Hematite (α-Fe_2O_3) crystallizes in the corundum type structure (spacegroup R-3c) with the magnetic ions on the threefold axis. Antiferromagnetic ordering takes place at 950 K, a magnetic phase transition occurs at ≃ 250 K, the so called Morin transition. Below the Morin transition the magnetic moments are ordered antiferromagneticaly parallel to [111]. Above, a slightly canted antiferromagnetic arrangement with the spins perpendicular to the [111] direction is observed, which leads to a weak ferromagnetic component (Morin phase). The magnetic ordering of the Morin phase is not in agreement with the crystal symmetry, since the magnetic moments are perpendicular to the threefold axis. This break of symmetry should either result in an orthorhombic distortion of the lattice, a shift of the magnetic ions off the axis (implying static disorder) or an orbital ordering of the valence electrons. None has been reported in the literature.

To investigate the points in question, electron density studies are carried out on a natural hematite. Convergent beam electron diffraction patterns were taken from the three symmetry zone axes [001], [100] and [210] (hex. setting) with the corresponding whole- and bright-pattern symmetries of 3m, 2 and m. The patterns were each measured at room temperature and 90K using a JEOL2010FEF microscope equipped with a Schottky-type field emission gun and a Wollnik-type Ω-Filter [1]. Distortion and background corrections were applied. A maximum of 91 reflections per pattern was fitted using the software package MBFIT, which provides a multi beam nonlinear least squares algorithm for zeroth order and higher order Laue zone (ZOLZ, HOLZ) reflections, fully based on dynamical diffraction theory [2]. The set of fitting parameters contains full structural information (atomic positions, anisotropic Debye-Waller-factors and low order structure factors). Precise lattice parameters and starting parameters for the structural data were taken from Rietveld refinement based on synchrotron powder diffraction data measured at the beamline BL20B2 at SPring8 / Japan [3] at the above mentioned temperatures. The charge density distribution is calculated from the refined low order structure factors.

[1] K. Tsuno et al., J. Electron Microsc.. 46 (1997) 357-368
[2] K. Tsuda and M. Tanaka, Acta Cryst. A55 (1999) 939-954
[3] E. Nishibori et al., Nucl. Instr. Meth. A467-468 (2001) 1045-48