553. *Excited States of Acetylene. Part V.* Measured and Calculated Frequencies in the Near-ultra-violet Absorption Spectra of Acetylene and Dideuteroacetylene: Vibrational and Rotational Energies of the* trans-*Bent Excited State.*

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Band and line frequencies are recorded which lead to vibrational frequencies of the excited states, and to their rotational constants. The results of some calculations are given on which rotational line assignments are based.

(1) Vibrational analysis

(a) *Normal Electronic State.*—The present spectra provide an opportunity for learning one new thing about the already very closely studied vibrations of the ground state of acetylene, namely, the variation of magnitude of successive quanta of the bending vibration π_g. As appears from Table 22, this vibration shows the opposite of the usual trend, its energy in acetylene *increasing* by about 1% per quantum over the first three quanta, and in dideuteroacetylene by slightly less than this. The trends suggest that the wall of resistance to hydrogen bending hardens somewhat sharply as the amplitude is increased.

Table 22. *Energies (cm.$^{-1}$) of the π_g vibration of normal acetylene and dideuteroacetylene.*

[v is the total and K the azimuthal quantum number of this vibration, while v' is the quantum number with which vibration A_g (α) is also excited in the measured bands.]

	Quantum Q_1 between quantum numbers (v^K) : $1^1 - 0^0$		Quantum Q_2 between quantum numbers (v^K) : $2^2 - 1^1$ (two estimates)			
	Band D — band B		Band G — band H		Band C — band E — Q_1	
v'	C_2H_2	C_2D_2	C_2H_2	C_2D_2	C_2H_2	C_2D_2
1	612·1	—	617·6	—	618·9	—
2	612·5	510·5	617·3	—	619·5	513·2
3	611·2	510·6	620·9	—	621·2	512·9
4	610·7	510·3	621·1	511·5	619·2	513·0
5	—	510·8	—	513·5	—	513·5

	Quantum Q_3 between quantum numbers (v^K) : $3^1 - 2^2$ (two estimates)			
	Band A — band J — Q_2		Band B — band F — Q_2	
v'	C_2H_2	C_2D_2	C_2H_2	C_2D_2
2	624·7	518·0	624·5	518·3
3	623·0	517·4	622·6	517·7
4	—	518·4	624·1	518·6
5	—	517·1	—	517·4

(b) *The Excited Electronic State.*—The vibration $A_g(\alpha)$ can be measured over the first five quanta in acetylene, and over four quanta, starting with the third, in dideuteroacetylene. The most direct source of data consists of the intervals in Table 23 between successive C

Table 23. *Energies (cm.$^{-1}$) of $A_g(\alpha)$ vibration of excited acetylene and dideuteroacetylene.*

	$C_1 - C_0$	$C_2 - C_1$	$C_3 - C_2$	$C_4 - C_3$	$C_5 - C_4$	$C_6 - C_5$
C_2H_2	1048·7	1032·1	1011·8	986·0	972·5	—
C_2D_2	—	—	823·8	814·4	802·6	781·4

bands, though it must be remembered that the acetylene bands C_4 and C_5 are appreciably perturbed. For both molecules the energies of successively added quanta fall by about 1·7% for each extra quantum.

* Part IV, preceding paper.

For both acetylene and dideuteroacetylene, the energy of the first quantum of vibration A_g(C) may be deduced from the frequencies of combinations with various quanta of vibration $A_g(\alpha)$, as is shown in Table 24. For dideuteroacetylene only, the energy of the first quantum of vibration A_g(H) can be similarly obtained, as shown in Table 25.

TABLE 24. *Energy (cm.$^{-1}$) of the first quantum of vibration A_g(C).*

[v' is the quantum number with which vibration $A_g(\alpha)$ is simultaneously excited.]

v'	a — A	b — B	c — C	e — E	f — F	j — J	h — H
				Acetylene			
0	1379·0	1385·3	—	—	—	—	—
1	1382·6	1384·2	1384·1	1384·8	—	—	1381·7
2	1383·0	1386·1	1385·8	1385·5	1384·6	1386·4	1384·1
3	1385·4	1384·3	1384·6	1385·4	1384·5	1381·4	1382·7
4	1386·3	1384·4	—	1387·0	1385·4	1382·2	1387·9
5	—	—	—	—	1385·7	—	—
				Dideuteroacetylene			
2	1299·8	1298·5	1299·3	1299·1	1298·4	1300·1	—
3	1295·4	1293·0	1294·2	1293·3	—	1294·4	—
4	1291·1	1289·1	1291·0	1289·0	—	1290·4	—
5	1288·5	1286·5	—	1288·6	1286·1	—	—

(Additional values for acetylene from " hot " bands : $k_1 - K_1 = 1381{\cdot}6$ cm.$^{-1}$; $l_1 - L_1 = 1385{\cdot}0$ cm.$^{-1}$.)

TABLE 25. *Energy (cm.$^{-1}$) of first quantum of vibration A_g(H) of dideuteroacetylene.*

(v' is the quantum number with which vibration $A_g(\alpha)$ is simultaneously excited.)

v'	p — A	q — B	r — C	t — E	u — F	w — H	y — J
2	2198·1	2198·6	—	2197·7	2200·2	—	2198·1
3	2191·2	2191·8	2191·6	2190·6	—	2191·5	2190·4
4	2183·1	2180·0	—	—	—	—	—

(2) ROTATIONAL ANALYSIS

For the normal acetylene molecule, we have taken the standard value $B'' = 1{\cdot}1769$ cm.$^{-1}$ as the rotational constant applying to all the vibrational states of concern to us. As to the bent excited molecule, the rotational constant A, depending as it does on an average de-

TABLE 26. *Calculated and observed line positions of band* C_1.

Spectral positions are in cm.$^{-1}$, but in the columns only the last three significant figures are noted. Lower state, $B'' = 1{\cdot}1769$ cm.$^{-1}$. Upper state, $A = 13{\cdot}80$ cm.$^{-1}$, $B = 1{\cdot}126$ cm.$^{-1}$, $C = 1{\cdot}030$ cm.$^{-1}$. Vibronic origin, $\nu_{00} = 43{,}245{\cdot}0$ cm.$^{-1}$. Gyrovibronic origin, $\nu_0 = 43{,}257{\cdot}7$ cm.$^{-1}$.

	R Branch		Q Branch		P Branch	
J''	Calc.	Obsd.	Calc.	Obsd.	Calc.	Obsd.
0	59·9	—	—	—	—	—
1	62·2	62·2	57·5		—	—
2	63·9	—	56·9	56·5	52·9	—
3	65·8	66·2	56·2		50·4	(50·9)
4	67·2	—	55·3	—	47·4	—
5	68·9	69·0	54·0	54·1	44·4	44·4
6	69·8	—	52·5	—	41·3	(41·4)
7	71·1		50·8	50·9	38·3	38·3
8	72·2	73·9	48·2	—	34·5	(35·0)
9	73·1	head	46·5	46·7	31·1	31·4
10	73·7		44·1	(44·4)	27·5	(27·6)
11	74·0		41·1	41·4	23·6	23·6
12	—	—	38·2	(38·3)	19·6	(19·4)
13	—	—	—	—	15·2	15·5

parture from linearity, is quite a sensitive function of the number of quanta with which the vibration $A_g(\alpha)$ is excited; while the constants B and C, depending as they do on an average molcular length, have a small but appreciable dependence on the vibration $A_g(\alpha)$. Thus for each value v' of the quantum member of this vibration, that is, for each repetition of the gyrovibronic pattern of bands, D, C, G, B, A, H, E, F, J, etc., we have to

determine a new set of constants A, B, C, such that, when they are introduced into the exact energy expression for the asymmetric rotor, they will yield energy levels so spaced relatively to the rotational levels of the linear ground molecule, as to give line positions agreeing with the observed fine structure. Examples are given in Tables 26, 27, and 28 of such calculations for three bands, C_1, A_1, and B_1, all of the one-quantum gyrovibronic pattern. The same rotational constants have been used in calculations, not illustrated, on the bands E_1, H_1, D_1, and G_1, of the same pattern, $v' = 1$. Similarly determined rotational constants, applying to the other gyrovibronic patterns, having quantum numbers v' from 0 to 3, are listed in Part IV, Table 17, p. 2735.

TABLE 27. *Calculated and observed line positions of band* A_1.

See notes at head of Table 26. Rotational constants as there stated. Vibronic origin ν_{00} = 42,633·0 cm.$^{-1}$. Gyrovibronic origin ν_0 = 42,633·0 cm.$^{-1}$.

	R Branch		Q Branch		P Branch	
J''	Calc.	Obsd.	Calc.	Obsd.	Calc.	Obsd.
0	—	—	—	—	—	—
1	—	—	32·8		30·1	—
2	—	—	32·4		28·1	28·3
3	—	—	31·8	31·9	25·3	—
4	—	—	31·0		22·4	23·8
5	—	—	30·0	30·1	19·3	(19·8)
6	43·7		28·7	—	15·7	16·0
7	44·4		27·2	28·3	12·3	(12·1)
8	44·7	44·5	25·5	—	08·4	08·3
9	44·9	(head)	23·6	23·8	04·4	(04·6)
10	44·7		21·3	—	00·0	00·4
11	44·0		18·8	19·8	95·9	—
12	—	—	16·1	(16·0)	90·5	91·2
13	—	—	—	—	85·5	(87·3)

TABLE 28. *Calculated and observed line positions of band* B_1.

See notes at head of Table 26. Rotational constants as there stated. Vibronic origin, ν_{00} = 42,633·0 cm.$^{-1}$. Gyrovibronic origin, ν_0 = 42,683·9 cm.$^{-1}$.

	R Branch		Q Branch		P Branch	
J''	Calc.	Obsd.	Calc.	Obsd.	Calc.	Obsd.
0	—	—	—	—	—	—
1	88·0	—	—	—	—	—
2	89·8	90·8	83·3			
3	91·3		82·7	82·7	76·2	(77·6)
4	92·8	—	81·9		73·3	73·5
5	94·0	—	81·1	80·6	70·1	—
6	95·1	—	79·9		67·0	68·3
7	95·9	—	78·6	77·6	63·2	63·0
8	96·8	—	76·8		59·8	60·3
9	97·5	97·1	75·0	—	55·6	56·8
10	98·1	—	73·0	—	52·9	52·9
11	98·5	—	72·2	—	47·1	48·4
12	—	—	70·2	—	44·0	Overlap
13	—	—	—	—	37·8	with A_1

(3) Observed frequencies and assignments

The following four Tables, referring to the absorption spectra of acetylene and of dideuteroacetylene at 20° and 200°, contain the measured peak frequencies and our assignments of them. The indications of intensity, s = strong, w = weak, d = diffuse, etc., are to be understood as applying relatively to the immediate spectral surroundings of any maximum so marked. The grouping of the maxima in bands is indicated by the labelled R-head, with which each band starts, when the observations are arranged, as here, in order of decreasing frequency. The labels of the assigned bands are placed opposite the frequencies of their R-heads. Almost all the clearly defined bands in these spectra have been assigned, excepting a few near the beginnings of Tables 29 and 31, which probably belong to gyrovibronic patterns headed by C bands lying beyond the high-frequency limits of the observed spectra.

TABLE 29. *Frequencies (cm.$^{-1}$) of absorption maxima of acetylene at 20°.*

Frequency	Assignment Band	Lines	Frequency	Assignment Band	Lines	Frequency	Assignment Band	Lines
47,315·3 wd	D_5	R-head	50·6 s	—	R-head	44·6 s		
47,282·9 w			46·8 w			39·3		
79·4 w			43·2			35·0 ss	A_5	R-head
75·2 ss	C_5	R-head	38·9			29·3		
67·3			32·2			23·8 ss	—	Q-head
59·1 s	—	Q-head	29·4 sd			21·2		
56·6			27·0			17·2		
52·8			21·8 s			13·9		
50·1			16·6 s			10·4		
47·6 s			13·2			07·4		
42·5			10·3			04·6		
40·3			04·2			02·2 wd		
35·9			46,888·0			46,599·7		
32·8			84·6			97·8		
27·9			82·0			93·6 s		
23·8 ss	—	R-head	77·4 ss	—		91·1 s	h_4	R-head
18·7			74·2			86·4 s		
14·9			69·0 w			82·3 d		
09·4			60·2 s			77·4		
04·3 s			54·6 s			73·0		
47,199·1			50·9 s	f_5	R-head	71·5		
96·2			46·7			68·9 w		
92·5			43·1			65·5		
89·9			40·7			63·3		
86·4 s			34·8 ss			60·8		
83·4			30·5 s			57·4		
79·9			26·9 w			53·0 wd		
75·6			18·1			49·5		
72·2			12·5 ss			40·1 s		
67·3			09·9			32·9 s		
63·9 s	—	R-head	07·3 ss			29·8 w		
60·8			04·1 ss			27·8 w		
58·1			46,796·7			25·8		
54·5			89·7 ss	G_5		23·9		
45·6			87·6 s			19·9 s		
42·8			85·5			18·0 s		
40·2			80·6			11·7		
35·3			77·7			07·8 w		
30·0			74·7 s			05·1		
23·6 ss	b_4	R-head	68·1 s			03·8		
20·2			65·7 w			01·0 w		
17·2			64·3 w			46,498·1		
11·8	—	Q-head	60·7 s			96·0		
07·8			53·7 ss	—	R-head	91·7 w		
04·8			49·9			87·8 w		
00·0			43·8	—	Q-head	79·1 s	—	R-head
47,095·8			42·3			76·0		
92·5			40·0			73·7 w		
88·4 s			37·1			71·5 w		
80·7			35·2			68·7		
74·2			33·2			67·5		
69·9			29·0			63·6 w		
64·3			24·2			60·4 ss	e_4	R-head
56·6 s	a_4	R-head	17·3 s			57·4		
45·5	—	Q-head	13·9			54·6 w		
43·3 s			09·8 s			46·6 s	—	Q-head
40·7			02·4 ss	$c_3 + B_5$	R-head	44·6 s		
36·6 s			46,695·7 s			42·9 s		
31·8			89·9			40·7 s		
30·0			85·6 s	—	Q-head	38·8 w		
25·7			83·0			35·9 w		
22·5			79·1			34·0 s		
19·0			77·2 w			30·1 s		
13·1			74·2			27·9 sd		
03·2			68·8 s			24·2 w		
46,993·1			65·4			21·8 w		
72·9			61·8 s			19·0 s		
69·0			57·7			14·4		
65·7			53·8 s			11·7		
60·5			49·4			07·9 w		

TABLE 29.—*Continued.*

Frequency	Assignment Band	Assignment Lines
05·9 w		
02·1 s		
46,397·0 s		
92·4 s		
89·0 w		
83·9 w		
81·6 s		
78·8		
75·9		
73·5		
70·4		
63·9		
57·8		
53·2		
49·9 s	D_4	R-head
47·8		
44·7		
41·2		
36·5		
24·9		
20·2		
17·3		
14·3		
03·3 ss	C_4	R-head
46,299·8 s		
96·1		
92·1		
86·5 s	—	Q1—3
84·1 s	—	Q5
80·7 s	—	Q7
78·1		
75·7 sd	—	Q9, P5
70·6	—	Q11
67·8	—	P7
64·1 s	—	Q13
61·0	—	P9
56·5	—	Q15
53·6		
51·9 w		
50·1 w		
47·4	—	Q17
45·1		
42·5 w		
40·9 w		
37·0 ss		
32·0		
26·6 s		
23·4 w		
21·1 w		
18·2		
16·3		
14·5		
07·1 s	H_5	R-head
06·3 s		
00·7		
46,194·2		
92·0		
86·5 d		
72·6 s		
70·7 s		
68·2 w		
57·3 w		
53·6 w		
49·6 w		
43·3		
37·5		
31·7 ss	b_3	R-head
25·2		
19·0 s	—	Q-head
13·0 d		
11·3		
07·1		
03·3		
00·3		
46,096·3 s		
92·2		
89·4		
87·6		
82·7 d		
78·0		
70·8 ss	$a_3 + E_5$	R-head
67·7		
62·9		
59·3 s	—	Q-head
57·2		
50·5 s		
45·7 s		
43·2 s		
39·8 s		
36·5 w		
33·2 w		
26·4 d		
21·5		
16·7 s		
06·2 s		
45,999·6		
94·3		
91·2		
85·4		
81·0		
73·7		
66·1		
63·9		
54·0		
51·1		
32·2 s		
29·0 s		
23·8		
19·1		
13·5 s		
08·4		
03·2		
45,880·2 ss	f_4	R-head
74·3		
67·8 s	—	Q-head
65·1		
63·1		
60·8		
58·3		
55·7		
52·6		
47·9		
44·4		
41·3		
35·7		
31·6 w		
28·9		
24·3 s	G_4	
21·8 s		
13·1 s		
09·5		
06·7		
02·1 sd		
45,798·5 sd		
96·1		
92·5 s	j_4	R-head
88·1		
85·7		
84·1		
82·0		
79·2		
77·4		
75·0		
72·7		
68·4		
64·3		
59·4		
39·2 ss	B_4	R-head
31·1		
27·9		
25·6 s	—	Q-head
23·2		
19·7		
15·4		
10·4		
04·3		
45,698·5		
91·1 ss	c_2	R-head
85·6		
81·4		
75·7		
70·3 ss	A_4	R-head
65·2		
58·1 s	—	Q-head
56·8 sd		
53·6		
49·5		
45·7 w		
41·7 sd		
34·4 s		
30·4 w		
26·4 s		
21·9 w		
17·2 s		
13·6 w		
06·6 s		
02·9 w		
45,596·2 d		
94·1		
89·1 s	h_3	R-head
84·2		
81·5		
77·4		
75·5 s		
70·6		
68·1		
64·0		
60·8		
57·9 w		
55·5 w		
52·8		
49·2 s		
44·9		
40·4 w		
36·4 sd		
32·7		
30·8		
28·4		
25·2		
23·0 wd		
21·2		
19·6		
13·8 s		
01·3		
45,470·8 ss	e_3	R-head
65·2 s	F_5	
59·9		
55·2 s		
53·2 s		
50·2		

TABLE 29.—*Continued.*

Frequency	Assignment Band	Lines
48·5		
43·5 s		
40·1		
38·2		
34·4		
33·4 wd		
30·6 s		
25·7		
22·2 s		
16·4		
12·9 s		
08·0 w		
06·2 w		
03·3		
45,399·1 d		
92·7 s		
88·8		
81·3 s		
76·9		
72·8		
68·3		
58·6 ss	D_3	R-head
54·9		
50·2 s		
45·9		
41·3		
37·9		
34·0		
28·9		
26·3		
23·1		
17·8 ss	C_3	R15
13·7	—	R5, 7
10·1	—	R3
06·5	—	R1
00·5 s	—	Q1, 3
45,298·3	—	Q5
94·7	—	Q7
90·6	—	Q9
88·6 w	—	P5
85·0	—	Q11
82·3 w	—	P7
78·5	—	Q13
75·2 w	—	P9
71·2	—	Q15
67·5 w	—	P11
62·1	—	Q17
60·1	—	P13
52·2	—	Q19
45·9 w		
41·4 s	—	Q21
35·1 w		
29·9 s	—	Q23
23·5 w		
18·3		
15·1		
12·8 w		
10·0 w		
03·2 ss	H_4	R-head
45,196·4		
94·2 w		
88·3 sd	—	Q-head
87·3 s		
85·0 s		
81·3		
79·3		
76·8		
74·7 s		
71·2 wd		
64·3 wd		
59·9		
17·3 ss	b_2	R-head
13·9		
03·1 s	—	Q-head
00·1		
45,097·7		
93·4 s		
88·5 s		
81·6		
73·4 ss	E_4	R-head
68·9 s		
62·3 s		
57·2 s	a_2	R-head
52·6		
50·7		
47·6		
42·0 s		
36·7		
34·5		
31·5		
28·2		
24·1 s		
19·5		
15·6		
09·2		
05·2		
44,996·3 d		
89·6		
84·0		
78·4 w		
71·9 s		
66·1 w		
59·1		
44,888·2 ss	f_3	R-head
73·7 sd		
71·1		
67·5		
64·3 s		
60·6 d		
56·6		
52·4		
48·4		
27·3 ss	G_3	
22·8 ss	j_3	R-head
14·9 d		
11·7		
07·2 s		
02·7		
44,799·7		
96·8 w		
89·4 ss		
82·7 s		
47·4 ss	B_3	~R8
43·7	—	R3, 4
40·9 w	—	R2
33·9	—	Q3
31·6		
28·2	—	P3
24·6	—	P4
19·1 sd	—	P6
13·4	—	P7, 8
07·1	—	P9
03·2	—	P10
44,699·0		
93·9	—	P12
85·4 ss	A_3	~R8
80·4	—	R2
73·0 ss	—	Q1—3
69·3 s		
65·7 d		
60·0 d		
58·0 d	(c_1)	
56·1 w	—	P7
49·6	—	P8
45·5 w	—	P9
41·2	—	P10
37·5	—	P11
32·6	—	P12
27·5		
21·4 wd		
18·0		
12·5		
10·3		
04·4		
00·0		
44,597·2		
90·6		
86·5 wd		
83·0		
75·4 wd		
67·7 s	h_2	R-head
58·3 w		
54·7 s		
52·4 w		
48·4 w		
39·2 w		
44,494·8 ss	F_4	R-head
80·1 s	—	Q-head
75·8		
70·4		
65·6		
59·3	e_2	R-head
49·8		
43·8 s	—	Q-head
41·6 s		
38·1		
33·1 s		
29·5		
26·2 s		
22·9 w		
19·2 w		
14·6		
10·3 s	J_4?	R-head
06·2		
01·7		
44,396·1		
90·5 d		
85·7 w		
81·6		
43·7 s	D_2	~R10
38·8 w		
05·8 ss	C_2	~R13
04·8	—	R9
01·7	—	R5
44,298·1	—	R3
94·4	—	R1
88·6 s	—	Q1—3
86·3	—	Q5
82·9	—	Q7
78·6	—	Q9
76·6 w	—	P5
73·3 s	—	Q11
70·3 w	—	P7; Q12
66·7 s	—	Q13; P8
63·2	—	P9; Q14
59·4	—	Q15; P10
55·7	—	P11; Q16
50·8	—	Q17; P12
47·2	—	P13
42·9	—	P14

TABLE 29.—*Continued.*

Frequency	Assignment Band	Lines
39·4	—	Q19
34·5 wd		
29·4 sd	—	Q21
24·3 wd		
18·5	—	Q23
13·5 wd		
06·4 ss	H_3	R-head
02·5		
44,195·8		
91·0 s	—	Q-head
87·7 s		
86·0 w		
83·6 s		
81·6 w		
78·8 s		
76·4 ww		
73·4 s		
70·2		
66·6		
57·6 d		
52·6 d		
48·5		
42·7 w		
44,085·4 ss	E_3	R-head
81·3 ss	b_1	R-head
75·2 w		
68·2 s	—	Q-head
66·5		
63·3 d		
60·3		
58·7		
54·9		
52·7		
50·3		
45·6 s		
40·9 w		
36·2 s		
30·8 w		
27·1 s	a_1	R-head
22·8 w		
17·7 s		
15·3		
13·6		
08·6		
06·1		
02·5		
00·0		
43,996·8		
94·9		
88·9 w		
85·3 s		
81·2 wd		
75·9 s		
73·0		
70·1		
65·6 s		
59·1 sd		
53·7		
43,872·9 ss	f_2	R-head
69·3		
60·1 sd	—	Q-head
48·7		
44·6		
41·0		
36·8		
33·5		
28·4		
17·5 s	J_3	R-head
14·2		
05·9		

Frequency	Assignment Band	Lines
00·9 ss	G_2	
43,797·5 ss		
93·2		
90·0		
86·8 d		
80·1		
72·6 s		
31·2 ss	B_2	R10
17·1 s	—	Q2—4
14·8	—	Q5, 6
11·8	—	Q8; P3
08·0 d	—	Q10; P4, 5
02·5 s	—	Q12; P6
43,697·0	—	P7
94·4	—	P8
90·7	—	P9
86·9 s	—	P10
82·8	—	P11
77·4 w	—	P12
74·2 ss	A_2	~R9
68·7	—	R2
60·4 sd	—	Q3—5
57·9	—	Q7; P2
54·1 s	—	Q9; P3
52·6 w	—	P4
49·7	—	Q10; P5
46·5 s	—	P6; Q11
44·7 w	—	P7; Q12
38·2 s	—	P8
34·4	—	P9
30·2 s	—	P10
26·3	—	P11
21·4	—	P12
10·5	—	P14
43,530·7 s		
25·5 ss	h_1	R-head
03·7 ss	F_3	~R8
43,489·8 s	—	Q2, 3
88·1 sd	—	Q4—7
84·6	—	Q8; P3
81·9	—	Q9, 10; P4
79·3	—	Q11
74·6	—	Q6; P12
71·6	—	P7
67·0	—	P8
62·8	—	P9
58·9	—	P10
54·5 d	—	P11
49·8	—	P12
44·7	—	P13
41·4 s	J_3	~R8
34·9 w	—	R1
27·7 ss	e_1	R-head
22·0		
17·2 w		
11·7 s	—	Q-head
05·6 s		
01·2 w		
43,397·2 s		
91·7		
87·7		
83·0 w		
77·9 s		
69·4		
64·6		
58·9		
48·7		
37·3		
09·2 d	D_1	
43,273·9 ss	C_1	~R13

Frequency	Assignment Band	Lines
69·0	—	R5
66·2 w	—	R3
62·2 w	—	R1
56·5 s	—	Q1—3
54·1	—	Q5
50·9 s	—	Q7
46·7	—	Q9
44·4 w	—	P5
41·4	—	Q11
38·3 w	—	P7
35·0	—	Q13
31·4	—	P9
27·6	—	Q15
23·6	—	P11
19·4	—	Q17
15·5	—	P13
12·0 w		
10·0 w	—	Q19
06·7	—	P15
03·8	—	Q21
43,198·1	—	P17
93·8 w		
83·6 ss	H_2	R-head
78·1		
73·8 w		
69·2 s	—	Q-head
67·1		
64·1		
60·3		
58·5		
56·1		
50·7 s		
47·7		
43·2		
29·9		
25·5		
20·4		
11·5 d		
43,073·8 ss	E_2	~R13
69·9	—	R5
67·3	—	R3
63·4	—	R2
56·9 s	—	Q2, 3
55·2		
51·8		
48·8 s	—	Q8
46·9	—	Q9
43·6	—	Q10
41·6	—	P6; Q11
38·5	—	P7; Q12
34·5	—	P8; Q13
31·7 s	—	P9; Q14
27·0	—	P10; Q15
24·3	—	P11; Q15
21·1	—	P12
15·3 s	—	P13
11·4 w		
06·1 s		
01·3 w		
42,995·9 s	b_0	R-head
90·9		
84·9		
73·2 s		
70·6		
67·2		
61·6 d		
55·5		
49·4 sd	a_0	R-head
46·3		
38·1 s		

TABLE 29.—*Continued.*

Frequency	Assignment Band	Lines	Frequency	Assignment Band	Lines	Frequency	Assignment Band	Lines
29·5 s			31·9 s	—	Q1—3	42,398·3 w	—	P7
26·3			30·1 s	—	Q5	95·3	—	P8
20·3			28·3 s	—	P2; Q7	90·1	—	P9
13·4 s			23·8 sd	—	P4; Q9	87·0	—	P10
11·3			19·8	—	Q11	82·8		
09·3			16·0 s	—	P6	77·8	—	P12
05·3			12·1	—	Q13	73·0		
02·6			08·3 s	—	P8	66·5		
42,799·5			04·6	—	Q15	61·4		
93·7			00·4 s	—	P10	54·6		
89·6 w			42,591·2	—	Q19; P12	48·9		
87·0 s			87·3 d			44·0		
80·2 w			80·5	—	Q21	42,225·5 ss	C_0	~R13
74·9			77·1			20·9	—	R5
71·3			69·3	—	Q23	17·5	—	R3
67·4			63·5			07·8 sd	—	Q1—3
61·4	G_1		56·7			02·5 s	—	Q7
56·5			42,488·3 ss	F_2	~R10	42,198·6 s	—	Q9
49·9 w			74·0 s	—	Q2, 3	96·0 w	—	P5
42·4			72·2 s	—	Q4, 5	92·9	—	Q11
32·2 w			68·9	—	Q7	90·2	—	P7
13·5 s			66·5	—	Q9	87·0	—	Q13
08·7 s			63·6	—	Q10	83·4	—	P9
42,679·1 ss	B_1	~R8	58·9	—	P6; Q12	79·1	—	Q15
90·8	—	R2	55·9	—	P7	75·3	—	P11
82·7 sd	—	Q2, 3	51·6	—	P8	71·9 s	—	Q17
80·6 d	—	Q4, 5	47·5 s	—	P9	66·8	—	P13
77·6 d	—	Q7, 8; P3	43·3	—	P10	63·1 d	—	Q19
73·5 s	—	P4; Q10	38·8	—	P11	57·5 s		
68·3	—	P6	31·1 ss	J_2	~R9	43·8 s	H_1	R-head
63·0 s	—	P7	24·2	—	R2	38·5		
60·3 w	—	P8	18·0 s	—	Q1, 3	33·5		
56·8 ss	—	P9	14·8	—	P2; Q7	28·4 s	—	Q-head
52·9	—	P10	11·3	—	P3; Q8	25·4 d		
48·4 w	—	P11	07·0			21·5		
44·5 ss	A_1	~R9	02·3	—	P6	10·8		
39·6	—	R2						

TABLE 30. *Additional frequencies (cm.$^{-1}$) of absorption maxima in acetylene at 200°.*

Frequency	Assignment Band	Lines	Frequency	Assignment Band	Lines	Frequency	Assignment Band	Lines
42,341·2 s	J_2 continuation		35·8 ss	—	R-head	51·2 ss		
37·2			30·7			44·1 ss	H_1	R-head
34·8			25·8			37·6		
28·4			22·3 s			32·3		
27·5			21·0			28·6 s	—	Q-head
25·6			18·6			23·8		
20·5			16·5			20·6		
17·5			14·1			19·4		
12·1			11·1			13·2		
09·1			06·3			08·2		
00·6			04·1			02·7		
42,295·4			42,198·9			42,097·0		
91·8			94·9			91·4		
89·9			90·8			85·8		
86·2			88·1			81·1 d		
81·7			86·2			75·8 w		
70·2 ss	k_1	R-head	82·5			72·8		
65·1 w			71·8 ss	l_1	R-head	66·8		
56·4 w			67·9 w			58·7		
50·8 ss			62·0 w			52·6		
46·3			57·6			42·9 ss	E_1	R-head
42·3			53·9			39·1		

TABLE 30.—*Continued.*

Frequency	Assignment Band	Lines
36·8		
32·6		
26·0 s	—	Q-head
24·2		
20·6		
16·0		
13·4		
11·0		
07·4 s		
04·0		
01·0 d		
41,995·9		
92·9		
91·5		
88·1 w		
84·4 s		
79·6 w		
75·5 s		
71·2		
65·8		
60·7		
55·0 s		
48·9 wd		
42·9		
36·9		
33·0		
28·3 ss	K_2	R-head
24·4		
16·4		
10·0 s	—	Q-head
08·3		
05·1		
03·1		
00·4		
41,897·3		
94·0		
88·2		
83·3		
79·5		
74·5		
70·1		
64·4		
58·5 wd		
53·4 s		
47·2 d		
41·6 s		
38·1		
35·1		
31·0		
28·7		
24·6		
17·7 ss	L_2	~R13
16·1		
08·7	—	R2
01·3	—	Q2, 3
41,799·9	—	Q4
96·6	—	Q6
93·4	—	Q8
91·7	—	P4; Q9
88·1 s	—	P5; Q10
85·5	—	P6; Q11
82·4 s	—	P7; Q12
78·7	—	P8; Q13
75·8	—	P9; Q14
72·0	—	P10; Q15
68·9 s	—	P11; Q16
65·9 s		
59·2		
56·2		
49·5 s		

Frequency	Assignment Band	Lines
44·8 w		
39·2 s		
33·4 w		
26·8 sd		
21·3		
15·5		
08·6		
06·9		
02·3 d		
41,694·5		
91·0		
88·0		
78·4		
70·3 s		
64·3 s		
56·8		
49·7		
46·3		
10·6 ss	B_0	R-head
06·8		
41,596·2 s	—	Q-head
91·8		
87·9		
85·1		
82·8		
80·5		
77·6		
70·4 ss	A_0?	R-head
66·6		
61·1		
56·4		
49·4 s	—	Q-head
46·2		
19·2 s		
13·4		
03·8 s		
41,499·8 s		
91·4		
88·5		
83·8		
79·3		
74·2		
68·4		
63·0		
53·7 ss	F_1	R-head
50·9		
46·4		
40·2 s	—	Q-head
37·9		
34·7		
32·1		
29·2		
24·7		
17·2		
09·7		
01·5 ss	J_1	R-head
41,395·6		
89·4 ss	—	Q-head
87·8		
85·5		
81·3		
77·2		
72·8 s		
68·1		
65·3		
61·6		
52·6		
48·4		
42·6		
36·6		

Frequency	Assignment Band	Lines
31·7		
25·0		
20·8		
14·9		
11·4		
03·8		
41,220·0 ss	M_2	~R10
15·5		
07·7 s	—	Q-head
04·7		
00·9		
41,198·5		
95·1	—	P5; Q10, 11
90·0	—	Q12
88·9	—	P6
83·2	—	P8
75·5	—	P10
69·7	—	P11
63·0 ss	N_2	R-head
59·8		
55·7 w		
50·7 sd	—	Q-head
47·1		
43·6		
39·1		
35·2		
30·5		
26·5		
22·8		
18·7		
13·5		
08·9		
04·4		
41,096·5 s	H_0	R-head
92·1		
88·2		
85·5 s		
40,994·4 s	E_0	R-head
90·3		
77·5 s	—	Q-head
08·6		
40,888·6 ss	K_1	R-head
85·2		
75·8		
71·0 s	—	Q-head
68·7		
65·8		
63·1		
60·3		
40,786·8 s	L_1	R-head
84·1		
70·9 d		
68·1 d		
65·5		
62·5		
60·8		
57·1		
51·5 s		
47·8 w		
44·5		
38·5		
36·0 s		
28·2 s		
18·6		
40,648·3 wd		
40,599·1 wd		
41·2 wd		
37·3 wd		
20·0 wd		

TABLE 31. *Frequencies (cm.$^{-1}$) of absorption maxima of dideuteroacetylene at 20°.*

(The label of each assigned band is placed opposite the frequency of its R-head.)

Frequency	Band	Frequency	Band	Frequency	Band	Frequency	Band	Frequency	Band
47,418·8 s		31·7		47·1		47·3 s	t_4	08·6	
04·1 sd		28·7		43·5		32·9		03·8	
47,375·6 sd		24·3 s		42·8		27·4		01·2	
10·5		22·1		39·1		24·9		45,399·1	
05·1 d		18·6		37·0 w		16·4 ss	B_5	95·1	
47,299·5		14·8 s		34·9		06·7 w		92·0	
93·0 s	q_5	13·2 s		30·7 s		45,896·4 s		88·1 s	
90·4		10·6		28·0		84·9 wd		85·9	
77·9 s		07·2		25·8		76·0 s	A_5	82·9 d	
75·3 s		02·6 s		23·0		71·9 w		72·9 ss	E_5
72·0 w		46,898·9		20·6 s		64·0		64·2	
57·0 s	p_5	91·5		17·2		60·3 s	e_4	60·4	
49·2		89·5		14·1		58·7		57·5 d	
46·6 s		85·6 s	c_4	12·2		56·4		52·6	
44·7		83·8		08·2		51·2		49·1	
39·1		81·7		06·8		29·6		47·3	
36·3 s		79·6		02·1	b_4	26·8		45·1	
31·2		76·9		46,397·2 ss	C_5	20·0 s		41·8	
22·6 s		73·0 s		93·4		45,689·3 dd		33·8 d	j_4
20·3		70·3		91·5		69·9 ss	F_6+q_3	28·8	r_2
08·0		66·8		88·5		62·7 w		26·3	
02·9 s	b_5	62·5		85·9 s		60·9		24·5	
47,195·2		59·9		84·9 s		58·8		45,255·7 wd	a_2
91·3		56·4 s		82·3		54·0 s		45,199·2 s	w_3
88·5		52·6		78·4 s		50·5		61·1	
83·0		45·2 s		75·1 s		48·4		57·8	G_4
78·6 sd	C_6	42·6		72·1		45·6		55·0	
74·7		35·3 sd		69·7		43·6		51·8	
71·9		31·7		65·2 ss	a_4	41·7 w		48·9	
69·6		19·7 w		63·7		35·3 ss	p_3	45·3	
64·5 s	a_5	46,785·4 d		61·4		29·1		42·8 s	
61·8		67·9 w		58·0		25·7		39·7	
59·0		64·9 s		51·5		23·0		37·0	
56·8		57·4		46,274·5 s		21·3		34·4	
55·1		54·9		71·2		19·0 s		30·4 s	t_3
52·2 d		37·8 sd		31·1		15·0		25·0	
47·4		35·8 sd		26·2 s	H_6	11·8		21·3	
43·2		21·7		18·8		10·2		17·3	
39·8		19·5		11·5		08·6		13·0 ss	B_4
32·7 s		09·9		06·4 wd		04·7		02·0 w	
30·0		05·1		46,198·1		02·0		45,095·3 s	
27·2		02·2 s	A_6	95·2 d		45,594·6 sd	C_4	93·7	
47,084·8 sd		46,694·8		92·5 s		89·7 sd	b_3	91·9	
44·2		89·5 w		90·7		87·7		89·1	
28·6 s		71·6		88·1		84·3		87·2	
26·6 s		61·5 ss	e_5	84·6 w		81·7 sd		84·8	
24·9		55·3 d		78·3 s		77·3		74·1 ss	A_4
22·0		45·2		71·6 sd	f_5	73·3		70·7	
17·6 d		42·9		67·9		70·3 w		66·2	
13·0		26·8		54·5 ss	E_6	68·5		62·8	
10·8		15·7		52·6		66·2		59·2	
07·9		05·2		49·7		63·4		50·0 sd	e_3
04·6		46,514·9 w		46·0		55·6 ss	a_3	46·7	
01·5		13·5		43·1		51·7		44·5	
46,999·2		11·8		39·5 s		48·9		41·1	
95·2 s		09·4		33·8		45·7		44,910·4 d	
91·9		07·3		32·0		43·4		44,885·5 s	F_5
89·5		46,488·5 ss	q_4	30·0		39·0 s		65·5 s	
87·7		83·3		27·8		35·4		64·9 s	
85·1		80·0		25·0		29·9		45·4 sd	J_5
71·8 s	r_4	76·7		21·4		25·0		39·4 sd	q_2
69·7		72·4 s		18·9		22·0		38·2	
68·0		70·9 s		46,087·4 s	d_3 ?	18·8 s		34·4	
66·3		68·8		74·4 sd	c_3	02·0 w		29·3 w	
63·2		66·6		68·5 w		45,479·2 d		25·8 d	
60·2		64·3		43·7		69·5		06·4 s	p_2
56·6		61·0		19·6 sd	w_4	58·0 s	H_5	05·1	
52·0 s		60·0		45,997·3		51·8 s		01·3	
46·1 sd		55·3		95·0		37·9 d		44,797·2	
43·6		51·4 ss	p_4	71·3 d	G_5	20·3 s	y_4	94·3	
34·6		49·9		62·0 d		13·7		90·4	

TABLE 31.—*Continued.*

Frequency	Band	Frequency	Band	Frequency	Band	Frequency	Band	Frequency	Band
88·2		85·7		44,366·7 wd		62·1 wd		46·5 d	
80·2 s	C_3	83·2		22·4 wd		43·5 s	J_4	43·4	
77·0		79·9 w		16·0 wd		43,998·0		38·2 s	f_2
75·3		71·3 ss	E_4	01·2 s	t_2	66·7 w		06·1 wd	j_2
69·8 sd	b_2	59·0		44,296·7 ss	B_3	56·4	C_2	43,610·4 w	
37·0 s	a_2	57·9		81·1 s		43,846·9 wd		43,535·0 w	
34·1		53·9 d		60·2 ss	A_3	28·1 s	H_3	43,471·3 s	B_2
44,661·8 dd		50·6 d		57·2		08·6 s	u_2	60·8 d	
46·3 s	H_4	48·0		52·5 w		43,781·6 d		37·2 s	A_2
39·2 s	u_3	43·2 s		49·5 w		75·5 d	y_2	33·8	
21·8 wd		39·3		31·8 d	e_2	71·7 d		43,373·6	
04·1 sd	y_3	36·8		44,194·9 w		68·3		43,284·0 wd	
44,598·7		31·4		63·7		65·5 w		66·1 s	F_3
96·3		24·3 s	j_3	44,094·6 w		56·7 ss	E_3	48·9	
93·1 w		44,416·0 wd		82·1 s	F_4	54·9		29·9 s	J_3
89·7									

TABLE 32. *Additional frequencies (cm.$^{-1}$) of absorption maxima in dideuteroacetylene at 200°.*

(The label of each assigned band is placed opposite the frequency of its R-head.)

Frequency	Band	Frequency	Band	Frequency	Band	Frequency	Band	Frequency	Band
43,196·6 wd		06·2 d		42,888·7 d		34·0		42,439·8 ss	F_2
77·1 wd		42,993·3		66·0		20·3 ss		24·8 s	
54·4 wd		90·6		19·2 d		12·1		06·0 s	J_2
15·0 wd		66·7 s		42,791·6 s		06·9		03·3	
43,087·2 d		55·8 s		69·2		03·2		42,398·5	
43·0 s		44·2 wd		56·5		42,564·7 wd		57·6	
24·6		32·7 ssd	E_2	44·5		41·0		32·6	

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