NEW ABSORPTION SPECTRA OF CH2 NEAR 780 NM

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The near infrared and visible spectrum $(\tilde{b}^1 B_1 - \tilde{a}^1 A_1)$ of singlet CH₂ has been the subject of much study. However, the region between the red end of the visible part of the spectrum and about 800 nm has not been recorded since the pioneering work of Herzberg and Johns.^{*a*} We have remeasured the absorption spectrum between approximately 769 and 806 nm at near shot-noise-limited sensitivity and Dopplerlimited resolution using a frequency-modulated extended cavity diode laser source. Rotational branches in 7 vibronic bands involving $K_a = 0 - 4$ have been assigned using known ground state combination differences. Most of them have not previously been observed and some reassignments of the Herzberg and Johns analysis have been made. Comparison with the most complete available calculated ro-vibronic energy level structure^{*b*} helped considerably in making the assignments, and the observed vibronic levels are assigned to levels of both \tilde{a} and \tilde{b} electronic character. The calculated energy levels show moderate, up to 10 cm⁻¹, apparently random, differences from the observed levels The new data will certainly help to refine the singlet potential and also provide additional avenues for future kinetics and dynamics studies of the radical.

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^aG. Herzberg and J. W. C. Johns Proc. R. Soc. London Ser. A, 295, 107 (1966)

^bJ. -P. Gu, G. Hirsch, R J Buenker, M. Brumm, G. Osmann, P. R. Bunker and P. Jensen J. Molec. Struc., 517-8, 247 (2000)