle X-ray diffractometer with MoKα radiation at a temperature of 150°C which was maintained by a nitrogen gas stream cooling device.

DL-serine: monoclinic, P2₁/a, Z=4, 10515 reflections measured, 3081 independent observed reflections, conventional refinement r_F = 0.029;
L-serine: orthorhombic, P2₁2₁2, Z=4, 7766 reflections measured, 2910 independent observed reflections, conventional refinement r_F = 0.030.

The L-forms of the molecule in the two different crystal structures are alike, showing the same overall conformation, but only the DL-serine crystal structure possesses a strong intramolecular hydrogen bond. So this is a special situation to look for the transferability of multipole parameters and the dependency of electronic and topological properties on intra- and intermolecular interactions.