and 18-electron complexes, respectively. Crystal Be1o
electron complex
and
all compounds studied that was
of 1.09(2)
In the series of the 16-.17 -.18-electron complexes a gradual occu­
ment with the
radiation up to
higher than any other of these bonds.
pancies were estimated using a multipole refinement procedure.
pancy of the different metal orbitals was observed that was in agree­
significantly shorter and with an electron density
shor1 quasi-linear hydrogen bond with an
3 for the longer bond. Both
and this effect is clearly seen in the defonnation electron density maps.

Electron density distribution using single crystal X-ray dif­
fraction data was studied for the the similar π-complexes (η3-
C3H5)M(n7-C5H5) where M=M,Ti, V and Cr. This series represents the
16-, 17- and 18-electron complexes, respectively. Crystal struc­
tures studied are isomorphous and compounds are isostructural (space group Pmmn. Zn=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 0.025-0.030. Similar
molecular structure has the 17-electron complex (η5C5H4)Ti(η5-
C5H5) that was also studied (data collection at 293K because of the
phase transition, ca 9000 reflections, R=0.025). All complexes
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
pancies of the 3d-metal orbitals. Numerical values of these occu­
pancies were estimated using a multipole refinement procedure.
In the series of the 16-,17-,18-electron complexes a gradual occu­
pancy of the different metal orbitals was observed that was in agree­
ment with the performed ab initio calculations and measured vapor-phase electronic absorption spectra of the compounds studied. It was found for Ti-complexes with the C5H5- and C6H6-
ligands that due to the different size of the ligand the ring energy sequence of the molecular el, e1 and e2 orbitals has been changed, and this effect is clearly seen in the deformation electron density maps.

Electron density studies on tetraaquabis (hydorgenmaleate)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 crystal of Fe(C6H5O2)4H2O 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 φ-2θ scan technique, using MoKα radiation up to sinθ/λ=0.20 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 O...O bonds is significantly shorter and with an electron density maximum twice higher than any other of 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.

Electron density studies on tetraaquabis (hydorgenmaleate)iron(II), Isolda M. de C. Mendes & Nelson G. Fernandes. Department of Chemistry, Federal University of Minas Gerais, CP702-31270 901- Belo Horizonte, Brazil.

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.