C-Band Gas-Phase EPR Spectra of the Rotational Excited $J=3$ Level of SO in the $^1\Delta$ State

Hiromichi Uehara and Yonezo Morino

Sagami Chemical Research Center, Sagamihara-shi, Kanagawa

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We report the gas-phase C-band electron paramagnetic resonance spectra of the rotational excited $J=3$ level of the electronically excited state $^1\Delta$ of SO. The EPR spectrum of SO in the $^1\Delta$ state was first observed by Carrington *et al.*[1] for the rotational ground state ($J=2$) by using X-band microwave frequencies (*ca.* 9 GHz). By lowering the microwave frequency from X- to C-band region we have succeeded in observing the spectrum in the next higher rotational level.

A Stark modulated cylindrical TE_{011} mode detection cavity resonated at about 4.46 GHz was used with the axis of the cylinder parallel to the dc magnetic field. The C-band spectrometer used was reported elsewhere.[2] Micowave discharged oxygen gas was introduced into the resonance cavity through a gas-inlet at a pressure of 0.3 Torr and carbonyl sulfide was introduced through another inlet at a pressure of 0.1 Torr and mixed the dischagre product immediately outside the detection cavity. A strong spectrum of SO ($^1\Delta$, $J=2$) was observed in a field of 4.7 kG at a signal-to-noise ratio of about 100. Five lines of the rotational excited $J=3$ state were observed in a field of 9.1 to 10 kG, as shown in Fig. 1. Although the spectrum of the $J=3$ level consists of a sextet according to the selection rule of $\Delta M=1$, the transition to be expected at the highest field was not observed because of the restriction of the magnetic field available to us (maximum field of 10000 G).

A preliminary calculation was made with the method presented by Carrington *et al.*[1] By using the matrix elements of $(J, \Lambda, M|\mathscr{H}|J, \Lambda M)$ and $(J, \Lambda, M|\mathscr{H}|J+1, \Lambda, M)$ of the Hamiltonian

$$\mathscr{H} = B_0(\boldsymbol{J}-\boldsymbol{L})^2 + g_l\beta\boldsymbol{L}\cdot\boldsymbol{H}, \qquad (1)$$

we set up a 4×4 matrix and diagonalized it. The molecular constants used were $B_0=0.709$ cm^{-1} [1] and $g_l=1.00000$. The main feature of the observed five transitions were well reproduced, although a fairly large discrepancy between the calculated and the observed was noted in the absolute (about 5 gauss) and relative (a few gauss) field positions of the resonance transitions. It is expected that the electronic g factor, l-uncoupling constants, and the rotational constant may be determined accurately by analyzing the spectra of the rotational excited state $J=3$, combined with those of the ground $J=2$ state.

Carrington *et al.*[1] presented the following three features for the identification of the lines for $^1\Delta$ SO: first, the spectrum consists of four lines of similar intensity, secondly, the center of the quartet pattern indicates a molecular g value very close to the expected value 2/3, and thirdly, analysis of the splitting between the lines leads to a value of the rotational constant B_0 which is very close to that known for the $^3\sum^-$ ground state. Similarly, the present observation of the spectral lines in the $J=3$ level close to the predicted positions with the relative intensities close to the expected ratios, 3 : 5 : 6 : 6 : 5, confirms the assignment of the spectra to the $^1\Delta$ of SO.

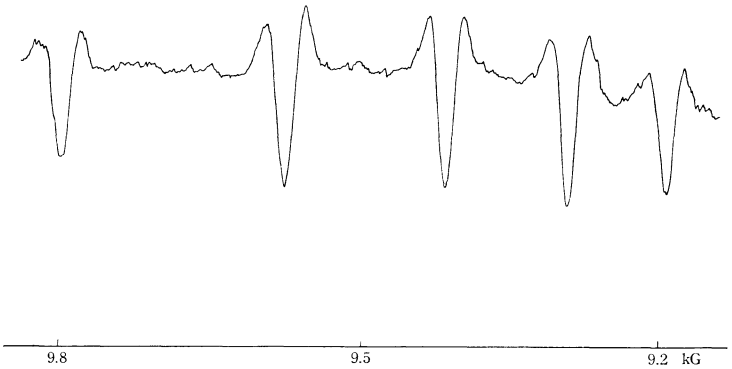

Fig. 1. Gas-phase EPR spectrum of rotationally excited $^1\Delta$ SO ($J=3$) observed with a microwave frequency of 4.46 GHz.

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[1] A. Carrington, D. H. Levy and T. A. Miller, *Proc. Roy. Soc.*, **A293**, 108 (1966).

[2] H. Uehara and Y. Morino, *J. Mol. Spectrosc.*, to be published.