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The Infra-Red Spectrum of C14O2

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THE INFRA-RED SPECTRUM OF $C^{14}O_2$

R. K. Shelton and J. W. Weigh

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Berkeley, California

THE INFRA-RED SPECTRUM OF $C^{14}O_2$

by

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Recently radio-carbon dioxide containing about 30% $C^{14}O_2$ has become available. We have used a Perkin-Elmer automatic infra-red spectrometer with a NaCl prism to obtain the spectrum of this CO_2 in the region 2-16 microns. The measurements were made at room temperature in a 9.4 cm. glass cell fitted with KBr windows. The total CO_2 pressure was 9.6 mm. The absorption curves are shown in Figure 1.

The calibration function of McKinney and Friedel (1), which gives a straight line when plotted against drum reading, permitted a more accurate determination of frequencies than the usual curve of ν itself vs. drum reading. This was important because the precision with which it was possible to determine the band centers limited the accuracy of the product rule check.

Table 1 shows our experimental results, as well as those of A. H. Nielsen for $C^{13}O_2$ (2). These data are compared to the frequencies calculated from the infra-red active fundamentals of $C^{12}O_2$ by the Redlich-Teller product rule (3). The agreement between the observed and calculated quantities is well within the precision of our measurements. The product rule applies strictly only to zero-order bands; however, the difference in ratio between the zero order bands and the fundamentals for CO_2 is so small as to be negligible, unless one has the accuracy of a grating spectrograph.

In view of recent interest in the isotope effect on bond energies, we hope to locate these band centers with a grating spectrometer, with the purpose of determining differences in the potential functions of the isotopic molecules. The authors are indebted to Professor M. Calvin for his interest in this work.

Table I

Isotope Shift of Band Centers

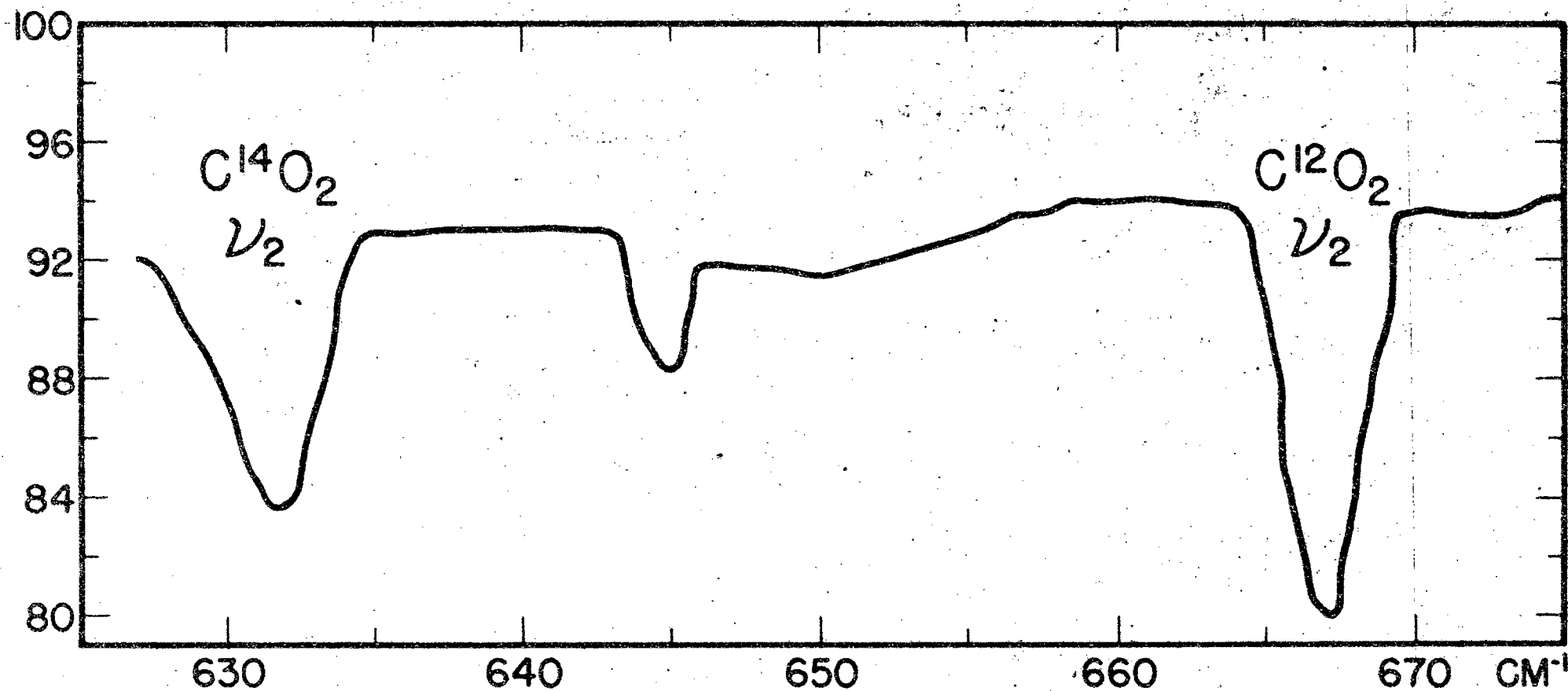
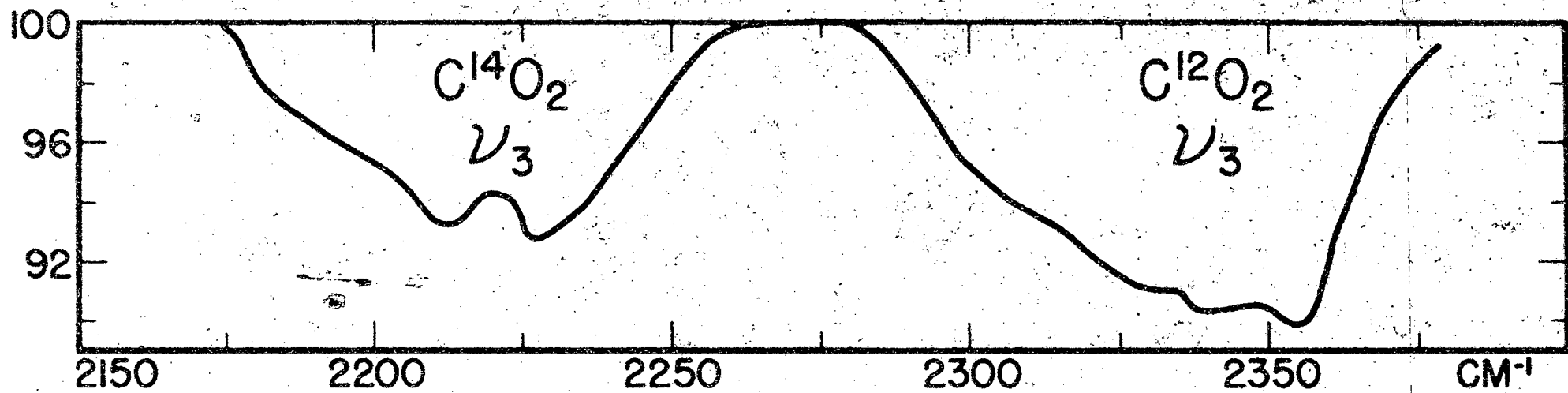
	ν_2	ν_3	Ratio $\left(\frac{\nu_i}{\nu}\right)_2$	Ratio $\left(\frac{\nu_i}{\nu}\right)_3$
$C^{12}O_2$ obs.	667.3	2349.3	1.0000	1.0000
calc.	---	---	1.0000	1.0000
$C^{13}O_2$ obs. (2)	---	2284.5	---	.97242
calc.	648.3	2282.4	.97154	.97154
$C^{14}O_2$ obs.	632 \pm 2	2220 \pm 5	.94710	.94496
calc.	631.6	2223.7	.94656	.94656

References:

- (1) D. S. McKinney and R. A. Friedel, J. Opt. Soc. Am. 38, 222 (1948).
- (2) A. H. Nielsen, Phys. Rev. 53, 983 (1938).
- (3) G. Herzberg, Infra-red and Raman Spectra of Polyatomic Molecules.
D. Van Nostrand Co., New York, (1947), p. 230.

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Fundamental Bands of $C^{12}O_2$ and $C^{14}O_2$