

Subfile name: Inorganic, Mineral, Alloy&Metal, Battery Material, Common Phase, Forensic, Pharmaceutical, ICSD Pattern

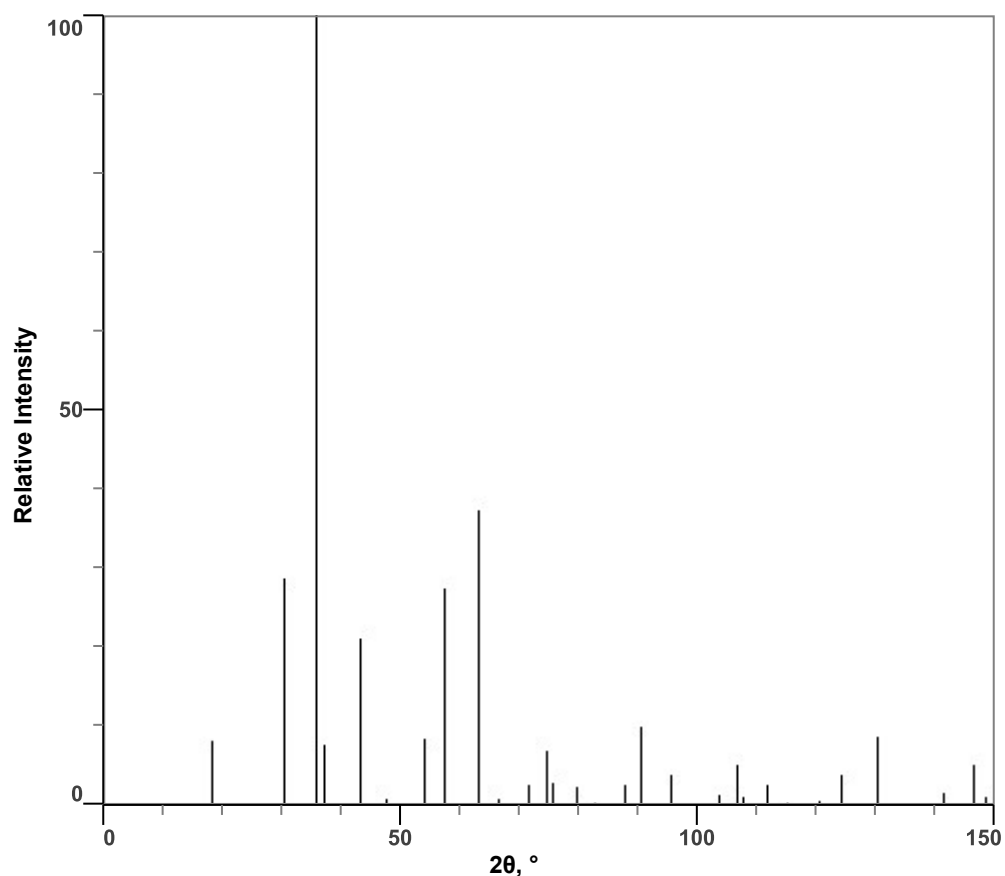
Chemical formula: Fe_3O_4
 Name: iron diiron(III) oxide, magnetite, syn I/Ic (RIR) = 5.070

Crystal system: Cubic Space group: 227 : Fd-3m Obs.density, g/cm³: 0.00000
 Lattice parameters: $a = 8.31980$ $b = 8.31980$ $c = 8.31980$
 $\alpha, ^\circ = 90.000$ $\beta, ^\circ = 90.000$ $\gamma, ^\circ = 90.000$
 Volume = 575.889 Z = 8.000

Reference : Gatta, G.D., Kantor, I., Boffa Ballaran, T., Dubrovinsky, L., McCammon, C. Phys. Chem. Miner.34(2007) 627.

Radiation: CuK α 1 Wavelength = 1.54060
 2 θ range: 0.00000 - 150.00000

Database comments: ANX: AB2X4. Analysis: Fe_3O_4 . Formula from original source: Fe_3O_4 . ICSD Collection Code: 158505. In Situ Condition: In diamond anvil cell with methanol:ethanol:water pressure-transmitting medium. Pressure of Datacollection: 4990 MPa. Sample Source or Locality: synthetic. Temperature of Data Collection: 293 K. Wyckoff Sequence: e d a (FD3-MZ). Unit Cell Data Source: Single Crystal.



No.	2 $\theta, ^\circ$	d-value	Norm. I.	h k l	No.	2 $\theta, ^\circ$	d-value	Norm. I.	h k l
1	18.46	4.803	8.30	1 1 1	17	90.66	1.083	9.80	7 3 1
2	30.36	2.941	28.80	2 2 0	18	95.58	1.040	3.80	8 0 0
3	35.77	2.509	100.00	3 1 1	19	98.55	1.016	0.10	7 3 3
4	37.41	2.402	7.60	2 2 2	20	103.56	0.980	1.20	8 2 2
5	43.47	2.080	21.10	4 0 0	21	106.61	0.961	5.20	7 5 1
6	47.60	1.909	0.70	3 3 1	22	107.64	0.954	1.00	6 6 2

No.	2 θ , °	d-value	Norm. I.	h k l	No.	2 θ , °	d-value	Norm. I.	h k l
9	63.17	1.471	37.30	4 4 0	25	120.58	0.887	0.60	6 6 4
10	66.43	1.406	0.80	5 3 1	26	124.06	0.872	3.80	9 3 1
11	71.69	1.315	2.70	6 2 0	27	130.23	0.849	8.60	8 4 4
12	74.76	1.269	6.80	5 3 3	28	134.21	0.836	0.10	9 3 3
13	75.78	1.254	2.80	6 2 2	29	141.54	0.816	1.60	10 2 0
14	79.80	1.201	2.40	4 4 4	30	146.56	0.804	5.10	9 5 1
15	82.78	1.165	0.40	5 5 1	31	148.38	0.801	1.00	10 2 2
16	87.71	1.112	2.70	6 4 2					

2 θ are calculated with wavelength=1.54059Å