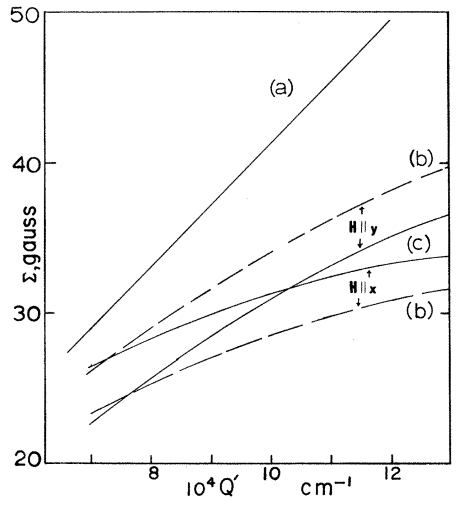

FIG. 1. Computed values of $\Sigma \equiv |a_i^2 - b_i^2| + |c_i^2 - d_i^2|$ for $i = x$ or y (i.e., the sum of the separations in the high-field and low-field pairs of $\Delta M_I = \pm 2$ lines; notation as in Ref. 4). (a) Calculated by the perturbation expressions (5.1c) of Ref. 4, $\Sigma = 4Q'h\nu/g_i\beta_i$; (b) computer diagonalization of $\mathcal{H}_{\text{spin}} = \beta \vec{H} \cdot \overleftrightarrow{g} \cdot \vec{S} + \vec{I} \cdot \overleftrightarrow{A} \cdot \vec{S} + \vec{I} \cdot \overleftrightarrow{P} \cdot \vec{I} - g_N \beta_N \vec{I} \cdot \vec{H}$, with $g_z = 2.346$, $g_x = 2.109$, $g_y = 2.094$, $A_z = -0.00875$, $A_x = 0.00187$, $A_y = 0.00272$ cm^{-1}, $Q' = 1.5P_z$, $\mathrm{Tr}\,\overleftrightarrow{P} = 0$, $P_x = P_y$; (c) same as (b) except $\eta \equiv (P_y - P_x)/P_z = 0.87 \times 10^{-4}$ cm$^{-1}/Q'$. The experimental values of Σ for TiO_2:Cu^{++} were in the vicinity of 30 G. See Ref. 4.

expressions are inadequate for certain transitions and that this inadequacy has severe consequences in the determination of quadrupole coupling parameters from EPR spectra.

An interesting case in point is provided by TiO_2:Cu^{++}, recently reported by Ensign, Chang, and Kahn.[4] They measured EPR spectra of ^{63}Cu and ^{65}Cu (natural-abundance mixture) doped into rutile and used the $\Delta M_I = \pm 2$ lines for $\vec{H}$ along the x and y axes, together with the perturbation expressions of Bleaney *et al*,[5] to extract a quadrupole tensor for ^{63}Cu: $Q' = 7.42 \pm 0.24 \times 10^{-4}$ cm^{-1}, $\eta = 0.03 \pm 0.03$. They also found that the results obtained from the $\Delta M_I = 0$ lines were not consistent with those from the $\Delta M_I = \pm 2$ lines. Applying their Eq. (5.1a) for the $\Delta M_I = 0$ lines in their x and y spectra, we obtain $Q' \approx 10.2 \times 10^{-4}$ cm^{-1} and $\eta \approx 0.15$.

We have examined the perturbation equations (5.1a) and (5.1c) of Ensign *et al*,[4] in comparison with exact 8×8 matrix-diagonalization expressions for the same quantities. Figure 1 shows a sample plot. Clearly, the perturbation expressions are apt to yield a quadrupole coupling tensor grossly in error.

Upon fitting the TiO_2:Cu^{++} spectra published by Ensign *et al.*[4] by a complete diagonalization of the spin Hamiltonian, we obtained values of $Q' = 9.7 \times 10^{-4}$ cm^{-1} and $\eta = 0.09$ from the $\Delta M_I = \pm 2$ lines. These values are close to those obtained from the $\Delta M_I = 0$ lines. Considering all the data and errors, we recommend $Q' = +10 \times 10^{-4}$ cm^{-1} and $\eta = 0.1$. These values, moreover, are in the range of expected values[1,4] for cupric ion in a slightly distorted octahedral site.

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ERRATA

Theory of the Nuclear Magnetic Resonance Chemical Shift of Xe in Xenon Gas, Frank J. Adrian [Phys. Rev. 136, A980 (1964)]. In the discussion following Eq. (33) there is a misprint in the statement "$(S_{\sigma\sigma} + S_{\pi\pi})^2 = 0.061$ at $R = 4$ Å." This should have read "$(S_{\sigma\sigma} + S_{\pi\pi})^2 = 0.0061$ at $R = 4$ Å." This misprint does not affect any other result or conclusion, and the value of $(S_{\sigma\sigma} + S_{\pi\pi})^2$ as a function of R is correctly given at the top of p. A987. The author is indebted to Dr. A. K. Jameson and Dr. C. J. Jameson for calling this misprint to his attention.

Spin Correlation and Entropy, H. Falk and Masuo Suzuki [Phys. Rev. B 1, 3051 (1970)]. Several typographical errors (which do not propagate to