

$$\alpha_{C1} = 608 (110), \quad \beta_{C1} = 2074 (760) \quad \text{and}$$

$$\alpha_v = 343 (74), \quad \beta_v = 200 (74),$$

when δ_2 is in units of 10^{-4} cm^{-1} . The standard deviation of the fit is $48.0 \times 10^{-4} \text{ cm}^{-1}$, rather worse than suggested by the results of I, but the variation of δ_2^0 and δ_2^{C1} over the range of interest are not greatly different to those proposed in I.

A major difference between I and III is that the simple superposition model,⁴ as used in III was extended in I to include contributions from the lattice vacancy. To check whether consistent results can be obtained within the framework of a common model, we have examined the application of the simple superposition model to the alkali chloride situation. We have used a simple linear dependence for $\delta_2^{C1}(R)$ and the distortions calculated in I. This analysis shows that the sign of the gradient of $\delta_2(R)$ required to fit the C_{2v} site data is opposite to that required for C_{4v} site and so a consistent interpretation is not possible. This is presumably the reason why the simple model was not considered in I.

We next consider the physical significance of the successful analysis of the alkali chloride data which can be achieved using the extended superposition model and the lattice distortions calculations in I. The vacancy contribution actually corresponds to that of the associated incomplete shell of cations, and for an undistorted cation sublattice we have $\delta_2(\text{vacancy}) = -\delta_2(\text{cations})$. Since the relevant cations are second or fourth nearest-neighbor ions of the Mn^{2+} ions, we expect the interaction, if significant, to be primarily electrostatic in character, and to scale with cation distance as R^{-3} , in contrast to the $R^{-1.6}$ variation found in I. The latter variation implies an interaction which is still increasing at the fourth nearest-neighbor position.

We conclude that the extended superposition model analysis of the alkali chlorides leads to physically implausible results, while no satisfactory fit can be obtained with the simple model using the distortions calculated in I. This suggests that the simple distortion model used there may be inadequate for a superposition model analysis of the alkali chloride situation, where the *differences* in relaxed bond lengths among the six ligands, rather than just an average change, play a crucial role. Only two distortional degrees of freedom are permitted in I for the C_{2v} site, whereas seven are allowed by the observed site symmetry. In particular, their model assumes that the Mn^{2+} ion remains at the exact lattice site, which is a severe constraint, since all of the bond angles and lengths are sensitive to the Mn^{2+} ion displacement.

From these considerations we conclude that a more extensive calculation of the lattice distortions must be performed before the applicability of the superposition model to the Mn^{2+} doped alkali chlorides can be assessed.

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ERRATA

Erratum: Direct determination of rotational correlation time by electron-spin echoes [*J. Chem. Phys.* **73**, 3507 (1980)]

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The summary that was given of our theoretical computations relating to the phase memory times T_M for a slowly tumbling nitroxide was inaccurate. Those results for the slowest decaying mode can be fit to the form: $\text{Re } E = a\tau_R^{-b}$ with a , b model dependent. Thus, for Brownian motion, $a \approx 2-13 \times 10^3 \text{ s}^{-1/2}$, $b \approx \frac{1}{2}$, while for approximate free diffusion, $a \approx 3-12 \times 10^2 \text{ s}^{-1/3}$, $b \approx \frac{2}{3}$. In both cases, the small and large values for a relate to the central and high field extremum spectral regions, respectively, with an intermediate value for the low extremum. For moderate jump, $a \approx 1$ for both extrema and $a \approx 2$ in the central region, while $b \approx 1$. Thus, our spin-echo results follow the *moderate jump* predictions most closely (when we identify $T_M^{-1} \approx \text{Re } E$) consistent with the CW study (cf. Ref. 4).