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Ishikawa, K., Kumauchi, T., Baba, M., & Katô, H. (1992). Hyperfine structure of the NaK c³Σ⁺ state and the effects of perturbation. *The Journal of Chemical Physics*, 96(9), 6423–6432. doi:10.1063/1.462856

we have

$$\begin{aligned} \langle 0 | \langle 10 | \langle v | \sum_i s_{i-1}(i) \delta(r_{i1}) | 0 \rangle | 11 \rangle | v \rangle \\ = (2)^{-1} [\langle \sigma s(i) | \delta(r_{i1}) | \sigma s(i) \rangle \\ + \langle \sigma p_0(i) | \delta(r_{i1}) | \sigma p_0(i) \rangle]. \end{aligned} \quad (22)$$

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Ishikawa *et al.*: Hyperfine structure of NaK c³Σ⁺

$|\sigma p_0\rangle = c|3p_z^{Na}\rangle + d|4p_z^K\rangle$, where $|\chi^n\rangle$ represents χ^n atomic orbitals of nucleus n , and a, b, c , and d are the coefficients, we have

$$\begin{aligned} K_1 = (8\pi/3)\zeta(1) [a^2 \langle 3s^{Na} | \delta(r_1) | 3s^{Na} \rangle \\ + 2ab \langle 3s^{Na} | \delta(r_1) | 4s^K \rangle + b^2 \langle 4s^K | \delta(r_1) | 4s^K \rangle \\ + c^2 \langle 3p_z^{Na} | \delta(r_1) | 3p_z^{Na} \rangle + 2cd \langle 3p_z^{Na} | \delta(r_1) | 4p_z^K \rangle \\ + d^2 \langle 4p_z^K | \delta(r_1) | 4p_z^K \rangle] / 2. \end{aligned} \quad (25)$$

The hyperfine constant of the c³Σ⁺ state induced by the Fermi contact interaction between the ²³Na nuclear moment and the electron spin is then expressed by neglecting small terms as

$$K_{Na}(c^3\Sigma^+) = (8\pi/3)\zeta(Na)a^2 \langle 3s^{Na} | \delta(r_{Na}) | 3s^{Na} \rangle / 2. \quad (26)$$

The hyperfine structure of the Na(3s²S_{1/2}) atom arises from the Fermi contact interaction and the value of $K_{Na}(3s^2S_{1/2}) = (8\pi/3)\zeta(Na)\langle 3s^{Na} | \delta(r_{Na}) | 3s^{Na} \rangle$ is reported to be $2.95 \times 10^{-2} \text{ cm}^{-1}$.¹⁸ From the observed hyperfine splitting, we determined the value of $K_{Na}(c^3\Sigma^+)$ to be

FIG. 10. Simulated hyperfine spectra of the c³Σ⁺ (v=0, J) transition [^RQ(J)] and the F₁–X¹Σ⁺ (v=0, J) transition [^RQ(J)]. The energy separation are calculated from the eigenvalues obtained by diagonalizing the matrix of H_0 for all perturbing states, whose molecular constants are assumed to be the same as those of the c³Σ⁺ state. The linewidth (fullwidth at half-maximum) is assumed to be 20 MHz.

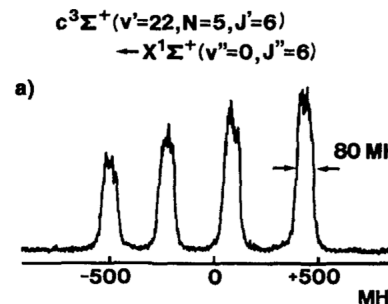


FIG. 11. (a) Observed hyperfine spectrum of the F₁–X¹Σ⁺ (v''=0, J''=6) transition [^RQ(6)] of the c³Σ⁺ (v'=22, N=25, F₂)–X¹Σ⁺ (v''=0, J''=6) transition [^RR(24)], which shows that our spectral resolution is

electric quadrupole interaction of the c³Σ⁺ state is much smaller than the magnetic dipole interaction of the c³Σ⁺ state.