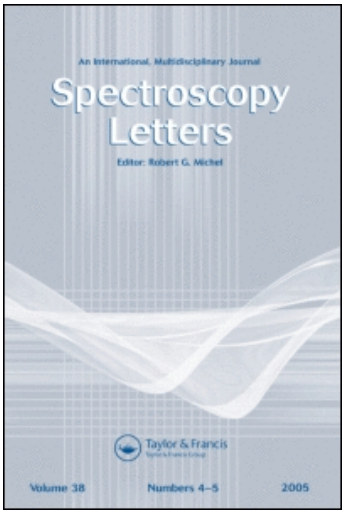

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Infra-Red Spectra of Monobromoethyne and Some Polyalkynes

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INFRA-RED SPECTRA OF MONOBROMOETHYNE AND SOME POLYALKYNES

by

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INTRODUCTION

In the course of an investigation into the reactions of ethynyl radicals with alkynes[1], monobromoethyne and certain polyalkynes were synthesized and their infra-red spectra were recorded. Although the spectra of certain of the compounds have been well-documented, others are less familiar and, in the case of two dialkynes, no record can be found of their vibrational spectra.

In the present communication, the spectra of monobromoethyne, buta-1,3-diyne, penta-1,3-diyne, 1,6-dichlorohexa-2,4-diyne and hexatriyne, are reported.

EXPERIMENTAL

Monobromoethyne was prepared by the method of Oppenheim and Shorr[2] and purified by eleven trap-to-trap distillations in vacuo. Gas chromatographic analysis revealed that the compound was 99.98% pure, the only impurity being dibromoethene. Butadiyne was prepared by the method of Armitage, Jones and Whiting[3] and, after purification, contained ca. 1% 1,4-dichlorobut-2-yne. Penta-1,3-diyne, 1,6-dichlorohexa-2,4-diyne and hexatriyne were also prepared by the methods of Armitage et al.[4,5]

Infra-red spectra from 600 - 4000 cm^{-1} were measured using a Perkin Elmer 257 Spectrophotometer.

RESULTS

Monobromoethyne

The infra-red spectrum of this compound has been extensively reported[6,7,8,9]. The present results are in good agreement with those of Hunt and Wilson[6] and Evans et al.[9] The three sets of data are shown in Table 1.

Table 1. Gas-phase, Infra-red Spectrum of Monobromoethyne (100 Torr)

This work (cm^{-1})	Ref.9(cm^{-1})	Ref.6(cm^{-1})	Assignment
3920	3920	-	Combination
3620	3630	-	Combination
3320	3333	3325	C-H stretch
-	3040	-	Combination
2710	2710	-	Combination
2090	2088	2085	C≡C stretch
1229,1210	1254,1226	1225	H-C≡C overtone
-	920	-	Combination
615	604,624	618	H-C≡C bend

Butadiyne

There have been several descriptions of the spectrum of this compound including those of Jones[10] and Freund and Halford[11]. In the present work, the gas-phase (100 Torr) spectrum of the butadiyne revealed the following absorptions (cm^{-1}):

3945 (combination band); 3330 (C-H stretch); 2000,2020 (C≡C stretch); 1250,1230 (H-C≡C overtone); 852 (C-C stretch); 704; 685 (possibly C≡C-C band); 600 (H-C≡C bend).

These results are very similar to those of Freund and Halford[11]

Penta-1,3-diyne

The spectrum of penta-1,3-diyne does not appear to have been published. The following absorptions (cm^{-1}) were recorded (gas-phase, 30 torr):

3920 (combination band); 3325 (C-H stretch); 2930,2865(CH_3 stretch); 2310; 2240; 2070 (C≡C stretch); 1725; 1412, 1430, 1442, 1445, 1469, 1481 (symmetric and asymmetric CH_3 bending); 1370, 1232, 1240 (H-C≡C, first overtone); 820 (C-C stretch); 610 (H-C≡C bend).

Compared with the spectrum of butadiyne, the substitution of a methyl group into the molecule produces a more complex structure and certain absorptions (2310, 2240, 1725 and 1370) were not satisfactorily identified.

1,6 dichlorohexa-2,4 diyne

This is another compound, for which the vibrational spectrum has not previously been reported. The liquid-phase spectrum found during the present measurements is:

2980, 2940; 2155; 1420; 1285; 1250; 963; 695 (cm^{-1}).

Table 2. Gas-phase, Infra-red Spectrum of Hexatriyne (7 Torr)

This work(cm^{-1})	Ref.12(cm^{-1})	Assignment
3320	3327,3318	C-H stretch
3940	-	Combination
2120	2115	C≡C stretch
1232, 1240	1234, 1243	H-C≡C, first overtone
685	-	
623	628,623,618	H-C≡C bend

Hexatriyne

Hexatriyne has recently been prepared and its infra-red spectrum has been recorded by Kloster-Jensen[12]. The present spectrum is in good agreement with that of Kloster-Jensen, as can be seen in Table 2.

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