point scatterer initially placed on the middle of the B-N bond (R = 0.0070, R_w = 0.0105 (set I) and R = 0.0105, R_w = 0.0153 (set II)), and b) the multipole model (Hirshfeld, Israel J. Chem. (1977) 16, 226) including atomic monopole-, octopole- and hexadecapole scattering functions (R = 0.0050, R_w = 0.0088 (set I) and presently R = 0.0127, R_w = 0.0160 (set II)). The refined multipole parameters served to calculate sections of the static deformation density distribution.

All results show that the B-N bond contains a considerable ionic contribution in agreement with the respective electronegativities of 2.0 (boron) and 3.0 (nitrogen).

06.2–35   RE-DETERMINATION OF THE CHARGE DENSITY DISTRIBUTION IN BERYLLIUM METAL. By V.G. Tsirel'son, N.N. Lobanov, R.P. Ozerov, Mendeleev Institute of Chemical Technology, Moscow, USSR.

The experimental deformation electron density distribution (DEDD) in beryllium metal was studied by the modern treatment of Brown, X-ray diffraction data with extinction-free (10$\bar{1}$0), (0002) and (10$\bar{1}$1) reflections measured by Suortti and the neutron thermal parameters. Maps of DEDD in (000z) planes with z= 0, 0.125, 0.250 were calculated. Positive peaks of "covalent" electron density (0.016 a.u.) have been found in interatomic space. Positive peaks (0.098 a.u.) have been observed on Be atoms positions. This indicates that Be atoms in the metal are contracted in comparison with free state. As it has been established earlier in diamond, V, Cr, etc. excess of electronic part of electrostatic potential at Be position was found on potential distribution maps. Accordingly to the Politzer functional density approach these features correspond to the bonded state of Be atoms in metal.

06.2–36 X-RAY DIFFRACTION STUDIES OF THE CHARGE DENSITY IN PORPHYRINS : MESOTETRAPHENYL PORPHINATO BIS (TETRAHYDROFURAN) IRON II. By C. Lecomte[a], P. Coppens[b], R.H. Blessing[c], and Liang Li[b]. a) Laboratoire Cristallographie ERA162 54506 VANDOEUVRE LES NANCY FRANCE. b) Chemistry Department STATE UNIVERSITY OF New York, BUFFALO, N.Y. 14214 USA. c) Medical fondation of Buffalo, 73 High street, BUFFALO, N.Y. 14203 USA.

The crystal structure and experimental electron density distribution of (meso-tetraphenyl porphinato) bis (tetrahydrofuran) iron II has been determined from high resolution single crystal X-ray diffraction measurements at 120K This complex contains a six coordinate iron II atom which has an unusual high spin electronic ground state.

The detailed analysis was based on 7300 unique independent reflections by averaging of 11610 and 9490 reflections respectively measured at 120K on two different crystals. Both data sets were scaled ($R_T(F^2)$ = 0.023 after scaling). An empirical TDS correction is applied and discussed.

Conventional least squares refinement was applied to the structure factors (R(L.O. data) = 0.037, R_w(L.O.) = 0.054, G.O.F(L.O) = 2.16; R (H.O data) = 0.040; R_w(H.O) = 0.041; G.O.F = 1.07) .
The iron- oxygen bond length contracts from 2.351 (3) Å at room temperature to 2.294 (2) Å at 120K corresponding to a higher binding of the axial THF ligands. Magnetic susceptibility measurements down to 10K show the absence of high spin-low spin transition.

The data sets are refined with the aspherical formalisms of Hansen and Coppens and of Hirshfeld and a comparison will be made.

The experimental d orbital occupancies calculated for iron from the deformation populations will be used to calculate the Mossbauer quadruple splitting.