

**substance: Fe<sub>3</sub>O<sub>4</sub>**

**property: crystal structure, high temperature phase**

Magnetite shows a highly unusual transition at 119 K– the Verwey transition. Above this temperature, the material shows the properties of a poor metal, but below  $T_V$  a distortion to a semiconducting phase of much lower symmetry is found.

**crystal structure** at room temperature: cubic, inverse spinel type, space group  $O_h^7 - Fd3m$ ,  $Z = 8$  [75S, 58H].

**positions of atoms in the unit cell**

O atoms at 32(e) sites  $u\ u\ u$ ;  $u\ -u\ -u$ ;  $1/4-u$ ,  $1/4-u$ ,  $1/4-u$ ;  $1/4-u$ ,  $u+1/4$ ,  $u+1/4$ ;

$-u$ ,  $-u$ ,  $u$ ;  $-u$ ,  $u$ ,  $-u$ ;  $u+1/4$ ,  $1/4-u$ ,  $u+1/4$ ;  $u+1/4$ ,  $u+1/4$ ,  $1/4-u$  + f.c. translations

Fe atoms at 16(d) sites  $5/8\ 5/8\ 5/8$ ;  $5/8\ 7/8\ 7/8$ ;  $7/8\ 5/8\ 7/8$ ;  $7/8\ 7/8\ 5/8$  + f.c. translations.

Fe atoms at 8(a) sites  $0\ 0\ 0$ ;  $1/4\ 1/4\ 1/4$  + f.c. translations.

The 16(d) sites are octahedral and the 8(a) sites are tetrahedral.

**value of  $u$**

$u$	0.379	25C
	0.3798	58H

**References:**

- 25C Claasen, A. A.: Proc. Phys. Soc. 38 (1925) 482.  
58H Hamilton, W. C.: Phys. Rev. 110 (1958) 1050.  
75S Samuelson, E. J.: J. Phys. C7 (1975) L 115.