

This article was downloaded by:

On: 30 January 2011

Access details: *Access Details: Free Access*

Publisher *Taylor & Francis*

Informa Ltd Registered in England and Wales Registered Number: 1072954 Registered office: Mortimer House, 37-41 Mortimer Street, London W1T 3JH, UK



Spectroscopy Letters

Publication details, including instructions for authors and subscription information:

<http://www.informaworld.com/smpp/title~content=t713597299>

Infra-Red Spectra of Monobromoethyne and Some Polyalkynes

D. J. Hucknall^a, J. V. Shepherd^a

^a Department of Chemistry, The City University, London, England

To cite this Article Hucknall, D. J. and Shepherd, J. V.(1974) 'Infra-Red Spectra of Monobromoethyne and Some Polyalkynes', *Spectroscopy Letters*, 7: 8, 381 — 384

To link to this Article: DOI: 10.1080/00387017408067262

URL: <http://dx.doi.org/10.1080/00387017408067262>

PLEASE SCROLL DOWN FOR ARTICLE

Full terms and conditions of use: <http://www.informaworld.com/terms-and-conditions-of-access.pdf>

This article may be used for research, teaching and private study purposes. Any substantial or systematic reproduction, re-distribution, re-selling, loan or sub-licensing, systematic supply or distribution in any form to anyone is expressly forbidden.

The publisher does not give any warranty express or implied or make any representation that the contents will be complete or accurate or up to date. The accuracy of any instructions, formulae and drug doses should be independently verified with primary sources. The publisher shall not be liable for any loss, actions, claims, proceedings, demand or costs or damages whatsoever or howsoever caused arising directly or indirectly in connection with or arising out of the use of this material.

INFRA-RED SPECTRA OF MONOBROMOETHYNE AND SOME POLYALKYNES

by

D. J. Hucknall and J. V. Shepherd
Department of Chemistry, The City University,
London EC1V 4PB, England

INTRODUCTION

In the course of an investigation into the reactions of ethynyl radicals with alkynes¹, 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 Shorr² 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 Whiting³ 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 Wilson⁶ 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)

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

Butadiyne

There have been several descriptions of the spectrum of this compound including those of Jones¹⁰ and Freund and Halford¹¹. 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 \equiv C stretch); 1250,1230 (H-C \equiv C overtone); 852 (C-C stretch); 704; 685 (possibly C \equiv C-C band); 600 (H-C \equiv C bend).

These results are very similar to those of Freund and Halford¹¹

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 ($\text{C}\equiv\text{C}$ stretch); 1725; 1412, 1430, 1442, 1445, 1469, 1481 (symmetric and asymmetric CH_3 bending); 1370, 1232, 1240 ($\text{H}-\text{C}\equiv\text{C}$, first overtone); 820 (C-C stretch); 610 ($\text{H}-\text{C}\equiv\text{C}$ 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)

<u>This work (cm^{-1})</u>	<u>Ref. 12 (cm^{-1})</u>	<u>Assignment</u>
3320	3327, 3318	C-H stretch
3940	-	Combination
2120	2115	$\text{C}\equiv\text{C}$ stretch
1232]	1234]	H-C \equiv C, first overtone
1240]	1243]	
685	-	
623	628, 623, 618	H-C \equiv C bend

Hexatriyne

Hexatriyne has recently been prepared and its infra-red spectrum has been recorded by Kloster-Jensen¹². The present spectrum is in good agreement with that of Kloster-Jensen, as can be seen in Table 2.

REFERENCES

- (1) C.F.Cullis, D.J.Hucknall and J.V.Shepherd, Proc. Roy. Soc. London, A335, 525 (1973).
- (2) W.Oppenheim and L.M.Shorr, Israel J. Chem., 2, 121 (1964).
- (3) J.B.Armitage, E.R.H.Jones and M.C.Whiting, J. Chem. Soc., 44 (1951).
- (4) J.B.Armitage, E.R.H.Jones and M.C.Whiting, J. Chem. Soc., 1993 (1952).
- (5) J.B.Armitage, C.L.Cook, E.R.H.Jones and M.C.Whiting, J. Chem. Soc. 2012 (1952).
- (6) G.R.Hunt and M.K.Wilson, J. Chem. Phys., 34, 1301 (1961).
- (7) R.Queignec and B.Wojtkowiak, Comp. Rend., Ser. A., B262B(7), 486 (1966).
- (8) E.D.Lubuzh and E.M.Popov, Zh. Prikl. Spektrosk., 5(4), 498 (1966); CA 66: 60454 y.
- (9) K.Evans, R.Scheps, S.A.Rice and D.Heller, JCS Faraday II. 69, 856 (1973).
- (10) A.V.Jones, Proc. Roy. Soc. Lond., A211, 285 (1952).
- (11) I.Freund and R.S.Halford, J. Chem. Phys., 42, 4132 (1965).
- (12) E. Kloster-Jensen, Angew. Chemie (Internat. Ed.), 11, 438 (1972).

Received June 18, 1974

Accepted July 8, 1974