American Mineralogist, Volume 87, pages 347–349, 2002

Monoclinic nearly stoichiometric wüstite at low temperatures

HELMER FJELLVÅG,[1] BJØRN C. HAUBACK,[2] TOM VOGT,[3] AND SVEIN STØLEN[1,*]

[1]Department of Chemistry, University of Oslo, Postbox 1033, N0315 Oslo, Norway
[2]Institute for Energy Technology, Kjeller, Norway
[3]Physics Department, 2-21, Building 510B, Brookhaven National Laboratory, Upton, New York 11973-5000, U.S.A.

ABSTRACT

The crystallographic and magnetic structures of $Fe_{0.99}O$ at 10 K have been determined by high-resolution neutron powder diffraction. $Fe_{0.99}O$ is found to be monoclinic, space group *C2/m*, with unit-cell dimensions $a = 5.2615(1)$, $b = 3.0334(1)$, $c = 3.0602$ (1) Å, and $\beta = 124.649(2)°$. The Fe-O distances in the distorted FeO_6 octahedron are 2.154 Å × 4 and 2.165 Å × 2. The magnetic unit cell is obtained by doubling one of the crystallographic axes, a (magn) = a_m, b (magn) = b_m, and c (magn) = $2c_m$. The refined magnetic components at 8 K are $M_x = 2.7(1)$ μB, $M_y = -0.9(2)$ μB, and $M_z = 4.77(2)$ μB, with resultant $M = 4.03(2)$ μB.