

The Raman Spectra of Deuteroacetones and Methyl Alcohol

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The Raman Spectra of Deutero-acetones and Methyl Alcohol-*d*

Raman spectra have been photographed for a series of equilibrium solutions of the several deutero-acetones produced by means of the exchange reaction of acetone with deuterium oxide¹ and containing progressively higher deuterium fractions up to 91 percent. The results are summarized in Table I, from which the changes of frequency may be seen as a function of the isotopic composition.

Acetones (percent D)	0	4	24	51	70	91
Raman Frequencies (cm ⁻¹)	396 531 796 1068 1706	533 790 1067 1707	402 532 760 794 1047 1703	396 502 714 750 1036 1703	393 484 702 744 1030 1700	488 706 1031 1704 2049 2072 2113 2160 2219 2251 2937
		2175	2163 2126 2182 2218	2126 2104 2151 2210	2060 2049 2072 2113 2160 2219 2251 2937	
	2918 2970 3000	2930 2963 3001	2934 2997	2256 2942 2992	2248 2948 3000	

As the deuterium fraction increases, the higher frequency of acetone at 2918 cm⁻¹ and possibly the frequencies 2970 and 3000 cm⁻¹, increase slightly and then fade out, only the high probability parallel frequency at 2937 cm⁻¹ appearing faintly in the most concentrated *d*-acetone. Simultaneously, at deuterium fraction = 4 percent, a line appears at 2175 cm⁻¹ and three are found in this region when D = 24 percent. The strong lines at about 2115, 2160, 2219 and 2250 cm⁻¹ appear at higher deuterium concentrations, with 2113 cm⁻¹ becoming the strongest line at the greatest deuterium concentration; weak lines at 2049 and 2072 cm⁻¹ also appear in the D = 91 percent acetone. The 1706 cm⁻¹ line, ascribed to C = 0, appears quite unchanged in all the acetones. The 795 cm⁻¹ line splits in the intermediate acetones to give a second line at 760 cm⁻¹. This second line becomes strong, splits to give a third at about 700 cm⁻¹ with the original line at 795 cm⁻¹ disappearing. Finally, the 750 cm⁻¹ line fades, leaving in the most concentrated *d*-acetone the 700 cm⁻¹ as the strongest line. Lines at 531 cm⁻¹ and 1069 cm⁻¹ are gradually displaced toward the exciting line as the concentration of deuterium is increased.

We are attempting to interpret these results by the use of the equations of Rosenthal,² comparing the data with frequencies calculated for the four possible isotopic methyl

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The line observed at 2970 cm⁻¹ with ordinary acetone is at present unexplained, CH₃ having theoretically only two frequencies near 3000 cm⁻¹.³ The usual explanation of resonance degeneracy apparently is not tenable in this case. The presence of the four strong and two weak lines at 2000–2250 cm⁻¹ in the acetones having the greatest deuterium fraction is also of interest, since never more than the 3 hydrogen lines from 2900–3050 cm⁻¹ appear in the acetones containing little deuterium.

Strong Raman lines appeared in acetone at 1157, 1224, 1340 and 1428 cm⁻¹. Lines at about these frequencies occur in the intermediate deutero-acetones and practically disappear in the 91 percent deutero-acetone. We have not tabulated these lines, however, because they may be due to excitation by the 4047 and 4078 Å lines of the mercury source. This point is being studied further.

The Raman spectra of methyl alcohol and methyl alcohol-*d* have been determined, using the mercury lines at 4358 and 2536 Å as exciting sources. Table II presents

TABLE II.

CH ₃ OH (cm ⁻¹)		CH ₃ OD (cm ⁻¹)	
From 2536	4358	2536	4358
1033	1031	1031	1034
	1056		1071
1109	1119	1153	1154
1153	1171		1179
1464	1451	1382	1370
2835	2839	2494 (Band)	2494 (Band)
2913	2914	2836	2839
2954	2948	2915	2918
2992	2982	2946	2947
3388 (Band)	3415 (Band)	2989	2986

the lines found. The OD band occurs at 2500 cm⁻¹ ± 10 and the OH band at 3400 cm⁻¹ ± 20.⁴ A line at about 1375 cm⁻¹ in the CH₃OD spectra and one at 115 cm⁻¹ in the CH₃OH were other differences noted. The four lines between frequencies 2840 and 3000 cm⁻¹ are very strong.

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¹ Halford, Anderson and Bates, J. Am. Chem. Soc. **56**, 491 (1934); Halford, Anderson, Bates and Swisher, *ibid.*, **57**, 1663 (1935).

² Rosenthal, Phys. Rev. **47**, 235 (1935).

³ Adel and Barker, J. Chem. Phys. **2**, 627 (1934).

⁴ Redlich and Pordes, Naturwiss. **22**, 808 (1934).