Polymer Journal, Vol. 2, No. 5, pp 815—816 (1971)

SHORT COMMUNICATION

Laser-Raman Scattering by $(CH_2)_{34}$ in the Low-Frequency Region

Robert F. SCHAUFELE*

Biophysics Department, Michigan State University, East Lansing, Michigan, U.S.A.

Mitsuo TASUMI**

Department of Chemistry, Faculty of Science, The University of Tokyo, Bunkyo-ku, Tokyo, Japan.

(Received May 24, 1971)

KEY WORDS Laser-Raman Scattering / Ring Molecule / $C_{34}H_{68}$ / Low-frequency Vibration /

In a previous paper[1] we reported the laser-Raman spectrum of the $(CH_2)_{34}$ ring molecule in the region above 130 cm.$^{-1}$ The assignments of the eight bands observed in the region between 130 and 600 cm^{-1} were discussed in terms of the results of a normal-coordinate treatment.

More recently we succeeded in measuring the Raman spectrum of the same compound in the region below 130 cm^{-1} and found several more bands. The observed spectra are shown in Figures 1a and 1b. The measurements were conducted using a Spex grating double monochromator together with d.c. photoelectric detection and the 5145 Å line of an Ar^+ gas laser (about 0.7 watts). Measurements were made to within 9 cm^{-1} of the exciting line. No filters were necessary inasmuch as the technique of focusing the laser beam into an internal cavity of the specimen to maximize the inelastic/elastic scattering intensity ratio was utilized. This technique has been described earlier[2] and later verified by Schrader[3] as being the most efficient geometry for maximizing this ratio. In this particular instance $(CH_2)_{34}$ was studied in the form of an unpressed powder, contained within 5-mm glass tubing. A scattering cavity was formed merely by pressing the tip of a sharpened match stick into the center of the powder. Figure 2 shows the experimental geometry.

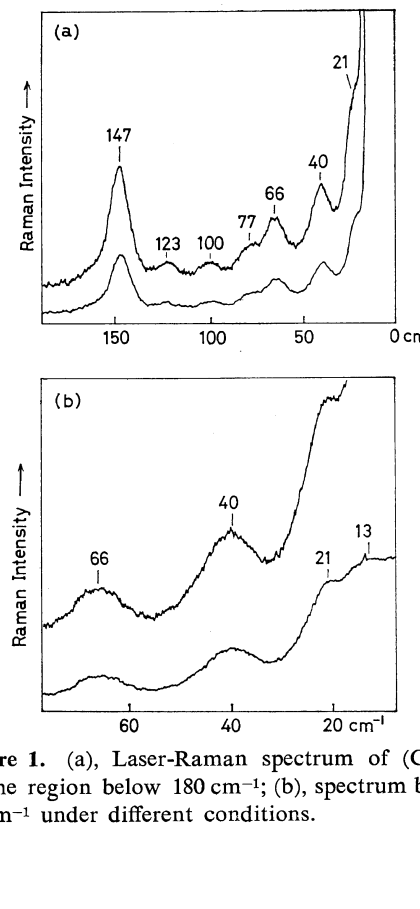

Figure 1. (a), Laser-Raman spectrum of $(CH_2)_{34}$ in the region below 180 cm^{-1}; (b), spectrum below 70 cm^{-1} under different conditions.

* Present address: *Human Biology Laboratories, College of Human Medicine, Michigan State University, East Lansing, Michigan, U.S.A.*

** Present address: *Department of Biophysics and Biochemistry, Faculty of Science, The University of Tokyo, Bunkyo-ku, Tokyo, Japan.*

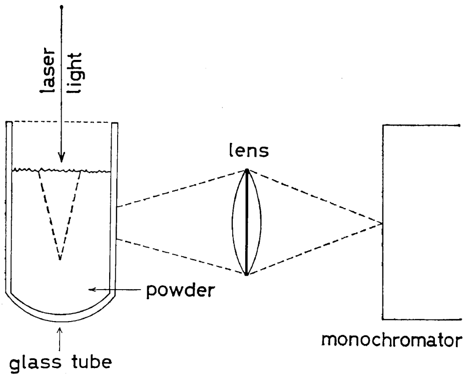

Figure 2. Geometry for scattering experiment.

Table I. Comparison of the observed and calculated frequencies of $(CH_2)_{34}$ in the region below 180 cm^{-1}

Obsd Raman frequency, cm^{-1}	Calcd frequency[a], cm^{-1}
13	13 (ν_{16})
21	21 (ν_{15})
40	42 (ν_{30})
66	53 (ν_{29})
77	68 (ν_{13})
100	94 (ν_{12})
123	120 (ν_{11})
147	145 (ν_{10})

[a] Calculated frequencies are taken from ref 1.

The observed frequencies are compared in Table I with those calculated. Three of the modes, ν_{16}, ν_{15}, and ν_{30}, have their vibrational patterns illustrated schematically in Figure 3. Although the vibrational modes of ν_{29}, ν_{13}, and ν_{12} are more complex, they also have long-wave

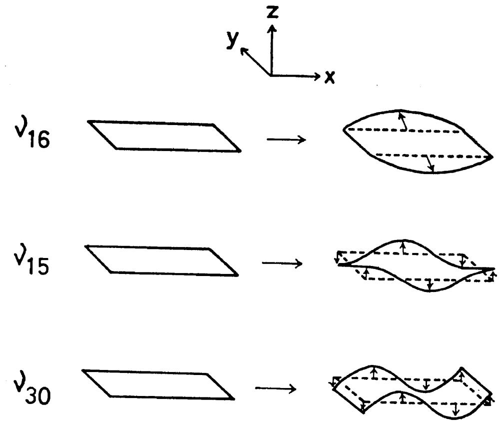

Figure 3. Approximate vibrational patterns of ν_{16}, ν_{15}, and ν_{30}.

components (atomic displacements in the z-direction). The mode ν_{11} has an accordion-type component. It is interesting to note that these low-frequency bands may be interpreted reasonably by the simple model calculation.[1] This increases the reliability of the assignments of the higher-frequency bands discussed in the previous paper.

Acknowledgement. One of us (RFS) wishes to thank Professor G. Leroi for permission to utilize his facilities.

REFERENCES

1. M. Tasumi, T. Shimanouchi, and R.F. Schaufele, *Polymer J.*, **2**, 740 (1971).
2. R. F. Schaufele, *J. Opt. Soc Amer.*,. **57**, 105 (1967).
3. B. Schrader and G. Bergmann, *Z. Anal. Chem.*, **2**, 230 (1967).