solids and will form one of the major topics of the following paper.

APPENDIX

Let us study more closely the oscillator strengths defined in (8.10). Since the relevant values of k are very small ($<\omega_p/c$), we may replace (8.10) by its limit for $k=0$. For the interband oscillator strengths, ω_{n0} is independent of k. We then see from (8.10) that the transverse oscillator strength $f_{0n}(k,\mu)$ is just equal to the corresponding longitudinal $f_{0n}(\boldsymbol{\varepsilon}_{k\mu})$, in the limit of small k. The interband oscillator strengths depend only on the polarization of the wave, and not on its direction of propagation.

In (8.10) we defined the intraband $f_{0n}(k,\mu)$ as being equal to the longitudinal $f_{0n}(\boldsymbol{\varepsilon}_{k\mu})$. The f-sum rule for the transverse $f_{0n}(k,\mu)$ is then a trivial consequence of the sum rule for the longitudinal $f_{0n}(\boldsymbol{\varepsilon}_{k\mu})$. If, however, we had defined the intraband oscillator strength by the same expression as the interband one,

$$f_{0n}{}^{\mathrm{intra}}(k,\mu)=\frac{2}{\hbar m}\,\frac{|\sum_i(\boldsymbol{\varepsilon}_{k\mu}\cdot\mathbf{p}_i e^{-i\mathbf{k}\cdot\mathbf{x}_i})_{0n}|^2}{\omega_{n0}},\qquad\text{(A1)}$$

we would not have an f-sum rule. Using (A1) in place of (8.10), one finds that

$$\sum_n f_{0n}(k,\mu)=N-\sum_{n\,(\mathrm{intra})}\sum_{\alpha,\beta}A_\alpha A_\beta\left(\frac{m}{m^*}\right)_{\alpha\beta}\qquad\text{(A2)}$$

where the vector $\mathbf{A}$ is given by

$$\mathbf{A}=\frac{(\boldsymbol{\varepsilon}_{k\mu}\times\boldsymbol{\varepsilon}_k)\times\boldsymbol{\nabla}_\kappa E}{\boldsymbol{\varepsilon}_k\cdot\boldsymbol{\nabla}_\kappa E}.\qquad\text{(A3)}$$

For a longitudinal polarization $\boldsymbol{\varepsilon}_{k\mu}$, $\mathbf{A}=0$ and the two definitions of the intraband oscillator strength are equivalent. It is not so, however, in the transverse case.

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Superexchange Interaction Energy for Fe^{3+}-O^{2-}-Fe^{3+} Linkages

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The superexchange interaction energy for an Fe^{3+}-O^{2-}-Fe^{3+} linkage is considered for seven oxides in which Fe^{3+} is the only magnetic ion present, and for magnetite. The superexchange energy may be estimated from the value of T_C/n, where T_C is the Curie temperature and n is the number of Fe^{3+}-O^{2-}-Fe^{3+} interactions per Fe^{3+} ion per formula unit. The average value of T_C/n is 115° (range 106 to 132°). The only compounds considered are antiferromagnetic oxides in which Fe^{3+} ions are present in one set of crystallographically equivalent positions and ferrimagnetic oxides in which Fe^{3+} ions are present in two different sets of crystallographically equivalent positions. No distinct correlation of superexchange energy with Fe^{3+}-O^{2-} distances or with the included angle in the linkages is evident. Superexchange coupling is considered only for contact distances and for included angles substantially greater than 90°.

INTRODUCTION

KRAMERS[1] first suggested that the coupling of magnetic moments of transition-metal ions in oxides could take place through excited states of intervening oxygen ions. The nature of this coupling, which is known as superexchange[2] interaction, has been investigated in more detail by Van Vleck[3] and Anderson.[4] Néel[5] has shown that the antiferromagnetism of transition-metal oxides and the spontaneous magnetization of iron spinels (ferrites), which he has called ferrimagnetism, may be understood on the basis of negative exchange (antiferromagnetic) interaction.

Thus far, attempts to estimate the exchange energy have not yielded entirely satisfactory results. Theoretical treatment of the problem is difficult and experimental data have been inadequate. Weisz[6] found a semiempirical relationship of the exchange energy to the magnetic moment of M, the M-O distances and the M-O-M angle, where M is a transition-metal ion. However, his relationship depends on the structure type involved.

The Curie temperature,[7] T_C, of a material may be considered to be the most direct measure of the interaction energy between magnetic ions. The number, n, of M-O-M interactions per magnetic ion per formula

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[1] H. A. Kramers, Physica **1**, 182 (1934).

[2] Superexchange hereafter will be called exchange for brevity.

[3] J. H. Van Vleck, J. phys. radium **12**, 262 (1951).

[4] P. W. Anderson, Phys. Rev. **79**, 350 (1950).

[5] L. Néel, Ann. phys. **3**, 137 (1948).

[6] R. S. Weisz, Phys. Rev. **81**, 626 (1951); Ceram. Age **59**, 35 (1952).

[7] The Curie temperature, T_C, will denote the temperature below which order appears in the orientation of the moments of the magnetic ions. Usually T_C corresponds to the appearance of spontaneous magnetization as a consequence of order in ferro- or ferrimagnetic materials, whereas the Néel temperature, T_N, designates the appearance of order in antiferromagnetic materials which have zero spontaneous magnetization.

TABLE I. T_C/n for oxides in which only iron ions are magnetic, where n is the number of Fe^{3+}-O^{2-}-Fe^{3+} negative exchange interactions of appreciable strength per Fe^{3+} ion per formula unit (see Appendix for sources of data).

Compound	Name	T_C(°K)	n	T_C/n(°K)
(a) Fe_3O_4	magnetite	848	8	106
(b) γ-Fe_2O_3	maghemite or siderac	850–950	$7\frac{1}{2}$	113–127
(c) $Li_{1/2}Fe_{5/2}O_4$	lithium-iron spinel	950	$7\frac{1}{5}$	132
(d) $Y_3Fe_2(FeO_4)_3$	yttrium-iron garnet	545	$4\frac{4}{5}$	114
(e) $Lu_3Fe_2(FeO_4)_3$	lutetium-iron garnet	549	$4\frac{4}{5}$	114
(f) $LaFeO_3$	lanthanum-iron perovskite	738	6	123
(g) $YFeO_3$	yttrium-iron perovskite	648	6	108
(h) α-Fe_2O_3	hematite	950	9	106

unit (i.e., the average number of interactions per magnetic ion) is an important factor which depends on structure and which must be taken into account in estimates of the interaction energy, J, per M ion per linkage. For n interactions, J would be expected to be proportional to kT_C/n.[8–10]

At present sufficient data are available for non-isostructural oxides in which Fe^{3+} is the only magnetic ion present so that J may be determined on the basis of kT_C/n in several independent cases.

Fe^{3+}-O^{2-}-Fe^{3+} INTERACTION ENERGY IN DIFFERENT STRUCTURE SYSTEMS

Oxides will be considered which contain Fe^{3+} as magnetic ions and which have the cubic structures of the garnet and spinel types, the rhombohedral structure of the corundum type and the orthorhombic structure of the perovskite type.* In all cases the exchange interaction is negative. The exchange interaction may, as discussed by Anderson,[4] increase in strength as the Fe^{3+}-O^{2-} distances decrease and as the Fe^{3+}-O^{2-}-Fe^{3+} angle approaches 180°; the interaction is assumed to be negligible for angles near 90°.

The number, n, of the interactions which determine the Curie temperature of these oxides is, accordingly, determined by the number of Fe^{3+}-O^{2-}-Fe^{3+} linkages in which the Fe^{3+}-O^{2-} distances correspond to the contact distance (about 2 A) and in which the angle is substantially greater than 90° (in almost all cases >125°).

In the antiferromagnetic oxides considered, all Fe^{3+} ions are in equivalent positions; the magnetic moments of Fe^{3+} ions are so arranged that there are equal numbers of antiparallel moments. In the ferrimagnetic oxides considered, the Fe^{3+} ions occupy two sets of nonequivalent positions in unequal numbers and are in antiparallel orientation so that there is a net moment. Oxides in which the Fe^{3+} ions occupy more than two positions, such as those with magnetoplumbite structure in which the Fe^{3+} ions occupy five different crystallographic positions, are not considered. Consideration of δ-Fe_2O_3 has been omitted for lack of sufficient data on structure and magnetism.[11,12]

A tabulation (Table I) of data obtained on this basis shows that for the eight oxides considered the average value of T_C/n is 115° with extremes of 106° and 132°. In no case has any allowance been made for the variation of interionic distances or angles from one compound to another (Table II).

DISCUSSION

From the data presented (Tables I and II) it is evident that the Curie temperature may depend primarily upon the number of interactions in the case of oxides in which the Fe^{3+}-O^{2-}-Fe^{3+} linkage is responsible for the only exchange interactions present. Although no obvious correlation of the variation of T_C/n from the average value of 115° with the distances and included angles can be seen, the probability of negligible interaction at 90°, as suggested by Anderson,[4] is thoroughly substantiated. Each case, however, should be con-

TABLE II. Contact distances and included angle of the Fe_a^{3+}-O^{2-}-Fe_b^{3+} linkages (see Appendix for sources of data).

Compound	Fe_a^{3+} position	Fe_a^{3+}-O^{2-} distance (A)	Included angle (deg)	Fe_b^{3+}-O^{2-} distance (A)	Fe_b^{3+} position	Number of interactions per formula unit[a]
(a) Fe_3O_4	16(d) 16(d)	2.07 2.07	124.0 91.9	1.88 2.07	8(a) 16(d)	*24* 24
(b) γ-Fe_2O_3	16(d) 16(d)	probably about the same as corresponding values for (c)			8(a) 16(d)	*15* $12\frac{1}{2}$
(c) $Li_{1/2}Fe_{5/2}O_4$	12(d) 12(d)	2.03 2.03	123.0 93.2	1.90 2.03	8(c) 12(d)	*18* $13\frac{1}{2}$
(d) $Y_3Fe_2(FeO_4)_3$	16(a)	2.00	126.6	1.88	24(d)	*24*
(e) $Lu_3Fe_2(FeO_4)_3$	16(a)		similar to (d)		24(d)	*24*
(f) $LaFeO_3$	4(b) 4(b)	1.97 2.11	176.8(O_I) 149.9(O_{II})	1.97 1.96	4(b) 4(b)	*2* *4*
(g) $YFeO_3$	4(b) 4(b)	1.92 2.02	163.8(O_I) 153.2(O_{II})	1.92 1.94	4(b) 4(b)	*2* *4*
(h) α-Fe_2O_3	4(c) 4(c) 4(c) 4(c)	2.06 1.98 2.06 2.06	132.6 116.2 94.5 88.9	1.98 1.98 1.98 2.06	4(c) 4(c) 4(c) 4(c)	*12* *6* 12 6

[a] Numbers in italics are used for the calculation of n.

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[8] The approximate proportionality of J to $1/n$ is shown by the work of Heisenberg[9] who was first to demonstrate the quantum-mechanical exchange interaction. Van Vleck[10] discusses the theory of T_C and the exchange interaction in more detail.

[9] W. Heisenberg, Z. Physik **49**, 619 (1928).

[10] J. H. Van Vleck, *The Theory of Electric and Magnetic Susceptibilities* (Oxford University Press, New York, 1932), Chap. XII.

* *Note added in proof.*—An article by E. W. Gorter [Advances in Phys. **6**, 336 (1957)] in which the interaction geometry of many ferrimagnetic oxides is clearly presented and instructively discussed has appeared since this paper was submitted for publication. Oxides containing many different transition-metal ions are considered.

[11] O. Glemser and E. Gwinner, Z. anorg. u. allgem. Chem. **240**, 161 (1939).

[12] L. Néel, Ann. phys. **4**, 249 (1949).

sidered separately for qualifications on the evaluation of T_C/n.

For spinels and garnets, the angles and distances observed are very nearly the same in the case of exchange interactions important to the Curie temperature. The similarity of these ferrimagnetic materials extends to the coordination of oxygen with iron. In spinel there are one tetrahedrally, 8(a), and three octahedrally, 16(d), coordinated iron ions per formula unit; in garnet there are three tetrahedrally, 24(d), and two octahedrally, 16(a), coordinated iron ions per formula unit. However, there is a difference of some consequence between the interactions in these two structures. In iron spinels there are twelve weak exchange interactions for each octahedral ion with other octahedral ions at contact distance[13]; in iron garnets there are no exchange interactions at contact distance other than those contributing to ferrimagnetism.[14]

Interaction between magnetic ions in octahedral sites in the spinel structure, which is not included in n, is known to yield only very low antiferromagnetic Curie temperatures. Two examples[13,15,16] are $ZnFe_2O_4$ ($T_C=9.5$°K) and $CdFe_2O_4$ ($T_C \simeq 10$°K) in which iron is located only in octahedral sites ("normal" spinel structure). This interaction would be expected to reduce the Curie temperature and, consequently, the apparent exchange energy (kT_C/n) in comparison with that of yttrium-iron garnet. In connection with the influence of interionic distance on exchange energy, Friedberg and Burk[15] have noted that the increase of lattice constant from $ZnFe_2O_4$ ($a=8.42$ A) to $CdFe_2O_4$ ($a=8.69$ A) does not seem to lower the Curie temperature (variation of the oxygen parameter is not known).

Although it has not been taken into account, the presence of Fe^{2+} ions in the octahedral sites[17] of magnetite ("inverse" spinel structure) probably affects the Fe^{3+}-O^{2-}-Fe^{3+} exchange energy. Valence exchange among iron ions in the octahedral sites as a consequence of electron transfer brings about a random distribution of Fe^{2+} in these sites, i.e., each octahedral iron ion is divalent or trivalent for one-half of the time on the average.

The difficulties attendant to evaluation of the Fe^{3+}-O^{2-}-Fe^{3+} exchange energy in magnetite as a consequence of valence exchange are not present in the case of γ-Fe_2O_3 and $Li_{1/2}Fe_{5/2}O_4$; no divalent iron is present. The structure of γ-Fe_2O_3 may be regarded as that of Fe_3O_4 in which one-third mole of Fe^{2+} has been removed from the octahedral positions and the remaining two-thirds mole of Fe^{2+} oxidized to Fe^{3+} to yield $Fe^{3+}[Fe^{3+}{}_{5/3}]O_4$.[17] The structure of $Li_{1/2}Fe_{5/2}O_4$ may, for convenience, also be regarded as that of magnetite in which one-half mole of Fe^{2+} has been removed from octahedral positions and replaced by Li^+, and the remaining one-half mole of Fe^{2+} oxidized to Fe^{3+} to yield $Fe^{3+}[Li^{+}{}_{1/2}Fe^{3+}{}_{3/2}]O_4$.[18]

It would appear, then, that $Li_{1/2}Fe_{5/2}O_4$ represents the best case from which the Fe^{3+}-O^{2-}-Fe^{3+} exchange energy may be estimated for a spinel-like structure: There is no Fe^{2+} present, in contrast to Fe_3O_4, and the average number of interactions between octahedral iron ions has been reduced from twelve for Fe_3O_4 to nine per octahedral iron ion (from twenty-four to thirteen and one-half per formula unit). Accordingly, the value of T_C/n would be expected to be somewhat higher than for magnetite; the reason for its being the highest observed, 132°, is not clear.

Although γ-Fe_2O_3 also contains no Fe^{2+}, it would be less satisfactory than $Li_{1/2}Fe_{5/2}O_4$ for estimation of the Fe^{3+}-O^{2-}-Fe^{3+} exchange energy in a spinel-like structure because the number of octahedral-octahedral iron-ion interactions is larger (sixteen and two-thirds per $Fe_{8/3}O_4$ formula unit *vs* thirteen and one-half for $Li_{1/2}Fe_{5/2}O_4$).

Among the compounds under discussion, the antiferromagnetic oxides (Table I) bear little resemblance in structure to each other or to the ferrimagnetic oxides. The perovskite-like structure is the simplest one of all. Each Fe^{3+} ion is octahedrally coordinated with O^{2-}; it interacts with another Fe^{3+} ion through each of the six O^{2-} ions in three nearly mutually perpendicular directions. There are no linkages with included angles near 90°. In $LaFeO_3$ six Fe^{3+} ions have moments antiparallel to a central Fe^{3+} ion according to the neutron diffraction data of Koehler and Wollan[19]; presumably a similar arrangement of moments applies to isostructural $YFeO_3$. Although the Fe^{3+}-O^{2-}-Fe^{3+} angles in these two perovskite-like compounds (Table II) approach 180° more closely than in any of the other compounds listed and the distances are not much different from each other, the values of T_C/n differ more with each other than with the average value of T_C/n.

In contrast to the simple interactions of perovskite-like compounds, the corundum structure of α-Fe_2O_3 presents the most complicated interaction picture to be considered. Because other previous treatments of this problem have been inadequate for the present discussion, the treatment of this case will be given in somewhat more detail.[20,21]

The magnetic structure has been established by Shull, Strauser, and Wollan[22] by means of neutron diffraction. Although the data were given in rhombohedral coordinates (Wyckoff notation), it is advisable

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[13] E. W. Gorter, Philips Research Repts. **9**, 295 (1954).

[14] S. Geller and M. A. Gilleo, J. Phys. Chem. Solids **3**, 30 (1957).

[15] S. A. Friedberg and D. L. Burk, Phys. Rev. **98**, 1200 (1956); *Conference on Magnetism and Magnetic Materials* (American Institute of Electrical Engineers, T-78, October, 1955), p. 62.

[16] J. M. Hastings and L. M. Corliss, Phys. Rev. **102**, 1460 (1956).

[17] E. J. W. Verwey and P. W. Haayman, Physica **8**, 979 (1941).

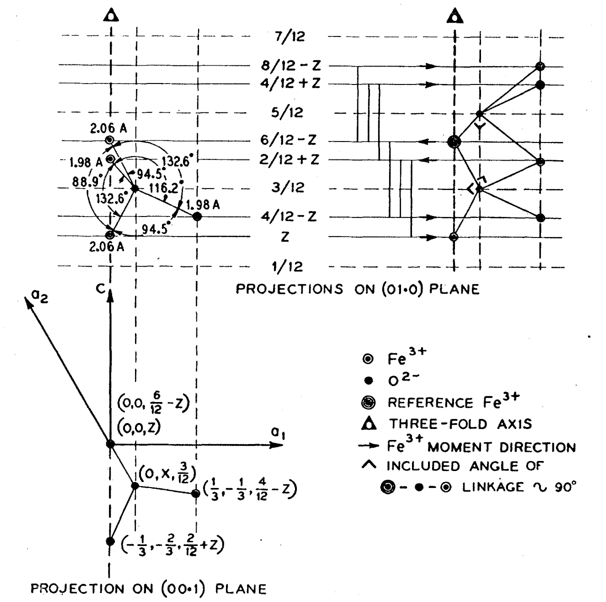
[18] P. B. Braun, Nature **170**, 1123 (1952).

[19] W. C. Koehler and E. O. Wollan, J. Phys. Chem. Solids **2**, 100 (1957).

[20] Y.-Y. Li, Phys. Rev. **102**, 1015 (1956).

[21] S. Iida, J. Phys. Soc. Japan **11**, 1300 (1956); **12**, 222 (1957).

[22] Shull, Strauser, and Wollan, Phys. Rev. **83**, 333 (1951).



(a) (b)

FIG. 1. Fe^{3+}-O^{2-}-Fe^{3+} linkages in α-Fe_2O_3. (a) Fe^{3+}-O^{2-}-Fe^{3+} angles and distances around O^{2-}. (b) All interactions of a reference Fe^{3+} ion with other Fe^{3+} ions (vertical bars between Fe^{3+} layers indicate exchange coupling).

to transform to hexagonal coordinates in which the layer nature of the structure is more clearly evident (Fig. 1).[23]

The number of interactions which must be considered is determined as follows: There are four Fe^{3+} in coordination with each O^{2-} so that six Fe^{3+}-O^{2-}-Fe^{3+} configurations are present; of these six configurations there are only four distinct ones—two pairs and two singles. One pair and one single have angles near 90°; the remaining pair and single have substantially greater angles so that they may be considered to be exchange interactions (Table II). Therefore, each Fe^{3+} ion appears in a total of eighteen Fe^{3+}-O^{2-}-Fe^{3+} configurations of which nine are important as exchange interactions.

With this knowledge the interactions may be presented on a layer diagram (Fig. 1) in which one-third are shown because the Fe^{3+} ions all lie on threefold axes. The magnetic structure is consistent with the negative exchange interaction always expected for the Fe^{3+}-O^{2-}-Fe^{3+} linkage.

A good first approximation of the exchange energy of the Fe^{3+}-O^{2-}-Fe^{3+} linkage has been achieved on the simple basis of T_C/n. The exact relationship between exchange energy and T_C would require more detailed knowledge and treatment of the problem. In particular an understanding of the influence on the exchange energy of the distances and angles in the Fe^{3+}-O^{2-}-Fe^{3+} exchange linkage would require that good structure data be obtained at T_C, the temperature of evaluation. Of the compounds considered, the data for $Y_3Fe_2(FeO_4)_3$ and $Li_{1/2}Fe_{5/2}O_4$ are the best. It would be desirable that all data for each compound be established for the same lot of material.

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APPENDIX

The data employed in the compilation of Tables I and II, and their origins, are given below for each compound. In every case room-temperature structure data are given. The notation is in accordance with *Internationale Tabellen*.[24] Lattice constants are given in the units of the references cited and have been used without revision.

(a) Fe_3O_4

Crystal structure[25]: $O_h(7)-Fd3m$, $Z=8$, $a=8.400$ A. Fe^{3+} in 8(a); $(\frac{1}{2}Fe^{3+}+\frac{1}{2}Fe^{2+})$ in 16(d); O^{2-} in 32(e), $x=0.379\pm0.001$.

Magnetic data: $Fe^{3+}[8(a)]$ antiparallel with $(\frac{1}{2}Fe^{3+}+\frac{1}{2}Fe^{2+})$ $[16(d)]$[26]; $T_C=848°K$.[27]

(b) γ-Fe_2O_3

Crystal structure: $O_h(7)-Fd3m$, $Z=32/3$, $a=8.338$ kx-units.[28] Fe^{3+} in 8(a); $\frac{5}{6}Fe^{3+}$ in 16(d); O^{2-} in 32(e), $x=0.382$.

Neither the structure nor composition of γ-Fe_2O_3 seems to be definitely known.[18,28,29] The above approximation is based upon the work of Braun[18] which gave evidence that the compound could be $Fe_2O_3\cdot xH_2O$ which could become isostructural with $Li_{1/2}Fe_{5/2}O_4$ for $x=\frac{1}{5}$. The structure given is also suggested by magnetization data.[30,31] The observed moment, 2.5 μ_B per formula unit, may be explained if the 8(a) positions are

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[23] In α-Fe_2O_3 the O^{2-} ions lie in (00·1) planes (or layers) separated by 2/12; the Fe^{3+} ions lie in two planes spaced $\pm(2/12-z)$ from a plane midway between the oxygen planes.

[24] *Internationale Tabellen zur Bestimmung von Kristallstrukturen* (Gebrüder Borntraeger, Berlin, 1935).

[25] A. A. Claassen, Proc. Phys. Soc. (London) **38**, 482 (1925–6).

[26] Shull, Wollan, and Strauser, Phys. Rev. **81**, 483 (1951).

[27] D. O. Smith, Phys. Rev. **101**, 959 (1956); see also W. Kopp, thesis, Zurich, 1919, as given in reference 5.

[28] I. David and A. J. E. Welch, Trans. Faraday Soc. **52**, 1642 (1956).

[29] I. Behar and R. Collongues, Compt. rend. **244**, 617 (1957).

[30] P. Weiss and R. Forrer, Ann. phys. **12**, 279 (1929); W. E. Henry and M. J. Boehm, Phys. Rev. **101**, 1253 (1956).

[31] Maxwell, Smart, and Brunauer, Phys. Rev. **76**, 459 (1949).

filled and the remainder of the Fe^{3+} ions are in 16(d). The Curie temperature has not been directly observed because the material becomes unstable at a lower temperature. However, data for $x\mathrm{FeO}\cdot\mathrm{Fe_2O_3}$, extrapolated to $x=0$, imply that T_C for γ-Fe_2O_3 may be about the same as for Fe_3O_4.[31] Data for sodium stabilized γ-Fe_2O_3 indicate a Curie temperature nearer that of α-Fe_2O_3.[32]

David and Welch[28] have also observed the importance of H_2O in γ-Fe_2O_3. Behar and Collongues[29] have found evidence for an order-disorder transition in γ-Fe_2O_3 which, it is felt, could be related to that observed by Braun[18] in $Li_{1/2}Fe_{5/2}O_4$.

(c) $\mathbf{Li_{\frac{1}{2}}Fe_{\frac{5}{2}}O_4}$

Crystal structure[18]: $O(6)-P4_33$, $Z=8$, $a=8.33$ A. Li^+ in 4(b); Fe^{3+} in 8(c), $x=0+\Delta_2$; O^{2-} in 8(c), $x=\frac{3}{8}+\Delta_6$; Fe^{3+} in 12(d), $x=\frac{3}{8}+\Delta_1$; O^{2-} in 24(e), $x=\frac{1}{8}+\Delta_3$, $y=-\frac{1}{8}-\Delta_4$, $z=\frac{1}{8}+\Delta_5$. The parameters Δ_3, Δ_4, Δ_5, and $\Delta_6\simeq0.007$; Δ_1 and Δ_2 are much smaller. For $\Delta_1=\Delta_2=0$ and for $\Delta_3=\Delta_4=\Delta_5=\Delta_6$ the space group becomes $O_h(7)-Fd3m$ for random distribution of Li^+ and Fe^{3+} in 16(d) which is observed above an order-disorder transition at 755°C.[18]

Magnetic data[13]: Fe^{3+} [8(c)] antiparallel with Fe^{3+} [12(d)] as deduced from a magnetic moment of 2.5 μ_B per formula unit; $T_C=950$°K.

(d) $\mathbf{Y_3Fe_2(FeO_4)_3}$

Crystal structure[14]: $O_h(10)-Ia3d$, $Z=8$, $a=12.376$ A. Fe^{3+} in 16(a); Y^{3+} in 24(c); Fe^{3+} in 24(d); O^{2-} in 96(h), $x=-0.027_4$, $y=0.057_2$, $z=0.149_2$. See also Bertaut and Forrat[33] and Prince.[34]

Magnetic data: Fe^{3+} [16(a)] antiparallel with Fe^{3+} [24(d)] from a magnetization of 5 μ_B per formula unit[35,36] and from neutron diffraction data[34,37]; $T_C=545$°K.[35,36]

(e) $\mathbf{Lu_3Fe_2(FeO_4)_3}$

Crystal structure[38]: $O_h(10)-Ia3d$, $Z=8$, $a=12.277$ A. Ion positions are the same as in (**d**) except that the 96(h) parameters have not been determined; presumably they are near those of (**d**).

Magnetic data[39]: presumably the same as for (**d**) except $T_C=549$°K.

(f) $\mathbf{LaFeO_3}$

Crystal structure[40]: $D_{2h}(16)-Pbnm$, $Z=4$, $a=5.556$, $b=5.565$, $c=7.862$ A. Fe^{3+} in 4(b); La^{3+} in 4(c), $x=-0.01$, $y=0.023$; $O_I{}^{2-}$ in 4(c), $x=0.01$, $y=0.50$; $O_{II}{}^{2-}$ in 8(d), $x=-0.29$, $y=0.27$, $z=0.06$. The parameters employed are those determined for the compound $La(Co_{0.2}Mn_{0.8})O_3$[41] as was suggested as a good approximation by Geller[42] and confirmed by Koehler and Wollan.[19]

Magnetic data: each Fe^{3+} is surrounded by 6 antiparallel Fe^{3+} nearest neighbors according to neutron diffraction data[19]; $T_C=738$°K.[19,43]

(g) $\mathbf{YFeO_3}$

Crystal structure[40]: $D_{2h}(16)-Pbnm$, $Z=4$, $a=5.302$, $b=5.589$, $c=7.622$ A. Fe^{3+} in 4(b); Y^{3+} in 4(c), $x=-0.018$, $y=0.060$; $O_I{}^{2-}$ in 4(c), $x=0.05$, $y=0.47$; $O_{II}{}^{2-}$ in 8(d), $x=-0.29$, $y=0.27_5$, $z=0.05$.

The parameters employed are those determined for $GdFeO_3$ by Geller[44] because of the close similarity of the lattice constants of these two isostructural compounds.

Magnetic data: the arrangement of Fe^{3+} moments is presumed to be identical with (**f**); $T_C=643$°K.[45]

(h) $\boldsymbol{\alpha}$-$\mathbf{Fe_2O_3}$

Crystal structure[46]: $D_{3d}(6)-R\bar{3}c$, $Z=6$, $a=5.03$, $c=13.73$ A. Fe^{3+} in 12(c), $z=0.145$; O^{2-} in 18(e), $x=-0.292$.[47]

Magnetic data: the magnetic structure has been deduced from susceptibility[12,48] and neutron diffraction[22] data. All Fe^{3+} ions, and moments thereof, are in (00·1) planes; all moments are parallel in the Fe^{3+} planes between O^{2-} planes; the moment direction reverses across O^{2-} planes; $T_C=950$°K.[12,48,49]

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