Errata : Infrared Absorption Spectrum of Deuterated Polyvinyl Alcohol Film

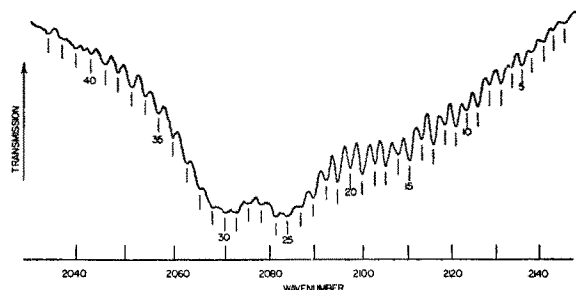Hiroyuki Tadokoro, Syûzô Seki, and Isamu Nitta

FIG. 1. ν_5 and ν_7 bands of digermane. Path length 10 cm, pressure 5.5 mm.

The spectrum of Ge_2H_6 in the region 2150 to 2025 cm^{-1} is shown in Fig. 1, and the line positions tabulated in Table I. The two broad maxima in absorption at 2083.1 and 2071.1 cm^{-1} are the R- and P-branches of the A_{2u} band ν_5, centered at 2077.1 cm^{-1}. The observed spacing, 12.0 cm^{-1}, agrees with the calculated value,[4]

TABLE I. Observed Q-branch frequencies.

Line	cm^{-1}	Line	cm^{-1}
1	2146.2	23	2089.5
2	2143.6	24	2086.7
3	2141.4	25	2083.9
4	2138.7	26	2081.1
5	2136.1	27	2078.4
6	2133.7	28	2076.0
7	2131.2	29	2073.0
8	2128.7	30	2070.2
9	2126.1	31	2067.8
10	2123.6	32	2065.1
11	2120.9	33	2062.4
12	2118.5	34	2059.6
13	2115.8	35	2056.6
14	2113.2	36	2053.8
15	2110.5	37	2051.1
16	2108.1	38	2048.3
17	2105.2	39	2045.7
18	2102.8	40	2042.7
19	2100.2	41	2039.4
20	2097.4	42	2036.8
21	2094.7	43	2033.7
22	2092.2		

11.8 cm^{-1}. The Q-branch of ν_5 is expected to be too weak to be observed because of the large ratio of moments of inertia I_B/I_A.

The lines numbered (arbitrarily) 1–43 are due mainly to the ^PQ- and ^RQ-branches of the E_u band ν_7. The intensities of the Q-branches are anomolous, every other branch having enhanced intensity instead of every third, as would be expected with a threefold symmetry axis. The expected intensity pattern was obtained for ν_8,[1] but it is interesting to note that disilane (Si_2H_6) appears to have the anomolous intensity pattern in ν_7.[5] The reason for this intensity effect is not known; it does not seem possible that it could be caused by the Coriolis interaction between ν_5 and ν_7, nor does there seem to be any relationship between the large and small moments of inertia that could cause the effect by coincidence of Q- and P- or R-branches. It is likely that "hot" bands are involved, since there are low-lying vibrational states with high populations at room temperature.

Because of the anomoly in intensities, the position of the band center can only be guessed at. From the over-all band contour it is near line 21, or about 2095 cm^{-1}, probably plus or minus 10 cm^{-1}.

Even though the assignment of the lines is not known, the approximate spacing of the Q-branches is given by $2A(1-\zeta_7)$, to the approximations mentioned in reference 1. The average spacing of the lines is found to be 2.69 ± 0.15 cm^{-1}; therefore $A(1-\zeta_7) = 1.35\pm0.08$ cm^{-1}. With the same assumptions as to structure as given in reference 1 the Coriolis constant ζ_7 is +0.02 or +0.07, which may be compared to the values for ethane, +0.095,[6] and disilane, -0.01.[5]

The authors wish to express their appreciation to the Light Division, National Physical Laboratories, Teddington, England, and in particular to Dr. L. A. Sayce, for the gift of the grating used in this work.

[1] D. A. Dows and R. M. Hexter, J. Chem. Phys. 24, 1117 (1956).
[2] See G. D. Dew, J. Sci. Instr. 30, 229 (1953) for description of grating and references. These gratings are available commercially from Hilger and Watts, Ltd. (London), Paton-Hawksley, Ltd. (London) and Sir Howard Grubb, Parsons, Ltd. (Newcastle).
[3] Lagemann, Nielsen, and Dickey, Phys. Rev. 72, 284 (1947).
[4] S. L. Gerhard and D. M. Dennison, Phys. Rev. 43, 197 (1933).
[5] H. S. Gutowsky and E. O. Stejskal, J. Chem. Phys. 22, 939 (1954), see Fig. 2.
[6] L. G. Smith, J. Chem. Phys. 17, 139 (1949).

Erratum: X-Ray Diffraction Study of Four Reinforcing Carbon Blacks

[J. Chem. Phys. 23, 594 (1955)]

LEROY ALEXANDER AND STEPHEN R. DARIN
Mellon Institute, Pittsburgh, Pennsylvania

THE equation in the second column is incorrect. It should read

$$\frac{4\pi n A_a s^2}{mF^2}\left(\frac{I-D}{1-D}\right) = \frac{s^2}{0.0606}\left(\frac{I-D}{1-D}\right).$$

Errata: Infrared Absorption Spectrum of Deuterated Polyvinyl Alcohol Film

[J. Chem. Phys. 23, 1351 (1955)]

HIROYUKI TADOKORO, SYÛZÔ SEKI, AND ISAMU NITTA
Department of Chemistry, Faculty of Science,
Osaka University, Osaka, Japan

THE following corrections are made for page 1352. In the explanation of Fig. 1, for "$\perp$ Parallel Band $\parallel$ Perpendicular Band" read "$\parallel$ Parallel Band $\perp$ Perpendicular Band." In column 2, line 5, for "M. T. Kanzawa" read "Mr. T. Kanzawa."

Erratum: Report on Notation for the Spectra of Polyatomic Molecules

[J. Chem. Phys. 23, 1997 (1955)]

ROBERT S. MULLIKEN
Department of Physics, The University of Chicago, Chicago, Illinois

THE name of the writer was inadvertently omitted when this Report was published.