

Infrared Absorption Spectrum of Butatriene in the LiF Region

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The butatriene molecule is of considerable interest, as it is the smallest hydrocarbon molecule with three double bonds. Its structure in the gaseous state has been investigated by Raman high-resolution spectroscopy,¹ and electron diffraction.² Neither of these investigations contradict the assumption of a planar structure with linear carbon chain (symmetry: D_{2h}) in the equilibrium position.

Some infrared bands of butatriene have been reported³ in connection with the synthesis of the compound, but no vibrational analysis has been attempted. Dr. Eggers⁴ kindly supplied to me a tentative assignment of some infrared bands, but still many uncertainties remain. We have taken up again this problem, trying to make an assignment of at least the infrared-active frequencies.⁵ Unfortunately there are great difficulties in taking a Raman spectrum in the liquid, due to rapid polymerization.⁴

In the present work the infrared absorption spectrum in the LiF region is reported. It has been recorded in 1958, using a sample prepared by Dr. Else Kloster-Jensen.² The observed maxima are given in Table 1. The four most prominent bands (band centra: 1607, 1711, 3001, and 3059 cm^{-1}) are reproduced in Figs. 1 and 2.

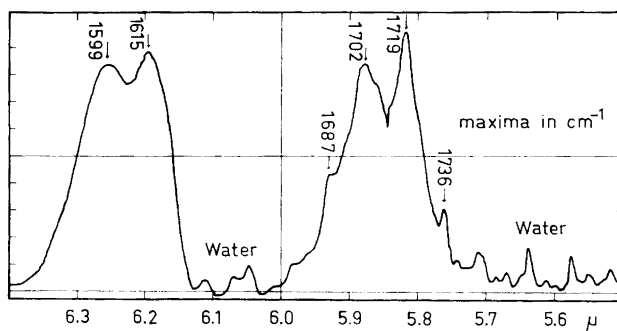


Fig. 1. I.R.-Spectrum of butatriene in the range 5.6 to 6.4 μ . Gas 10 cm, equilibrium temperature -19°C , prism LiF.

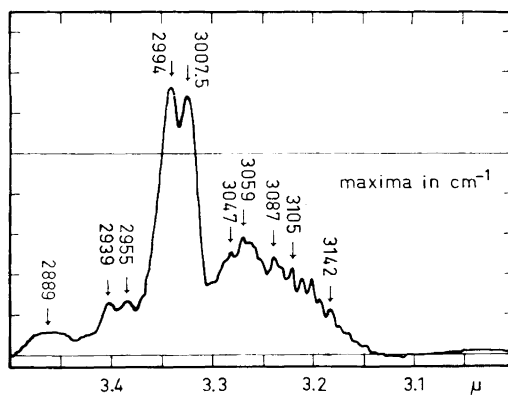


Fig. 2. I.R.-Spectrum of butatriene in the range 3.0 to 3.5 μ . Experimental conditions as in Fig. 1.

Table 1. Observed infrared LiF spectrum of butatriene: gas 10 cm, equilibrium temperature -19°C .

Band centra (cm^{-1})	Maxima (cm^{-1})	Intensity	
1607	1599	vs	
	1615	vs	
	1687	s	
1711	1702	vs	
	1719	vs	
	1736	s	
	1969	w	
2034	2026	s	
	2041	s	
	2475	w	
	2889	w	
	2939	w	
3001	2955	w	
	2994	vs	
	3007.5	vs	
	3030	fine structure	
	3040		
	3047		
	3059		
	3066	s	
	3076	fine structure	
	3087		
3095			
3105			
3115			
3123			
3132			
3059	3142	fine structure	
	3152		
	3160		
	3170		
	3178		
	3448		w
	4082		w
	4141		w
	4484		w
	4651		w

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Effect of Irradiation Temperature on the Yield of Solute Radicals in Frozen Aqueous Solutions

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In the present communication data are reported on the effect of the irradiation temperature on the efficiency of the indirect action of ionizing radiation.

When solutions are exposed to ionizing radiation, free radicals are induced in the solvent as well as in the solute. At 77°K or lower, there is little or no interaction between solvent radicals and solute molecules. Under these conditions the solute radicals, as revealed by electron spin resonance (ESR) spectroscopy, are formed predominantly by direct action.¹⁻³ When frozen aqueous solutions are heat-treated after irradiation, the radicals induced in the water disappear in the temperature range 100° to 130°K , largely by recombination reactions. Some of the radicals will, however, interact with the solute molecules with the result that radiation energy is transferred to the solute. The extent of this indirect effect in frozen aqueous solutions irradiated at 77°K is small compared to that observed after irradiation in the liquid state.^{3,4} Although the state of the solution is the most important factor in this respect,^{5,6} the possibility exists that the irradiation temperature as such may have a significant influence on the interaction of water radicals with solute molecules.

Frozen aqueous solutions of DL- α -alanine were irradiated in vacuum with X-rays at different temperatures in the range 77° to 195°K . During the exposure (104 min) secondary reactions will occur in the solvent as well as in the solute. In order to eliminate possible differences in the extent of the secondary reactions at the different temperatures used, all samples were heat-treated for 3 min after the exposure. A temperature was chosen (250°K) that was appreciably higher than the highest irradiation temperature. The ESR spectra were recorded at 77°K . The

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