$$P'_{7,2}(2,1) = \frac{\binom{4}{2}\binom{1}{1}}{\binom{5}{3}}$$

Thus, the total abundance P''_7 of this particular species is given by the following simple product (*2*, *1*).

$$P''_7 = P_7 \times P'_{7,2}$$

Appendix 2

Construction of the Stick Diagram

The construction of the stick diagrams was carried out on the basis of four assumptions, as follows.

- The total number of lines in the stick diagram, which equals the number of allowed transitions

$$|-\tfrac{1}{2}, m_I^{Cr}, m_I^{N}, m_I^{C}\rangle \rightarrow |+\tfrac{1}{2}, m_I^{Cr}, m_I^{N}, m_I^{C}\rangle$$

for

$$-\frac{3}{2} \le m_I^{Cr} \le \frac{3}{2}$$

$$-1 \le m_I^{N} \le 1$$

and

$$-\frac{1}{2} \le m_I^{C} \le \frac{1}{2}$$

was calculated from eq 3. Their positions are given by eq 4, and the intensities $\Im_j$'s are calculated by combining eq 5 with eqs 6 and 7.

$$\Im_j = \frac{P''_j}{\prod_i (2I^{(i)} + 1)} \qquad (8)$$

- The contribution of the significantly less abundant multi-labeled species **4**–**12** was neglected.
- The values of the hyperfine splittings of particular nuclei used for the construction of the stick diagrams were taken as those listed above under the subheading "The Simulated Spectra".
- For practical reasons, the intensity of the weakest line(s) on the stick diagram was taken as unity.

The stick diagram of $K_3[Cr(CN)_5NO]$ EPR spectrum (Fig. 1b) is built up by successive addition of partial subdiagrams arising from the interaction of the unpaired electron with ^{53}Cr (I = 3/2), ^{14}N (I = 1), and ^{13}C (I = 1/2) nuclei of the three most abundant isotopomers. In Table 2 are specified the allowed transitions, line positions, and intensities for the species that effectively contribute to the experimental spectrum.

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