RE-ANALYSIS OF THE SPIN-ORBIT PERTURBATION FOR THE PHILLIPS SYSTEM AND THE BALLIK-RAMSAY SYSTEM OF THE SPECTRA OF C_2

WANG CHEN, JIAN TANG and KENTAROU KAWAGUCHI, *Graduate School of Natural Science and Technology Okayama University, 3-1-1 Tsushima-Naka, Okayama 700-8530, Japan.*

The Phillips system and the Ballik-Ramsay system of the spectra of C_2 have been studied extensively before, and the energy difference between the ground $X^1\Sigma_g^+$ state and the first triplet $a^3\Pi_u$ state has been determined by analyzing the spin-orbit interaction between the $X^1\Sigma_g^+$ and $b^3\Sigma_g^-$ states. However, the analysis was carried out previously for the individual vibronic bands, and the perturbation parameters $< v|H_{SO}|v' >$ of the spin-orbit interaction determined for the different vibronic states lead to the very different values of A_{so}^{bX}.[a,b] In the present study, we re-analyzed the previous spectral data[a,c,d] by using the overlap integrals (Franck-Condon factors) and r-centroids between the vibronic states of $X^1\Sigma_g^+$ and $b^3\Sigma_g^-$ calculated from the RKR potential and by fitting all the vibronic states simultaneously. A new set of molecular parameters was obtained, including the single-valued spin-orbit interaction constant $A_{so}^{bX} = 3.067(9)$ cm^{-1} and the energy difference $\Delta E = 719.84(6)$ cm^{-1} between the $X^1\Sigma_g^+$ and $a^3\Pi_u$ states, the latter of which is about 1.5 cm^{-1} larger than the previously determined value.[a] This new result may guide for searching the forbidden transitions between the singlet and triplet states of C_2.

[a]C. Amiot, J. Chauville and J. -P. Maillard, J. Mol. Spectrosc. 75, 19 (1979).

[b]S. P. Davis et al., J. Opt. Sol. Am. B. 5, 1838 (1988).

[c]M. Douay, R. Nietmann and P. -F. Bernath, J. Mol. Spectrosc. 131, 250 (1988).

[d]M-C. Chan et al., Chem. Phys. Lett. 390, 340 (2004).