where μ_8^* and μ_{31}^* are the atomic moments in the low-temperature $B8_1$ and the intermediate temperature B31 phases respectively. Interpretation of the first-order phase change appears to require[13] a $\beta \sim 10$.

A $d\mu/dV > 0$ requires a high-spin $\rightleftarrows$ low-spin transition in the critical molar volume interval, and hence

$$\langle d(\epsilon_{ex} - \epsilon_{cf})/dV \rangle \, \Delta V > 0.1 \text{ eV}$$

within this interval ΔV. Here ϵ_{ex} and ϵ_{cf} are intra-atomic exchange and crystal-field splittings, respectively, and 0.1 eV is taken as the lower limit of the d-band width for orbitals of e_g symmetry. Since

$$\Delta(-\epsilon_{cf}) \approx \frac{1}{3} \, \epsilon_{cf} \, \Delta V/V \approx 0.01 \text{ eV} \quad ,$$

it follows that the sharp transition requires

$$\Delta\epsilon_{ex} = \langle d\epsilon_{ex}/dV \rangle \, \Delta V \geqslant 0.1 \text{ eV} \quad .$$

Stoner[14] has pointed out that there is a maximum bandwidth, and hence a maximum overlap integral Δ_c^f for orbitals on neighboring cations, that will support spontaneous band ferromagnetism. Further, the bandwidth for bonding orbitals is greater than that for antibonding orbitals, so that $\Delta_{ab} < \Delta_b$, where the subscripts refer to antibonding and bonding orbitals, respectively. Thus the two conditions for spontaneous band ferromagnetism are

$$\Delta_b < \Delta_c^f \quad \text{and} \quad \Delta_{ab} < \Delta_c^f < \Delta_b \quad ,$$

where high-spin manganese requires the first and low-spin manganese implies the second. It is concluded that the unusual occurrence of a $d\mu/dV > 0$ over a small volume interval ΔV manifests the transition

$$\Delta_b < \Delta_c^f \rightarrow \Delta_{ab} < \Delta_c^f < \Delta_b$$

and demonstrates that Δ_c^f is quite sharply defined.

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