3.2.1.2.1 C_2H

Microwave data for $^{12}C^{12}C^{1}H$

Transition rotational N′ – N″	fine J′ – J″	hyperfine [a]) F′ – F″	ν [MHz]	Ref.
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (0,0,0)				
1 ← 0	$1\frac{1}{2} \leftarrow \frac{1}{2}$	1 ← 1	87 284.156(30) [b])	83Go
		2 ← 1	87 316.925(4)	
		1 ← 0	87 328.624(6)	
	$\frac{1}{2} \leftarrow \frac{1}{2}$	1 ← 1	87 402.004(5)	
		0 ← 1	87 407.165(11)	
		1 ← 0	87 446.512(23)	
2 ← 1	$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	3 ← 2	174 663.222(8)	
		2 ← 1	174 667.685(17)	
	$1\frac{1}{2} \leftarrow \frac{1}{2}$	2 ← 1	174 721.777(26)	
		1 ← 0	174 728.074(30)	
3 ← 2	$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	4 ← 3	262 004.260(50)	81Sa
		3 ← 2	262 006.482(50)	
	$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	3 ← 2	262 064.986(50)	
		2 ← 1	262 067.469(50)	
7 ← 6	$7\frac{1}{2} \leftarrow 6\frac{1}{2}$	[c])	611 267.201(80)	00Mü
	$6\frac{1}{2} \leftarrow 5\frac{1}{2}$	[c])	611 329.708(80)	
8 ← 7	$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	[c])	698 544.778(150)	
	$7\frac{1}{2} \leftarrow 6\frac{1}{2}$	[c])	698 607.457(100)	
9 ← 8	$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	[c])	785 802.090(120)	
	$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	[c])	785 864.969(120)	
10 ← 9	$10\frac{1}{2} \leftarrow 9\frac{1}{2}$	[c])	873 036.391(80)	
	$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	[c])	873 099.537(150)	
11 ← 10	$11\frac{1}{2} \leftarrow 10\frac{1}{2}$	[c])	960 245.718(120)	
	$10\frac{1}{2} \leftarrow 9\frac{1}{2}$	[c])	960 308.867(120)	

[a]) Coupling scheme: $\boldsymbol{J} = \boldsymbol{N} + \boldsymbol{S}$; $\boldsymbol{F} = \boldsymbol{J} + \boldsymbol{I}$ where $\boldsymbol{I}$ is the ^{1}H nuclear spin
[b]) The figures in parentheses are the authors' estimates of experimental uncertainty, in units of the last quoted decimal place.
[c]) Proton hyperfine structure not resolved.

Molecular parameters for $^{12}C^{12}C^{1}H$

Parameter [a])		Value	Method	Ref.
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (0,0,0)				
B	[MHz]	43 674.528 94(115) [b])	MW	00Mü
D	[MHz]	0.105 687(51)		
H	[Hz]	0.32(32)		
γ	[MHz]	– 62.602 9(43)		
γ_D	[kHz]	– 2.313(255)		
$b_F(^1H)$	[MHz]	44.492 2(183)		
$b_F^D(^1H)$	[MHz]	– 0.011 0(38)		
$c(^1H)$	[MHz]	12.225 6(261)		

[a]) The parameter values in this table supersede those of Gottlieb *et al*. [83 Go], given in L-B II/12 D.
[b]) The numbers in parentheses are 1 standard deviation of the least-squares fit, in units of the last quoted decimal place.

Microwave data for $^{13}C^{12}C^{1}H$

Transition				ν	Ref.
rotational $N'-N''$	fine $J'-J''$	hyperfine [a]) $F_1'-F_1''$	$F'-F''$	[MHz]	
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (0,0,0)					
$1 \leftarrow 0$	$1\frac{1}{2} \leftarrow \frac{1}{2}$	$2 \leftarrow 1$	$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	84 119.33 (01) [b])	95McC
			$1\frac{1}{2} \leftarrow \frac{1}{2}$	84 124.11 (01)	
		$1 \leftarrow 0$	$\frac{1}{2} \leftarrow \frac{1}{2}$	84 151.33 (01)	
			$1\frac{1}{2} \leftarrow \frac{1}{2}$	84 153.30 (01)	
	$\frac{1}{2} \leftarrow \frac{1}{2}$	$0 \leftarrow 1$	$\frac{1}{2} \leftarrow \frac{1}{2}$	84 184.02 (02)	
		$1 \leftarrow 1$	$\frac{1}{2} \leftarrow 1\frac{1}{2}$	84 192.53 (03)	
			$1\frac{1}{2} \leftarrow 1\frac{1}{2}$	84 206.86 (02)	
$2 \leftarrow 1$	$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	$3 \leftarrow 2$	$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	168 274.45 (01)	
			$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	168 276.58 (01)	
	$1\frac{1}{2} \leftarrow \frac{1}{2}$	$2 \leftarrow 1$	$1\frac{1}{2} \leftarrow \frac{1}{2}$	168 300.48 (03)	
	$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	$2 \leftarrow 1$	$1\frac{1}{2} \leftarrow \frac{1}{2}$	168 302.33 (01)	
			$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	168 303.60 (01)	
	$1\frac{1}{2} \leftarrow \frac{1}{2}$	$2 \leftarrow 1$	$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	168 307.68 (01)	
		$1 \leftarrow 1$	$1\frac{1}{2} \leftarrow 1\frac{1}{2}$	168 317.47 (02)	
			$1\frac{1}{2} \leftarrow \frac{1}{2}$	168 331.80 (03)	
			$\frac{1}{2} \leftarrow \frac{1}{2}$	168 333.00 (02)	
		$2 \leftarrow 0$	$1\frac{1}{2} \leftarrow \frac{1}{2}$	168 341.88 (02)	
		$1 \leftarrow 0$	$1\frac{1}{2} \leftarrow \frac{1}{2}$	168 373.20 (03)	
	$1\frac{1}{2} \leftarrow 1\frac{1}{2}$	$2 \leftarrow 2$	$2\frac{1}{2} \leftarrow 2\frac{1}{2}$	168 395.22 (02)	
			$1\frac{1}{2} \leftarrow 1\frac{1}{2}$	168 401.80 (02)	
$3 \leftarrow 2$	$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	$4 \leftarrow 3$	$4\frac{1}{2} \leftarrow 3\frac{1}{2}$	252 422.90 (01)	
			$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	252 424.12 (01)	
		$3 \leftarrow 2$	$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	252 447.99 (01)	
			$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	252 449.23 (01)	
	$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	$3 \leftarrow 2$	$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	252 457.90 (01)	
			$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	252 468.77 (01)	
		$2 \leftarrow 1$	$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	252 480.97 (01)	
			$1\frac{1}{2} \leftarrow \frac{1}{2}$	252 489.38 (01)	
			$1\frac{1}{2} \leftarrow 1\frac{1}{2}$	252 490.58 (02)	
		$2 \leftarrow 2$	$2\frac{1}{2} \leftarrow 2\frac{1}{2}$	252 490.76 (02)	
$4 \leftarrow 3$	$4\frac{1}{2} \leftarrow 3\frac{1}{2}$	$5 \leftarrow 4$	$5\frac{1}{2} \leftarrow 4\frac{1}{2}$	336 563.75 (01)	
			$4\frac{1}{2} \leftarrow 3\frac{1}{2}$	336 564.54 (01)	
		$4 \leftarrow 3$	$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	336 586.66 (02)	
			$4\frac{1}{2} \leftarrow 3\frac{1}{2}$	336 587.85 (01)	
	$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	$4 \leftarrow 3$	$4\frac{1}{2} \leftarrow 3\frac{1}{2}$	336 600.51 (01)	
			$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	336 605.89 (02)	
		$3 \leftarrow 2$	$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	336 623.43 (01)	
			$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	336 626.83 (01)	

[a]) Coupling scheme: $\boldsymbol{J} = \boldsymbol{N} + \boldsymbol{S}$; $\boldsymbol{F}_1 = \boldsymbol{J} + \boldsymbol{I}_1$; $\boldsymbol{F} = \boldsymbol{F}_1 + \boldsymbol{I}_2$ where $\boldsymbol{I}_1$ is the ^{13}C nuclear spin and $\boldsymbol{I}_2$ is the ^{1}H nuclear spin
[b]) The figures in parentheses are the authors' estimates of experimental uncertainty, in units of the last quoted decimal place.

Molecular parameters for $^{13}C^{12}C^{1}H$

Parameter [a])		Value	Method	Ref.
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (0,0,0)				
B	[MHz]	42 077.462(1) [b])	MW	95McC
D	[MHz]	0.098 13(4)		
γ	[MHz]	– 60.080(6)		
$b_F(^{13}C)$	[MHz]	900.7(6)		
$c(^{13}C)$	[MHz]	142.87(3)		
$b_F(^{1}H)$	[MHz]	44.42(3)		
$c(^{1}H)$	[MHz]	12.17(5)		

[a]) The parameter values in this table supersede those of Bogey *et al*. [89 Bo], given in L-B II/19 D.
[b]) The numbers in parentheses are 1 standard deviation of the least-squares fit, in units of the last quoted decimal place.

Microwave data for $^{12}C^{13}C^{1}H$

Transition rotational $N'-N''$	fine $J'-J''$	hyperfine [a]) $F_1'-F_1''$	$F'-F''$	ν [MHz]	Ref.
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (0,0,0)					
1 ← 0	$1\frac{1}{2} \leftarrow \frac{1}{2}$	2 ← 1	$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	85 229.27 (01) [b])	95McC
			$1\frac{1}{2} \leftarrow \frac{1}{2}$	85 232.76 (01)	
		1 ← 0	$\frac{1}{2} \leftarrow \frac{1}{2}$	85 247.65 (01)	
			$1\frac{1}{2} \leftarrow \frac{1}{2}$	85 256.96 (01)	
	$\frac{1}{2} \leftarrow \frac{1}{2}$	1 ← 1	$\frac{1}{2} \leftarrow 1\frac{1}{2}$	85 303.98 (03)	
			$1\frac{1}{2} \leftarrow 1\frac{1}{2}$	85 307.59 (02)	
		0 ← 1	$\frac{1}{2} \leftarrow \frac{1}{2}$	85 314.28 (02)	
2 ← 1	$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	3 ← 2	$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	170 490.65 (01)	
			$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	170 492.38 (01)	
		2 ← 1	$1\frac{1}{2} \leftarrow 1\frac{1}{2}$	170 495.70 (02)	
			$1\frac{1}{2} \leftarrow \frac{1}{2}$	170 505.01 (01)	
			$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	170 509.26 (01)	
	$1\frac{1}{2} \leftarrow \frac{1}{2}$	2 ← 1	$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	170 533.57 (01)	
		1 ← 1	$1\frac{1}{2} \leftarrow 1\frac{1}{2}$	170 550.16 (02)	
		2 ← 0	$1\frac{1}{2} \leftarrow \frac{1}{2}$	170 551.37 (02)	
			$1\frac{1}{2} \leftarrow \frac{1}{2}$	170 553.77 (03)	
		1 ← 0	$\frac{1}{2} \leftarrow \frac{1}{2}$	170 559.49 (02)	
			$1\frac{1}{2} \leftarrow \frac{1}{2}$	170 574.38 (03)	
	$1\frac{1}{2} \leftarrow 1\frac{1}{2}$	2 ← 2	$2\frac{1}{2} \leftarrow 2\frac{1}{2}$	170 611.89 (03)	
3 ← 2	$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	4 ← 3	$4\frac{1}{2} \leftarrow 3\frac{1}{2}$	255 746.18 (01)	
			$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	255 747.23 (01)	
		3 ← 2	$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	255 756.00 (01)	
			$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	255 758.75 (01)	
	$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	3 ← 2	$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	255 794.85 (01)	
			$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	255 803.66 (01)	
		2 ← 1	$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	255 805.41 (01)	
			$1\frac{1}{2} \leftarrow \frac{1}{2}$	255 810.42 (01)	
		2 ← 2	$2\frac{1}{2} \leftarrow 2\frac{1}{2}$	255 822.00 (03)	
4 ← 3	$4\frac{1}{2} \leftarrow 3\frac{1}{2}$	5 ← 4	$5\frac{1}{2} \leftarrow 4\frac{1}{2}$	340 994.13 (02)	
			$4\frac{1}{2} \leftarrow 3\frac{1}{2}$	340 994.85 (02)	

	$4 \leftarrow 3$	$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	341 001.11 (01)
		$4\frac{1}{2} \leftarrow 3\frac{1}{2}$	341 002.80 (02)
$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	$4 \leftarrow 3$	$4\frac{1}{2} \leftarrow 3\frac{1}{2}$	341 046.60 (02)
		$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	341 051.65 (02)
	$3 \leftarrow 2$	$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	341 054.05 (02)
		$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	341 056.69 (01)
		$2\frac{1}{2} \leftarrow 2\frac{1}{2}$	341 067.42 (02)
	$3 \leftarrow 3$	$3\frac{1}{2} \leftarrow 3\frac{1}{2}$	341 081.20 (03)

a) Coupling scheme: $\boldsymbol{J} = \boldsymbol{N} + \boldsymbol{S}$; $\boldsymbol{F}_1 = \boldsymbol{J} + \boldsymbol{I}_1$; $\boldsymbol{F} = \boldsymbol{F}_1 + \boldsymbol{I}_2$ where $\boldsymbol{I}_1$ is the ^{13}C nuclear spin and $\boldsymbol{I}_2$ is the ^{1}H nuclear spin
b) The figures in parentheses are the authors' estimates of experimental uncertainty, in units of the last quoted decimal place.

Molecular parameters for $^{12}C^{13}C^{1}H$

Parameter a)		Value	Method	Ref.
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (0,0,0)				
B	[MHz]	42 631.383(1) b)	MW	95McC
D	[MHz]	0.101 57(6)		
γ	[MHz]	– 61.073(8)		
$b_F(^{13}C)$	[MHz]	161.63(10)		
$c(^{13}C)$	[MHz]	64.07(5)		
$b_F(^{1}H)$	[MHz]	44.75(4)		
$c(^{1}H)$	[MHz]	12.64(5)		

a) The parameter values in this table supersede those of Bogey *et al*. [89 Bo], given in L-B II/19 D.
b) The numbers in parentheses are 1 standard deviation of the least-squares fit, in units of the last quoted decimal place.

References for C_2H

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3.2.1.2.2 C_3H

Microwave data for $^{13}C^{12}C^{12}C^{1}H$

Transition				ν	Ref.
spin Ω	rotational $J' - J''$	parity e/f a)	hyperfine $F' - F''$	[MHz]	
State: electronic $\tilde{X}\,^2\Pi$; vibrational zero point level					
$\frac{1}{2}$	$7\frac{1}{2} \leftarrow 6\frac{1}{2}$	e	$7 \leftarrow 6$	157 303.599	96Ka
			$8 \leftarrow 7$	157 304.894	
		f	b)	157 398.453	
$\frac{3}{2}$	$7\frac{1}{2} \leftarrow 6\frac{1}{2}$	e	$7 \leftarrow 6$	165 289.276	
			$8 \leftarrow 7$	165 285.918	
		f	$7 \leftarrow 6$	165 166.959	
			$8 \leftarrow 7$	165 164.689	
$\frac{1}{2}$	$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	e	$8 \leftarrow 7$	178 347.867	
			$9 \leftarrow 8$	178 349.342	
			b)	178 475.179	
$\frac{3}{2}$	$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	e	$8 \leftarrow 7$	187 247.799	
			$9 \leftarrow 8$	187 247.799	
		f	$8 \leftarrow 7$	187 096.224	

			9 ← 8	187 094.389
$\frac{1}{2}$	$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	*e*	9 ← 8	199 415.626
			10 ← 9	199 417.082
		f	[b])	199 577.221
$\frac{3}{2}$	$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	*e*	9 ← 8	209 180.529
			10 ← 9	209 177.820
		f	9 ← 8	208 998.460
			10 ← 9	208 996.950
$\frac{1}{2}$	$10\frac{1}{2} \leftarrow 9\frac{1}{2}$	*e*	10 ← 9	220 506.956
			11 ← 10	220 508.385
		f	[b])	220 704.234
$\frac{3}{2}$	$10\frac{1}{2} \leftarrow 9\frac{1}{2}$	*e*	10 ← 9	231 086.635
			11 ← 10	231 084.165
		f	10 ← 9	230 873.544
			11 ← 10	230 872.297
$\frac{1}{2}$	$11\frac{1}{2} \leftarrow 10\frac{1}{2}$	*e*	11 ← 10	241 621.888
			12 ← 11	214 623.321
		f	[b])	241 856.027
$\frac{3}{2}$	$11\frac{1}{2} \leftarrow 10\frac{1}{2}$	*e*	11 ← 10	252 965.859
			12 ← 11	252 963.571
		f	11 ← 10	252 721.752
			12 ← 11	252 720.698
$\frac{1}{2}$	$12\frac{1}{2} \leftarrow 11\frac{1}{2}$	*e*	12 ← 11	262 761.311
			13 ← 12	262 759.907
		f	[b])	263 031.596
$\frac{3}{2}$	$12\frac{1}{2} \leftarrow 11\frac{1}{2}$	*e*	12 ← 11	274 815.901
			13 ← 12	274 818.088
		f	12 ← 11	274 542.723
			13 ← 12	274 543.564
$\frac{1}{2}$	$13\frac{1}{2} \leftarrow 12\frac{1}{2}$	*e*	13 ← 12	283 920.136
			14 ← 13	283 921.498
		f	[b])	284 229.914
$\frac{3}{2}$	$13\frac{1}{2} \leftarrow 12\frac{1}{2}$	*e*	13 ← 12	296 643.401
			14 ← 13	296 641.433
		f	13 ← 12	296 339.924
			14 ← 13	296 339.237
$\frac{1}{2}$	$14\frac{1}{2} \leftarrow 13\frac{1}{2}$	*e*	14 ← 13	305 101.608
			15 ← 14	305 103.014
		f	[b])	305 449.677
$\frac{3}{2}$	$14\frac{1}{2} \leftarrow 13\frac{1}{2}$	*e*	14 ← 13	318 442.105
			15 ← 14	318 440.262
		f	14 ← 13	318 111.607
			15 ← 14	326 303.160

[a]) States with parity equal to ± $(-1)^{J-0.5}$ are labeled *e* and *f* respectively.
[b]) ^{13}C hyperfine structure not resolved.

Microwave data for $^{13}C^{12}C^{12}C^{1}H$

Transition		ν [MHz]	Ref.
rotational $N' - N''$	fine structure $J' - J''$ [a])		
State: electronic $\tilde{X}\,^2\Pi$; vibrational v_4 = 1, lower vibronic component ($\mu^2\Sigma$)			
11 ← 10	$11\frac{1}{2} \leftarrow 10\frac{1}{2}$	237 224.824	96Ka
	$10\frac{1}{2} \leftarrow 9\frac{1}{2}$	237 229.347	
12 ← 11	$12\frac{1}{2} \leftarrow 11\frac{1}{2}$	258 791.080	
	$11\frac{1}{2} \leftarrow 10\frac{1}{2}$	258 788.472	
13 ← 12	$13\frac{1}{2} \leftarrow 12\frac{1}{2}$	280 357.800	
	$12\frac{1}{2} \leftarrow 11\frac{1}{2}$	280 346.155	
14 ← 13	$14\frac{1}{2} \leftarrow 13\frac{1}{2}$	301 925.346	
	$13\frac{1}{2} \leftarrow 12\frac{1}{2}$	301 902.272	
15 ← 14	$15\frac{1}{2} \leftarrow 14\frac{1}{2}$	323 494.612	
	$14\frac{1}{2} \leftarrow 13\frac{1}{2}$	323 456.715	

[a]) ^{13}C hyperfine structure not resolved.

Molecular parameters for $^{13}C^{12}C^{12}C^{1}H$

Parameter		Value	Method	Ref.
State: electronic $\tilde{X}\,^2\Pi$; vibrational zero point level				
B	[MHz]	10 755.824(31) [a])	MW	96Ka
D	[kHz]	4.783 8(56)		
A	[MHz]	432 416(21)		
γ	[MHz]	– 51.61(51)		
p	[MHz]	– 6.870(102)		
q	[MHz]	– 11.902(52)		
$a(^{13}C)$	[MHz]	63.0(59)		
$b(^{13}C)$	[MHz]	62.0(47)		
$c(^{13}C)$	[MHz]	– 81(24)		
$d^{13}C)$	[MHz]	125.9(53)		
$c(^{1}H)$	[MHz]	12.17(5)		
State: electronic $\tilde{X}\,^2\Pi$; vibrational v_4 = 1, lower vibronic component ($\mu^2\Sigma$)				
B	[MHz]	10 778.585(65)	MW	96Ka
D	[kHz]	4.641 7(187)		
γ	[MHz]	-34.57(31)		
γ_D	[kHz]	0.54(62)		
$b(^{13}C)$	[MHz]	62.0 [b])		
$c(^{13}C)$	[MHz]	– 81 [b])		
ΔE [c])	[GHz]	608.280(1320)		
β [d])	[MHz]	– 1 203.1(87)		

[a]) The numbers in parentheses are 3 standard deviation of the least-squares fit, in units of the last quoted decimal place.
[b]) Constrained to the corresponding value for the zero-point vibrational level.
[c]) The energy difference between the vibrational ground state and the v_4 = 1, $\mu^2\Sigma$ vibronic state.
[d]) Interaction parameter linking the vibrational ground state and the v_4 = 1, $\mu^2\Sigma$ vibronic state.

Microwave data for $^{12}C^{13}C^{12}C^{1}H$

Transition spin Ω	rotational $J' - J''$	parity e/f [a])	Hyperfine [b]) $F_1' - F_1''$	$F' - F''$	ν [MHz]	Ref.
State: electronic $\tilde{X}\,^2\Pi$; vibrational zero point level						
$\frac{1}{2}$	$7\frac{1}{2} \leftarrow 6\frac{1}{2}$	e	$7 \leftarrow 6$	[c])	163 468.621	96Ka
			$8 \leftarrow 7$		163 466.730	
		f	$7 \leftarrow 6$	$6\frac{1}{2} \leftarrow 5\frac{1}{2}$	163 574.845	
				$7\frac{1}{2} \leftarrow 6\frac{1}{2}$	163 574.158	
			$8 \leftarrow 7$	$7\frac{1}{2} \leftarrow 6\frac{1}{2}$	163 573.519	
				$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	163 572.844	
$\frac{3}{2}$	$7\frac{1}{2} \leftarrow 6\frac{1}{2}$	f	$7 \leftarrow 6$	[c])	172 078.259	
			$8 \leftarrow 7$		172 079.573	
$\frac{1}{2}$	$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	e	$8 \leftarrow 7$		185 346.347	
			$9 \leftarrow 8$		185 344.994	
		f	$8 \leftarrow 7$	$7\frac{1}{2} \leftarrow 6\frac{1}{2}$	185 488.688	
				$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	185 488.052	
			$9 \leftarrow 8$	$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	185 487.416	
				$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	185 486.805	
$\frac{3}{2}$	$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	e	$8 \leftarrow 7$	[c])	194 929.692	
			$9 \leftarrow 8$		194 931.039	
		f	$8 \leftarrow 7$		194 761.946	
			$9 \leftarrow 8$		194 763.213	
$\frac{1}{2}$	$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	e	$9 \leftarrow 8$		207 250.971	
			$10 \leftarrow 9$		207 249.704	
$\frac{3}{2}$	$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	e	$9 \leftarrow 8$		217 751.710	
			$10 \leftarrow 9$		217 752.974	
		f	$9 \leftarrow 8$		217 550.778	
			$10 \leftarrow 9$		217 551.954	
$\frac{1}{2}$	$10\frac{1}{2} \leftarrow 9\frac{1}{2}$	e	$10 \leftarrow 9$		229 182.497	
			$11 \leftarrow 10$		229 181.308	
$\frac{3}{2}$	$10\frac{1}{2} \leftarrow 9\frac{1}{2}$	e	$10 \leftarrow 9$		240 543.533	
			$11 \leftarrow 10$		240 544.683	
		f	$10 \leftarrow 9$		240 309.003	
			$11 \leftarrow 10$		240 310.087	
$\frac{1}{2}$	$11\frac{1}{2} \leftarrow 10\frac{1}{2}$	e	$11 \leftarrow 10$		251 140.588	
			$12 \leftarrow 11$		251 139.502	
$\frac{3}{2}$	$11\frac{1}{2} \leftarrow 10\frac{1}{2}$	e	$11 \leftarrow 10$		263 304.848	
			$12 \leftarrow 11$		263 305.975	
		f	$11 \leftarrow 10$		263 037.178	
			$12 \leftarrow 11$		263 038.210	
$\frac{1}{2}$	$12\frac{1}{2} \leftarrow 11\frac{1}{2}$	e	$12 \leftarrow 11$		273 124.498	
			$13 \leftarrow 12$		273 124.498	
$\frac{3}{2}$	$12\frac{1}{2} \leftarrow 11\frac{1}{2}$	e	$12 \leftarrow 11$		286 035.820	
			$13 \leftarrow 12$		286 036.842	
		f	$12 \leftarrow 11$		285 736.147	
			$13 \leftarrow 12$		285 737.124	
$\frac{1}{2}$	$13\frac{1}{2} \leftarrow 12\frac{1}{2}$	e	$13 \leftarrow 12$		295 133.094	

			14 ← 13	295 132.185
$\frac{3}{2}$	$13\frac{1}{2} \leftarrow 12\frac{1}{2}$	*e*	[d])	308 737.116
		f	[d])	308 407.556
$\frac{1}{2}$	$14\frac{1}{2} \leftarrow 13\frac{1}{2}$	*e*	[d])	317 164.673
		f	[d])	317 548.336

[a]) States with parity equal to $\pm(-1)^{J-0.5}$ are labeled *e* and *f* respectively.
[b]) Coupling scheme: $\boldsymbol{F}_1 = \boldsymbol{J} + \boldsymbol{I}_1$; $\boldsymbol{F} = \boldsymbol{F}_1 + \boldsymbol{I}_2$ where $\boldsymbol{I}_1$ is the ^{13}C nuclear spin and $\boldsymbol{I}_2$ is the ^{1}H nuclear spin
[c]) ^{1}H hyperfine structure not resolved.
[d]) ^{13}C hyperfine structure not resolved.

Transition		ν	Ref.
rotational $N' - N''$	fine structure $J' - J''$ [a])	[MHz]	
State: electronic $\tilde{X}\,^2\Pi$; vibrational $v_4 = 1$, lower vibronic component ($\mu^2\Sigma$)			
10 ← 9	$10\frac{1}{2} \leftarrow 9\frac{1}{2}$	224 320.486	96Ka
	$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	224 328.482	
11 ← 10	$11\frac{1}{2} \leftarrow 10\frac{1}{2}$	246 753.498	
	$10\frac{1}{2} \leftarrow 9\frac{1}{2}$	246 754.468	
12 ← 11	$12\frac{1}{2} \leftarrow 11\frac{1}{2}$	269 186.980	
	$11\frac{1}{2} \leftarrow 10\frac{1}{2}$	269 178.975	
13 ← 12	$13\frac{1}{2} \leftarrow 12\frac{1}{2}$	291 621.391	
	$12\frac{1}{2} \leftarrow 11\frac{1}{2}$	291 601.937	

[a]) ^{13}C hyperfine structure not resolved.

Molecular parameters for $^{12}C^{13}C^{12}C^{1}H$

Parameter		Value	Method	Ref.
State: electronic $\tilde{X}\,^2\Pi$; vibrational zero point level				
B	[MHz]	11 187.908(42) [a])	MW	96Ka
D	[kHz]	5.114 8(85)		
A	[MHz]	432 273(27)		
γ	[MHz]	– 50.95(72)		
p	[MHz]	– 7.474(121)		
q	[MHz]	– 12.835(66)		
$a(^{13}C)$	[MHz]	– 5.0(59)		
$b(^{13}C)$	[MHz]	– 68.3(56)		
$c(^{13}C)$	[MHz]	88(28)		
$d^{13}C)$	[MHz]	0.0 [b])		
$a(^1H)$	[MHz]	16.2(80)		
$b(^1H)$	[MHz]	– 22.54 [b])		
$c(^1H)$	[MHz]	27.49 [b])		
$d(^1H)$	[MHz]	16.241 [b])		
State: electronic $\tilde{X}\,^2\Pi$; vibrational $v_4 = 1$, lower vibronic component ($\mu^2\Sigma$)				
B	[MHz]	11 211.147(85)	MW	96Ka
D	[kHz]	4.976 (23)		
γ	[MHz]	– 35.960 (199)		
$b(^{13}C)$	[MHz]	– 68.3 [b])		
$c(^{13}C)$	[MHz]	88 [b])		
ΔE[c])	[GHz]	605.070(1450)		
β[d])	[MHz]	– 1 253.4(107)		

[a]) The numbers in parentheses are 3 standard deviation of the least-squares fit, in units of the last quoted decimal place.
[b]) Constrained to this value.
[c]) The energy difference between the vibrational ground state and the $v_4 = 1$, $\mu^2\Sigma$ vibronic state.
[d]) Interaction parameter linking the vibrational ground state and the $v_4 = 1$, $\mu^2\Sigma$ vibronic state.

Microwave data for $^{12}C^{12}C^{13}C^{1}H$

Transition						
Spin Ω	rotational $J' - J''$	parity e/f [a])	hyperfine $F' - F''$		ν [MHz]	Ref.
State: electronic $\tilde{X}\,^2\Pi$; vibrational zero point level						
$\frac{1}{2}$	$7\frac{1}{2} \leftarrow 6\frac{1}{2}$	f	$7 \leftarrow 6$	$6\frac{1}{2} \leftarrow 5\frac{1}{2}$	158 632.043	96Ka
				$7\frac{1}{2} \leftarrow 6\frac{1}{2}$	158 631.400	
			$8 \leftarrow 7$	$7\frac{1}{2} \leftarrow 6\frac{1}{2}$	158 634.513	
				$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	158 633.838	
$\frac{3}{2}$	$7\frac{1}{2} \leftarrow 6\frac{1}{2}$	e	$7 \leftarrow 6$	[c])	166 658.032	
			$8 \leftarrow 7$		166 652.519	
		f	$7 \leftarrow 6$		166 531.019	
			$8 \leftarrow 7$		166 526.367	
$\frac{1}{2}$	$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	f	$8 \leftarrow 7$	$7\frac{1}{2} \leftarrow 6\frac{1}{2}$	179 876.839	
				$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	179 876.235	
			$9 \leftarrow 8$	$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	179 879.122	
				$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	179 878.520	
$\frac{3}{2}$	$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	e	$8 \leftarrow 7$	[c])	188 795.840	
			$9 \leftarrow 8$		188 790.946	
		f	$8 \leftarrow 7$		188 638.568	
			$9 \leftarrow 8$		188 634.633	
$\frac{1}{2}$	$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	f	$9 \leftarrow 8$	$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	201 147.684	
			$10 \leftarrow 9$	$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	201 147.110	
			$9 \leftarrow 8$	$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	201 149.752	
			$10 \leftarrow 9$	$10\frac{1}{2} \leftarrow 9\frac{1}{2}$	201 149.155	
$\frac{3}{2}$	$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	e	$9 \leftarrow 8$	[c])	210 906.984	
			$10 \leftarrow 9$		210 902.572	
		f	$9 \leftarrow 8$		210 718.490	
			$10 \leftarrow 9$		210 715.018	
$\frac{1}{2}$	$10\frac{1}{2} \leftarrow 9\frac{1}{2}$	e	$10 \leftarrow 9$		222 238.453	
			$11 \leftarrow 10$		222 241.288	
		f	$10 \leftarrow 9$	$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	222 444.340	
				$10\frac{1}{2} \leftarrow 9\frac{1}{2}$	222 443.828	
			$11 \leftarrow 10$	$10\frac{1}{2} \leftarrow 9\frac{1}{2}$	222 446.284	
				$11\frac{1}{2} \leftarrow 10\frac{1}{2}$	222 445.747	
$\frac{3}{2}$	$10\frac{1}{2} \leftarrow 9\frac{1}{2}$	e	$10 \leftarrow 9$		232 990.568	
			$11 \leftarrow 10$		232 986.593	
		f	$10 \leftarrow 9$		232 770.442	
			$11 \leftarrow 10$		232 767.392	
$\frac{1}{2}$	$11\frac{1}{2} \leftarrow 10\frac{1}{2}$	e	$11 \leftarrow 10$		243 522.082	
			$12 \leftarrow 11$		243 524.828	
		f	$11 \leftarrow 10$		243 766.067	
			$12 \leftarrow 11$		243 767.881	
$\frac{3}{2}$	$11\frac{1}{2} \leftarrow 10\frac{1}{2}$	f	$11 \leftarrow 10$		254 794.816	
			$12 \leftarrow 11$		254 792.094	
$\frac{1}{2}$	$12\frac{1}{2} \leftarrow 11\frac{1}{2}$	e	$11 \leftarrow 10$		264 829.413	
			$12 \leftarrow 11$		264 832.022	
		f	$11 \leftarrow 10$		265 112.665	

			12 ← 11	265 114.302
$\frac{3}{2}$	$12\frac{1}{2} \leftarrow 11\frac{1}{2}$	*e*	12 ← 11	277 074.093
			13 ← 12	277 070.720
		f	12 ← 11	276 792.238
			13 ← 12	276 789.850
$\frac{1}{2}$	$13\frac{1}{2} \leftarrow 12\frac{1}{2}$	*e*	13 ← 12	286 159.597
			14 ← 13	286 162.031
		f	13 ← 12	286 482.478
			14 ← 13	286 483.963
$\frac{3}{2}$	$13\frac{1}{2} \leftarrow 12\frac{1}{2}$	*e*	13 ← 12	299 073.772
			14 ← 13	299 070.699
		f	13 ← 12	298 763.631
			14 ← 13	298 761.504
$\frac{1}{2}$	$14\frac{1}{2} \leftarrow 13\frac{1}{2}$	*e*	14 ← 13	307 511.459
			15 ← 14	307 513.754
		f	14 ← 13	307 874.176
			15 ← 14	307 875.626
$\frac{3}{2}$	$14\frac{1}{2} \leftarrow 13\frac{1}{2}$	*e*	14 ← 13	321 045.517
			15 ← 14	321 042.640
		f	14 ← 13	320 710.121
			15 ← 14	320 708.211
$\frac{1}{2}$	$15\frac{1}{2} \leftarrow 14\frac{1}{2}$	*e*	15 ← 14	328 883.829
			16 ← 15	328 885.967
		f	15 ← 14	329 286.445
			16 ← 15	329 287.717

[a]) States with parity equal to $\pm(-1)^{J-0.5}$ are labeled *e* and *f* respectively.
[b]) Coupling scheme: $\boldsymbol{F}_1 = \boldsymbol{J} + \boldsymbol{I}_1$; $\boldsymbol{F} = \boldsymbol{F}_1 + \boldsymbol{I}_2$ where $\boldsymbol{I}_1$ is the ^{13}C nuclear spin and $\boldsymbol{I}_2$ is the ^{1}H nuclear spin
[c]) ^{1}H hyperfine structure not resolved.

Microwave data for $^{12}C^{12}C^{13}C^{1}H$

Transition: Rotational $N' - N''$	Transition: fine structure $J' - J''$ [a])	Transition: hyperfine $F_1' - F_1''$ [b])	ν [MHz]	Ref.
State: electronic $\tilde{X}\,^2\Pi$; vibrational $v_4 = 1$, lower vibronic component ($\mu^2\Sigma$)				
12 ← 11	$12\frac{1}{2} \leftarrow 11\frac{1}{2}$	13 ← 12	260 831.758	96Ka
	$11\frac{1}{2} \leftarrow 10\frac{1}{2}$	12 ← 11	260 823.974	
13 ← 12	$13\frac{1}{2} \leftarrow 12\frac{1}{2}$	14 ← 13	282 570.255	
		13 ← 12	282 569.159	
	$12\frac{1}{2} \leftarrow 11\frac{1}{2}$	13 ← 12	282 552.050	
		12 ← 11	282 550.946	
14 ← 13	$14\frac{1}{2} \leftarrow 13\frac{1}{2}$	15 ← 14	304 310.350	
		14 ← 13	304 307.931	
	$13\frac{1}{2} \leftarrow 12\frac{1}{2}$	14 ← 13	304 279.032	
		13 ← 12	304 276.560	
15 ← 14	$15\frac{1}{2} \leftarrow 14\frac{1}{2}$	16 ← 15	326 053.539	
		15 ← 14	326 047.957	
	$14\frac{1}{2} \leftarrow 13\frac{1}{2}$	15 ← 14	326 006.068	
		14 ← 13	326 000.439	

[a]) Coupling scheme: $\boldsymbol{J} = \boldsymbol{N} + \boldsymbol{S}$; $\boldsymbol{F}_1 = \boldsymbol{J} + \boldsymbol{I}_1$; $\boldsymbol{F} = \boldsymbol{F}_1 + \boldsymbol{I}_2$ where $\boldsymbol{I}_1$ is the ^{13}C nuclear spin and $\boldsymbol{I}_2$ is the ^{1}H nuclear spin.
[b]) ^{1}H hyperfine structure not resolved.

Molecular parameters for $^{12}C^{12}C^{13}C^{1}H$

Parameter		Value	Method	Ref.
State: electronic $\tilde{X}\,^2\Pi$; vibrational zero point level				
B	[MHz]	10 842.577(36) [a])	MW	96Ka
D	[kHz]	4.788 9(68)		
A	[MHz]	431 462(31)		
γ	[MHz]	– 47.14(91)		
p	[MHz]	– 7.954(164)		
q	[MHz]	– 12.314(56)		
$a(^{13}C)$	[MHz]	44.2(68)		
$b(^{13}C)$	[MHz]	137.1(52)		
$c(^{13}C)$	[MHz]	– 75(28)		
$d^{13}C)$	[MHz]	90.9 (55)		
$a(^{1}H)$	[MHz]	17.1(99)		
$b(^{1}H)$	[MHz]	– 22.54 [b])		
$c(^{1}H)$	[MHz]	27.49 [b])		
$d(^{1}H)$	[MHz]	14.5 (99)		
State: electronic $\tilde{X}\,^2\Pi$; vibrational $v_4 = 1$, lower vibronic component ($\mu\,^2\Sigma$)				
B	[MHz]	10 863.109(75)	MW	96Ka
D	[kHz]	4.673 (25)		
γ	[MHz]	– 35.59 (21)		
$b(^{13}C)$	[MHz]	169.1 (139)		
$c(^{13}C)$	[MHz]	– 75 [b])		
ΔE [c])	[GHz]	594.330(1210)		
β [d])	[MHz]	– 1 219.9(92)		

[a]) The numbers in parentheses are 3 standard deviation of the least-squares fit, in units of the last quoted decimal place.
[b]) Constrained to this value.
[c]) The energy difference between the vibrational ground state and the $v_4 = 1$, $\mu\,^2\Sigma$ vibronic state.
[d]) Interaction parameter linking the vibrational ground state and the $v_4 = 1$, $\mu\,^2\Sigma$ vibronic state.

References for C_3H

96Ka Kanada, M., Yamamoto, S., Saito, S., Osamura, Y. : J. Chem. Phys. **104** (1996) 2192.

3.2.1.2.3 C_4H

Microwave data for $^{12}C^{12}C^{12}C^{12}C^{1}H$

Transition			ν	Ref.
rotational $N' - N''$	fine structure $J' - J''$	hyperfine $F' - F''$ [a])	[MHz]	
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational zero point level				
1 ← 0	$1\frac{1}{2} \leftarrow \frac{1}{2}$	1 ← 0	9 493.060	95Ch
		2 ← 1	9 497.615	
		1 ← 1	9 508.005	
	$\frac{1}{2} \leftarrow \frac{1}{2}$	1 ← 0	9 547.960	
		0← 1	9 551.720	
		1 ← 1	9 562.905	

[a]) Coupling scheme: $\boldsymbol{J} = \boldsymbol{N} + \boldsymbol{S}$; $\boldsymbol{F} = \boldsymbol{J} + \boldsymbol{I}$ where $\boldsymbol{I}$ is the ^{1}H nuclear spin.

Molecular parameters for $^{12}C^{12}C^{12}C^{12}C^{1}H$

Parameter		Value	Method	Ref.
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational zero point level				
B	[MHz]	4 758.655 7(7) [a])	MW	83Go, 95Ch
D	[kHz]	0.862 7(10)		
γ	[MHz]	– 38.555 (2)		
γ_D	[kHz]	0.127(9)		
$b_F(^1H)$	[MHz]	– 14.943(7)		
$c(^1H)$	[MHz]	12.44(1)		

[a]) The numbers in parentheses are 1 standard deviation of the least-squares fit, in units of the last quoted decimal place.

Microwave data for $^{13}C^{12}C^{12}C^{12}C^{1}H$

Transition				ν	Ref.
rotational	fine structure	hyperfine			
$N' - N''$	$J' - J''$	$F_1' - F_1''$ [a])	$F' - F''$ [a])	[MHz]	
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational zero point level					
$1 \leftarrow 0$	$1\frac{1}{2} \leftarrow \frac{1}{2}$	$1 \leftarrow 0$	$1\frac{1}{2} \leftarrow \frac{1}{2}$	9 166.245(5) [b])	95Ch
		$2 \leftarrow 1$	$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	9 167.370(5)	
			$1\frac{1}{2} \leftarrow \frac{1}{2}$	9 187.120(5)	
		$1 \leftarrow 1$	$\frac{1}{2} \leftarrow \frac{1}{2}$	9 188.325(5)	
	$\frac{1}{2} \leftarrow \frac{1}{2}$	$1 \leftarrow 1$	$\frac{1}{2} \leftarrow 1\frac{1}{2}$	9 198.330(5)	
		$0 \leftarrow 0$	$\frac{1}{2} \leftarrow \frac{1}{2}$	9 218.700(5)	
		$1 \leftarrow 1$	$1\frac{1}{2} \leftarrow 1\frac{1}{2}$	9 227.440(5)	
$15 \leftarrow 14$	$14\frac{1}{2} \leftarrow 13\frac{1}{2}$	$15 \leftarrow 14$	[c])	137 839.782(51)	
		$14 \leftarrow 13$	[c])	137 843.607(51)	
$16 \leftarrow 15$	$16\frac{1}{2} \leftarrow 15\frac{1}{2}$	$17 \leftarrow 16$	[c])	146 993.604(46)	
		$16 \leftarrow 15$	[c])	146 997.285(66)	
$24 \leftarrow 23$	$24\frac{1}{2} \leftarrow 23\frac{1}{2}$	$25 \leftarrow 24$	[c])	220 474.853(162)	
		$24 \leftarrow 23$	[c])	220 476.620(86)	
$26 \leftarrow 25$	$26\frac{1}{2} \leftarrow 25\frac{1}{2}$	$27 \leftarrow 26$	[c])	238 840.678(93)	
		$26 \leftarrow 25$	[c])	238 842.336(50)	
	$25\frac{1}{2} \leftarrow 24\frac{1}{2}$	$26 \leftarrow 25$	[c])	238 875.579(34)	
		$25 \leftarrow 24$	[c])	238 877.208(57)	
$27 \leftarrow 26$	$27\frac{1}{2} \leftarrow 26\frac{1}{2}$	$28 \leftarrow 27$	[c])	248 022.963(44)	
		$27 \leftarrow 26$	[c])	248 024.499(35)	
	$26\frac{1}{2} \leftarrow 25\frac{1}{2}$	$27 \leftarrow 26$	[c])	248 057.854(45)	
		$26 \leftarrow 25$	[c])	248 059.452(46)	
$28 \leftarrow 27$	$28\frac{1}{2} \leftarrow 27\frac{1}{2}$	$29 \leftarrow 28$	[c])	257 204.762(44)	
		$28 \leftarrow 27$	[c])	257 206.305(60)	
$30 \leftarrow 29$	$29\frac{1}{2} \leftarrow 28\frac{1}{2}$	$30 \leftarrow 29$	[c])	275 601.571(56)	
		$29 \leftarrow 28$	[c])	275 602.965(65)	

[a]) Coupling scheme: $\boldsymbol{J} = \boldsymbol{N} + \boldsymbol{S}$; $\boldsymbol{F}_1 = \boldsymbol{J} + \boldsymbol{I}_1$; $\boldsymbol{F} = \boldsymbol{F}_1 + \boldsymbol{I}_2$ where $\boldsymbol{I}_1$ is the ^1H nuclear spin and $\boldsymbol{I}_2$ is the ^{13}C nuclear spin.
[b]) Authors' estimate of experimental uncertainty in units of the last quoted decimal place.
[c]) ^1H hyperfine splitting not resolved.

Molecular parameters for $^{13}C^{12}C^{12}C^{12}C^{1}H$

Parameter		Value	Method	Ref.
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational zero point level				
B	[MHz]	4 594.540 9(3) [a])	MW	95Ch
D	[kHz]	0.812 7(1)		
γ	[MHz]	– 36.670(4)		
γ_D	[kHz]	0.121(12)		
$b_F(^{13}C)$	[MHz]	396.6(6)		
$c(^{13}C)$	[MHz]	89.12(1)		
$b_F(^{1}H)$	[MHz]	– 14.91(1)		
$c(^{1}H)$	[MHz]	12.42(3)		

[a]) The numbers in parentheses are 1 standard deviation of the least-squares fit, in units of the last quoted decimal place.

Microwave data for $^{12}C^{13}C^{12}C^{12}C^{1}H$

Transition				ν	Ref.
rotational	fine structure	hyperfine			
$N' - N''$	$J' - J''$	$F_1' - F_1''$ [a])	$F' - F''$ [a])	[MHz]	
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational zero point level					
1 ← 0	$1\frac{1}{2} \leftarrow \frac{1}{2}$	1 ← 0	$1\frac{1}{2} \leftarrow \frac{1}{2}$	9 448.165(5) [c])	95Ch
		2 ← 1	$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	9 449.910(5)	
			$1\frac{1}{2} \leftarrow \frac{1}{2}$	9 458.940(5)	
		1 ← 1	$\frac{1}{2} \leftarrow \frac{1}{2}$	9 464.915(5)	
	$\frac{1}{2} \leftarrow \frac{1}{2}$	0 ← 1	$\frac{1}{2} \leftarrow 1\frac{1}{2}$	9 495.830(5)	
		1 ← 1	$\frac{1}{2} \leftarrow \frac{1}{2}$	9 502.830(5)	
		1 ← 0	$1\frac{1}{2} \leftarrow 1\frac{1}{2}$	9 502.270(5)	
14 ← 13	$14\frac{1}{2} \leftarrow 13\frac{1}{2}$	[c])	[c])	132 541.486(59)	
	$13\frac{1}{2} \leftarrow 12\frac{1}{2}$	[c])	[c])	132 579.251(58)	
15 ← 14	$15\frac{1}{2} \leftarrow 14\frac{1}{2}$	[c])	[c])	142 008.592(27)	
	$14\frac{1}{2} \leftarrow 13\frac{1}{2}$	[c])	[c])	142 046.383(29)	
26 ← 25	$26\frac{1}{2} \leftarrow 25\frac{1}{2}$	[c])	[c])	246 122.193(23)	
	$25\frac{1}{2} \leftarrow 24\frac{1}{2}$	[c])	[c])	246 159.800(25)	
27 ← 26	$27\frac{1}{2} \leftarrow 26\frac{1}{2}$	[c])	[c])	255 584.279(23)	
	$26\frac{1}{2} \leftarrow 25\frac{1}{2}$	[c])	[c])	255 621.916(24)	
28 ← 27	$28\frac{1}{2} \leftarrow 27\frac{1}{2}$	[c])	[c])	265 045.845(33)	
	$27\frac{1}{2} \leftarrow 26\frac{1}{2}$	[c])	[c])	265 083.442(28)	
29 ← 28	$29\frac{1}{2} \leftarrow 28\frac{1}{2}$	[c])	[c])	274 506.780(29)	
30 ← 29	$30\frac{1}{2} \leftarrow 29\frac{1}{2}$	[c])	[c])	283 967.247(24)	
	$29\frac{1}{2} \leftarrow 28\frac{1}{2}$	[c])	[c])	284 004.639(19)	

[a]) Coupling scheme: $\boldsymbol{J} = \boldsymbol{N} + \boldsymbol{S}$; $\boldsymbol{F}_1 = \boldsymbol{J} + \boldsymbol{I}_1$; $\boldsymbol{F} = \boldsymbol{F}_1 + \boldsymbol{I}_2$ where $\boldsymbol{I}_1$ is the ^{1}H nuclear spin and $\boldsymbol{I}_2$ is the ^{13}C nuclear spin.
[b]) Authors' estimate of experimental uncertainty in units of the last quoted decimal place.
[c]) ^{13}C and ^{1}H hyperfine splitting not resolved.

Molecular parameters for $^{12}C^{13}C^{12}C^{12}C^{1}H$

Parameter		Value	Method	Ref.
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational zero point level				
B	[MHz]	4 734.632 9(6) [a])	MW	95Ch
D	[kHz]	0.852 1(4)		
γ	[MHz]	– 38.001(5)		
γ_D	[kHz]	0.176(7)		
$b_F(^{13}C)$	[MHz]	57.49(5)		
$c(^{13}C)$	[MHz]	– 1.91(3)		
$b_F(^{1}H)$	[MHz]	– 14.99(2)		
$c(^{1}H)$	[MHz]	12.51(2)		

[a]) The numbers in parentheses are 1 standard deviation of the least-squares fit, in units of the last quoted decimal place.

Microwave data for $^{12}C^{12}C^{13}C^{12}C^{1}H$

Transition: rotational $N'-N''$	fine structure $J'-J''$	hyperfine $F_1'-F_1''$ [a])	$F'-F''$ [a])	ν [MHz]	Ref.
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational zero point level					
1 ← 0	$1\frac{1}{2} \leftarrow \frac{1}{2}$	1 ← 0	$\frac{1}{2} \leftarrow \frac{1}{2}$	9 462.615(5) [b])	95Ch
		2 ← 1	$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	9 463.810(5)	
			$1\frac{1}{2} \leftarrow \frac{1}{2}$	9 464.295(5)	
		1 ← 1	$1\frac{1}{2} \leftarrow 1\frac{1}{2}$	9 474.860(5)	
	$\frac{1}{2} \leftarrow \frac{1}{2}$	1 ← 0	$1\frac{1}{2} \leftarrow \frac{1}{2}$	9 515.015(5)	
		0 ← 1	$\frac{1}{2} \leftarrow 1\frac{1}{2}$	9 519.530(5)	
		1 ← 1	$\frac{1}{2} \leftarrow \frac{1}{2}$	9 522.870(5)	
			$1\frac{1}{2} \leftarrow 1\frac{1}{2}$	9 533.800(5)	
14 ← 13	$14\frac{1}{2} \leftarrow 13\frac{1}{2}$	[c])	[c])	132 743.681(43)	
	$13\frac{1}{2} \leftarrow 12\frac{1}{2}$	[c])	[c])	132 782.090(38)	
28 ← 27	$28\frac{1}{2} \leftarrow 27\frac{1}{2}$	[c])	[c])	265 450.325(26)	
	$27\frac{1}{2} \leftarrow 26\frac{1}{2}$	[c])	[c])	265 488.427(25)	
30 ← 29	$30\frac{1}{2} \leftarrow 29\frac{1}{2}$	[c])	[c])	284 400.501(47)	
31 ← 30	$31\frac{1}{2} \leftarrow 30\frac{1}{2}$	[c])	[c])	293 874.734(18)	
	$30\frac{1}{2} \leftarrow 29\frac{1}{2}$	[c])	[c])	293 912.807(21)	
32 ← 31	$32\frac{1}{2} \leftarrow 31\frac{1}{2}$	[c])	[c])	303 348.290(21)	
	$31\frac{1}{2} \leftarrow 30\frac{1}{2}$	[c])	[c])	303 386.279(22)	

[a]) Coupling scheme: $\boldsymbol{J} = \boldsymbol{N} + \boldsymbol{S}$; $\boldsymbol{F}_1 = \boldsymbol{J} + \boldsymbol{I}_1$; $\boldsymbol{F} = \boldsymbol{F}_1 + \boldsymbol{I}_2$ where $\boldsymbol{I}_1$ is the ^1H nuclear spin and $\boldsymbol{I}_2$ is the ^{13}C nuclear spin.
[b]) Authors' estimate of experimental uncertainty in units of the last quoted decimal place.
[c]) ^{13}C and ^1H hyperfine splitting not resolved.

Molecular parameters for $^{12}C^{12}C^{13}C^{12}C^{1}H$

Parameter		Value	Method	Ref.
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational zero point level				
B	[MHz]	4 741.867 2(7) [a])	MW	95Ch
D	[kHz]	0.856 1(4)		
γ	[MHz]	– 38.363(2)		
γ_D	[kHz]	0.113(6)		
$b_F(^{13}C)$	[MHz]	– 9.54(2)		
$c(^{13}C)$	[MHz]	9.84(8)		
$b_F(^{1}H)$	[MHz]	– 14.93(2)		
$c(^{1}H)$	[MHz]	12.50(6)		

[a]) The numbers in parentheses are 1 standard deviation of the least-squares fit, in units of the last quoted decimal place.

Microwave data for $^{12}C^{12}C^{12}C^{13}C^{1}H$

Transition				ν [MHz]	Ref.
rotational $N' - N''$	fine structure $J' - J''$	hyperfine $F_1' - F_1''$ [a])	hyperfine $F' - F''$ [a])		
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational zero point level					
$1 \leftarrow 0$	$1\frac{1}{2} \leftarrow \frac{1}{2}$	$1 \leftarrow 0$	$1\frac{1}{2} \leftarrow \frac{1}{2}$	9 208.770(5) [b])	95Ch
		$2 \leftarrow 1$	$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	9 211.425(5)	
			$1\frac{1}{2} \leftarrow \frac{1}{2}$	9 213.470(5)	
		$1 \leftarrow 1$	$1\frac{1}{2} \leftarrow 1\frac{1}{2}$	9 221.490(5)	
			$\frac{1}{2} \leftarrow \frac{1}{2}$	9 222.440(5)	
	$\frac{1}{2} \leftarrow \frac{1}{2}$	$1 \leftarrow 0$	$1\frac{1}{2} \leftarrow \frac{1}{2}$	9 253.940(5)	
		$1 \leftarrow 1$	$1\frac{1}{2} \leftarrow 1\frac{1}{2}$	9 266.650(5)	
$11 \leftarrow 10$	$11\frac{1}{2} \leftarrow 10\frac{1}{2}$	[c])	[c])	101 506.343(54)	
	$10\frac{1}{2} \leftarrow 9\frac{1}{2}$	[c])	[c])	101 543.766(41)	
$12 \leftarrow 11$	$12\frac{1}{2} \leftarrow 11\frac{1}{2}$	[c])	[c])	110 735.027(28)	
	$11\frac{1}{2} \leftarrow 10\frac{1}{2}$	[c])	[c])	110 772.434(25)	
$26 \leftarrow 25$	$25\frac{1}{2} \leftarrow 24\frac{1}{2}$	[c])	[c])	239 940.459(24)	
$28 \leftarrow 27$	$28\frac{1}{2} \leftarrow 27\frac{1}{2}$	[c])	[c])	258 348.994(28)	
	$27\frac{1}{2} \leftarrow 26\frac{1}{2}$	[c])	[c])	258 386.269(35)	
$29 \leftarrow 28$	$29\frac{1}{2} \leftarrow 28\frac{1}{2}$	[c])	[c])	267 571.223(45)	
	$28\frac{1}{2} \leftarrow 27\frac{1}{2}$	[c])	[c])	267 608.304(33)	

[a]) Coupling scheme: $\boldsymbol{J} = \boldsymbol{N} + \boldsymbol{S}$; $\boldsymbol{F}_1 = \boldsymbol{J} + \boldsymbol{I}_1$; $\boldsymbol{F} = \boldsymbol{F}_1 + \boldsymbol{I}_2$ where $\boldsymbol{I}_1$ is the ^{1}H nuclear spin and $\boldsymbol{I}_2$ is the ^{13}C nuclear spin.
[b]) Authors' estimate of experimental uncertainty in units of the last quoted decimal place.
[c]) ^{13}C and ^{1}H hyperfine splitting not resolved.

Molecular parameters for $^{12}C^{12}C^{12}C^{13}C^1H$

Parameter		Value	Method	Ref.
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational zero point level				
B	[MHz]	4 614.970 5(8) [a])	MW	95Ch
D	[kHz]	0.805 5(6)		
γ	[MHz]	– 37.491(11)		
γ_D	[kHz]	0.107(15)		
$b_F(^{13}C)$	[MHz]	18.56(4)		
$c(^{13}C)$	[MHz]	– 19.23(7)		
$b_F(^1H)$	[MHz]	– 14.935(5)		
$c(^1H)$	[MHz]	12.43(4)		

[a]) The numbers in parentheses are 1 standard deviation of the least-squares fit, in units of the last quoted decimal place.

References for C_4H

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3.2.1.2.4 C_5H

Microwave data for $^{12}C_5{}^1H$

Transition spin Ω	rotational $J' - J''$	parity e/f [a]	hyperfine $F' - F''$	ν [MHz]	Ref.
State: electronic $\tilde{X}\,^2\Pi$; vibrational zero point level					
$\frac{1}{2}$	$1\frac{1}{2} \leftarrow \frac{1}{2}$	e	$2 \leftarrow 1$	7 157.665(2) [b]	98McC
			$1 \leftarrow 1$	7 159.213(2)	
		f	$2 \leftarrow 1$	7 162.042(2)	
			$1 \leftarrow 1$	7 152.172(2)	
	$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	e	$3 \leftarrow 2$	11 932.472(2)	
			$2 \leftarrow 1$	11 933.922(2)	
			$2 \leftarrow 2$	11 935.475(2)	
		f	$3 \leftarrow 2$	11 936.468(2)	
			$2 \leftarrow 1$	11 938.323(2)	
			$2 \leftarrow 2$	11 928.453(2)	
	$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	e	$4 \leftarrow 3$	16 706.720(2)	
			$3 \leftarrow 2$	16 707.475(2)	
			$3 \leftarrow 3$	16 710.478(2)	
		f	$4 \leftarrow 3$	16 710.619(2)	
			$3 \leftarrow 2$	16 711.510(2)	
			$3 \leftarrow 3$	16 703.494(2)	
	$4\frac{1}{2} \leftarrow 3\frac{1}{2}$	e	$5 \leftarrow 4$	21 480.809(2)	
			$4 \leftarrow 3$	21 481.299(2)	
		f	$5 \leftarrow 4$	21 484.695(2)	
			$4 \leftarrow 3$	21 485.248(2)	
$\frac{1}{2}$	$22\frac{1}{2} \leftarrow 21\frac{1}{2}$	e	[c]	107 409.91(10)	86Go
		f	[c]	107 416.65(10)	
$\frac{1}{2}$	$23\frac{1}{2} \leftarrow 22\frac{1}{2}$	e	[c]	112 183.49(10)	
		f	[c]	112 190.58(10)	
$\frac{1}{2}$	$24\frac{1}{2} \leftarrow 23\frac{1}{2}$	e	[c]	116 957.11(10)	
		f	[c]	116 964.39(10)	
$\frac{3}{2}$	$34\frac{1}{2} \leftarrow 33\frac{1}{2}$	e	[c]	165 785.43(10)	
		f	[c]	165 792.36(10)	
$\frac{1}{2}$	$35\frac{1}{2} \leftarrow 34\frac{1}{2}$	e	[c]	169 464.50(10)	
		f	[c]	169 475.49(10)	
$\frac{3}{2}$		e	[c]	170 588.58(10)	
		f	[c]	170 595.94(10)	
$\frac{1}{2}$	$38\frac{1}{2} \leftarrow 37\frac{1}{2}$	e	[c]	183 783.87(10)	
		f	[c]	183 796.03(10)	
$\frac{3}{2}$		e	[c]	184 997.07(10)	
		f	[c]	185 005.57(10)	
$\frac{1}{2}$	$39\frac{1}{2} \leftarrow 38\frac{1}{2}$	e	[c]	188 556.91(10)	
		f	[c]	188 569.50(10)	
$\frac{3}{2}$		e	[c]	189 799.43(10)	
		f	[c]	189 808.36(10)	

[a]) States with parity equal to $\pm(-1)^{J-0.5}$ are labeled *e* and *f* respectively.
[b]) The figures in parentheses are the authors' estimates of experimental uncertainty (1σ).
[c]) Proton hyperfine structure not resolved.

Molecular parameters for $^{12}C_5{}^1H$

Parameter		Value	Method	Ref.
State: electronic $\tilde{X}\,^2\Pi$; vibrational zero point level				
B	[MHz]	2 395.126 50(12) [a])	MW	99McC
D	[kHz]	0.127 41(3)		
A	[GHz]	725. 880(260)		
γ	[MHz]	– 51.6(8)		
p	[MHz]	4.275(1)		
q	[MHz]	– 0.310 8(6)		
q_D	[Hz]	1.6(2)		
$h_{1/2}(^1H)$ [b])	[MHz]	16.19(6)		
$b(^1H)$	[MHz]	– 29.12(12)		
$d(^1H)$	[MHz]	10.711(2)		

[a]) The numbers in parentheses are 1 standard deviation of the least-squares fit, in units of the last quoted decimal place.
[b]) $h_{1/2}(^1H) = a - (b+c)/2$.

Microwave data for $^{12}C_5{}^2H$ (C_5D)

Transition: spin Ω	rotational $J' - J''$	parity e/f [a])	hyperfine $F' - F''$	ν [MHz]	Ref.
State: electronic $\tilde{X}\,^2\Pi$; vibrational zero point level					
$\frac{1}{2}$	$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	e	$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	11 272.326	95Hi
			$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	11 272.583	
			$1\frac{1}{2} \leftarrow \frac{1}{2}$	11 272.799	
		f	$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	11 275.892	
			$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	11 276.369	
			$1\frac{1}{2} \leftarrow \frac{1}{2}$	11 276.369	
	$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	e	$4\frac{1}{2} \leftarrow 3\frac{1}{2}$	15 782.101	
			$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	15 782.222	
			$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	15 782.353	
		f	$4\frac{1}{2} \leftarrow 3\frac{1}{2}$	15 785.666	
$\frac{1}{2}$	$38\frac{1}{2} \leftarrow 37\frac{1}{2}$	e	[b])	173 608.921	
		f	[b])	173 620.872	
$\frac{3}{2}$		e	[b])	174 706.590	
		f	[b])	174 698.106	
$\frac{1}{2}$	$39\frac{1}{2} \leftarrow 38\frac{1}{2}$	e	[b])	178 117.651	
		f	[b])	178 130.052	
$\frac{1}{2}$	$40\frac{1}{2} \leftarrow 39\frac{1}{2}$	e	[b])	182 626.357	
		f	[b])	182 639.190	
$\frac{1}{2}$	$42\frac{1}{2} \leftarrow 41\frac{1}{2}$	e	[b])	191 643.588	
		f	[b])	191 657.216	
$\frac{3}{2}$		e	[b])	192 848.446	
		f	[b])	192 838.253	
$\frac{1}{2}$	$43\frac{1}{2} \leftarrow 42\frac{1}{2}$	e	[b])	196 152.151	
		f	[b])	196 166.253	
$\frac{3}{2}$		e	[b])	197 383.518	
		f	[b])	197 372.890	
$\frac{1}{2}$	$44\frac{1}{2} \leftarrow 43\frac{1}{2}$	e	[b])	200 660.626	
		f	[b])	200 675.210	
$\frac{3}{2}$		e	[b])	201 918.420	

		f	[b])	201 907.258
$\frac{1}{2}$	$45\frac{1}{2} \leftarrow 44\frac{1}{2}$	*e*	[b])	205 169.086
		f	[b])	205 184.116
$\frac{3}{2}$		*e*	[b])	206 453.057
		f	[b])	206 441.483
$\frac{1}{2}$	$46\frac{1}{2} \leftarrow 45\frac{1}{2}$	*e*	[b])	209 677.413
		f	[b])	209 692.963
$\frac{3}{2}$		*e*	[b])	210 987.578
		f	[b])	210 975.570
$\frac{1}{2}$	$57\frac{1}{2} \leftarrow 56\frac{1}{2}$	*e*	[b])	259 265.265
		f	[b])	259 286.436
$\frac{3}{2}$		*e*	[b])	260 854.041
		f	[b])	260 836.403
$\frac{1}{2}$	$58\frac{1}{2} \leftarrow 57\frac{1}{2}$	*e*	[b])	263 772.820
		f	[b])	263 794.521
$\frac{3}{2}$		*e*	[b])	265 386.017
		f	[b])	265 367.830
$\frac{1}{2}$	$59\frac{1}{2} \leftarrow 58\frac{1}{2}$	*e*	[b])	268 280.256
		f	[b])	268 302.549
$\frac{3}{2}$		*e*	[b])	269 917.840
		f	[b])	269 899.128
$\frac{1}{2}$	$60\frac{1}{2} \leftarrow 59\frac{1}{2}$	*e*	[b])	272 787.651
		f	[b])	272 810.479
$\frac{3}{2}$		*e*	[b])	274 449.397
		f	[b])	274 430.115
$\frac{1}{2}$	$61\frac{1}{2} \leftarrow 60\frac{1}{2}$	*e*	[b])	277 294.960

[a]) States with parity equal to $\pm(-1)^{J-0.5}$ are labeled *e* and *f* respectively.
[b]) Deuteron hyperfine structure not resolved.

Molecular parameters for $^{12}C_5{}^2H$ (C_5D)

Parameter		Value	Method	Ref.
State: electronic $\tilde{X}\,^2\Pi$; vibrational zero point level				
B	[MHz]	2 626.128 64(40) [a])	MW	95Hi
D	[kHz]	0.110 828(67)		
A	[GHz]	724. 77(78)		
γ	[MHz]	– 53.1(23)		
p	[MHz]	4.084 0(106)		
q	[MHz]	– 0.324 44(198)		
q_D	[Hz]	1.52(38)		
$h_{1/2}(^2H)$ [b])	[MHz]	2.658(77)		
$b(^2H)$	[MHz]	– 4.32(196)		
$d(^2H)$	[MHz]	1.645(92)		

[a]) The numbers in parentheses are 3 standard deviation of the least-squares fit, in units of the last quoted decimal place.
[b]) $h_{1/2}(^2H) = a - (b+c)/2$.

References for C_5H

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3.2.1.2.5 C_6H

Microwave data for $^{12}C_6{}^1H$

Transition				ν [MHz]	Ref.
spin Ω	rotational $J' - J''$	parity e/f [a])	hyperfine $F' - F''$		
State: electronic $\tilde{X}\,^2\Pi$; vibrational zero point level					
$\frac{3}{2}$	$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	e	$4 \leftarrow 3$	9 703.508(10) [b])	99McC
			$3 \leftarrow 2$	9 703.600(10)	
		f	$4 \leftarrow 3$	9 703.835(10)	
			$3 \leftarrow 2$	9 703 936(10)	
	$4\frac{1}{2} \leftarrow 3\frac{1}{2}$	e	$5 \leftarrow 4$	12 475.888(5)	
			$4 \leftarrow 3$	12 475.973(5)	
		f	$5 \leftarrow 4$	12 476.448(5)	
			$4 \leftarrow 3$	12 476.534(5)	
	$5\frac{1}{2} \leftarrow 4\frac{1}{2}$	e	$6 \leftarrow 5$	15 248.247(5)	
			$5 \leftarrow 4$	15 248.322(5)	
		f	$6 \leftarrow 5$	15 249.084(5)	
			$5 \leftarrow 4$	15 249 158(5)	
	$6\frac{1}{2} \leftarrow 5\frac{1}{2}$	e	$7 \leftarrow 6$	18 020.574(5)	
			$6 \leftarrow 5$	18 020.644(5)	
		f	$7 \leftarrow 6$	18 021.752(5)	
			$6 \leftarrow 5$	18 021.818(5)	
	$7\frac{1}{2} \leftarrow 6\frac{1}{2}$	e	$8 \leftarrow 7$	20 792.872(5)	
			$7 \leftarrow 6$	20 792.945(5)	
		f	$8 \leftarrow 7$	20 794.444(5)	
			$7 \leftarrow 6$	20 794.512(5)	
$\frac{3}{2}$	$25\frac{1}{2} \leftarrow 24\frac{1}{2}$	e	[c])	70 690.390(15)	99Li
		f	[c])	70 708.060(15)	
$\frac{1}{2}$		f	[c])	71 176.466(15)	
		e	[c])	71 216.384(15)	
$\frac{3}{2}$	$26\frac{1}{2} \leftarrow 25\frac{1}{2}$	e	[c])	73 462.273(15)	
		f	[c])	73 481.301(15)	
$\frac{1}{2}$		f	[c])	73 967.516(15)	
		e	[c])	74 008.360(15)	
$\frac{3}{2}$	$27\frac{1}{2} \leftarrow 26\frac{1}{2}$	e	[c])	76 234.155(15)	
		f	[c])	76 254.587(15)	
$\frac{1}{2}$		f	[c])	76 758.492(15)	
		e	[c])	76 800.308(15)	
$\frac{3}{2}$	$28\frac{1}{2} \leftarrow 27\frac{1}{2}$	e	[c])	79 006.011(15)	
		f	[c])	79 027.898(15)	
$\frac{1}{2}$		f	[c])	79 549.383(15)	
		e	[c])	79 592.201(15)	
$\frac{3}{2}$	$29\frac{1}{2} \leftarrow 28\frac{1}{2}$	e	[c])	81 777.856(15)	
		f	[c])	81 801.237(15)	
$\frac{1}{2}$		f	[c])	82 340.201(15)	
		e	[c])	82 384.050(15)	
$\frac{3}{2}$	$30\frac{1}{2} \leftarrow 29\frac{1}{2}$	e	[c])	84 549.688(15)	
		f	[c])	84 574.600(15)	
$\frac{1}{2}$		f	[c])	85 130.946(15)	
		e	[c])	85 175.846(15)	

$\frac{3}{2}$	$31\frac{1}{2} \leftarrow 30\frac{1}{2}$	*e*	c)	87 321.504(15)
		f	c)	87 347.994(15)
$\frac{1}{2}$		*f*	c)	87 921.593(15)
		e	c)	87 967.595(15)
$\frac{3}{2}$	$32\frac{1}{2} \leftarrow 31\frac{1}{2}$	*e*	c)	90 093.295(15)
		f	c)	90 121.407(15)
$\frac{1}{2}$		*f*	c)	90 712.181(15)
		e	c)	90 759.297(15)
$\frac{3}{2}$	$33\frac{1}{2} \leftarrow 32\frac{1}{2}$	*e*	c)	92 865.078(15)
		f	c)	92 894.848(15)
$\frac{1}{2}$		*f*	c)	93 502.677(15)
		e	c)	93 550.939(15)
$\frac{3}{2}$	$34\frac{1}{2} \leftarrow 33\frac{1}{2}$	*e*	c)	95 636.852(15)
		f	c)	95 668.308(15)
$\frac{1}{2}$		*f*	c)	96 293.084(15)
		e	c)	96 342.532(15)
$\frac{3}{2}$	$35\frac{1}{2} \leftarrow 34\frac{1}{2}$	*e*	c)	98 408.607(15)
		f	c)	98 441.812(15)
$\frac{1}{2}$		*f*	c)	99 083.408(15)
		e	c)	99 134.050(15)
$\frac{3}{2}$	$36\frac{1}{2} \leftarrow 35\frac{1}{2}$	*e*	c)	101 180.347(15)
		f	c)	101 215.315(15)
$\frac{1}{2}$		*f*	c)	101 873.640(15)
		e	c)	101 925.512(15)
$\frac{3}{2}$	$37\frac{1}{2} \leftarrow 36\frac{1}{2}$	*e*	c)	103 952.075(15)
		f	c)	103 988.861(15)
$\frac{1}{2}$		*f*	c)	104 663.787(15)
		e	c)	104 716.909(15)
$\frac{3}{2}$	$38\frac{1}{2} \leftarrow 37\frac{1}{2}$	*e*	c)	106 723.796(15)
		f	c)	106 762.421(15)
$\frac{1}{2}$		*f*	c)	107 453.845(15)
		e	c)	107 508.254(15)
$\frac{3}{2}$	$39\frac{1}{2} \leftarrow 38\frac{1}{2}$	*e*	c)	109 495.493(15)
		f	c)	109 535.996(15)
$\frac{1}{2}$		*f*	c)	110 243.798(15)
		e	c)	110 299.519(15)
$\frac{3}{2}$	$40\frac{1}{2} \leftarrow 39\frac{1}{2}$	*e*	c)	112 267.200(15)
		f	c)	112 309.594(15)
$\frac{1}{2}$		*f*	c)	113 003.681(15)
		e	c)	113 090.722(15)
$\frac{3}{2}$	$41\frac{1}{2} \leftarrow 40\frac{1}{2}$	*e*	c)	115 038.882(15)
		f	c)	115 083.223(15)
$\frac{1}{2}$		*f*	c)	115 823.453(15)
		e	c)	115 881.842(15)
$\frac{3}{2}$	$42\frac{1}{2} \leftarrow 41\frac{1}{2}$	*e*	c)	117 810.539(15)
		f	c)	117 856.886(15)
$\frac{1}{2}$		*f*	c)	118 613.134(15)
		e	c)	118 672.897(15)
$\frac{3}{2}$	$43\frac{1}{2} \leftarrow 42\frac{1}{2}$	*e*	c)	120 582.196(15)

		f	[c])	120 630.543(15)
$\frac{3}{2}$	$60\frac{1}{2} \leftarrow 59\frac{1}{2}$	*e*	[c])	167 698.922(15)
		f	[c])	167 784.918(15)
$\frac{1}{2}$		*f*	[c])	168 809.442(15)
		e	[c])	168 897.082(15)
$\frac{3}{2}$	$62\frac{1}{2} \leftarrow 61\frac{1}{2}$	*e*	[c])	173 241.877(15)
		f	[c])	173 332.621(15)
$\frac{1}{2}$		*f*	[c])	174 384.556(15)
		e	[c])	174 475.572(15)
$\frac{1}{2}$	$64\frac{1}{2} \leftarrow 63\frac{1}{2}$	*f*	[c])	179 959.198(15)
$\frac{3}{2}$	$67\frac{1}{2} \leftarrow 66\frac{1}{2}$	*e*	[c])	187 099.101(15)
$\frac{1}{2}$		*f*	[c])	188 320.242(15)
		e	[c])	188 419.784(15)
$\frac{3}{2}$	$77\frac{1}{2} \leftarrow 76\frac{1}{2}$	*e*	[c])	214 812.643(15)
		f	[c])	214 939.775(15)
$\frac{1}{2}$		*f*	[c])	216 182.376(15)
		e	[c])	216 299.186(15)
$\frac{3}{2}$	$78\frac{1}{2} \leftarrow 77\frac{1}{2}$	*e*	[c])	217 583.914(15)
		f	[c])	217 713.497(15)
$\frac{1}{2}$		*f*	[c])	218 967.931(15)
		e	[c])	219 086.404(15)

[a]) States with parity equal to $\pm(-1)^{J-0.5}$ are labeled *e* and *f* respectively.
[b]) The figures in parentheses are the authors' estimates of experimental uncertainty (1σ).
[c]) Proton hyperfine structure not resolved.

Molecular parameters for $^{12}C_6{}^1H$

Parameter		Value	Method	Ref.
State: electronic $\tilde{X}\,^2\Pi$; vibrational zero point level				
B	[MHz]	1 391.186 12(3) [a])	MW	99Li
D	[Hz]	40.49(1)		
A	[GHz]	– 450. 961(46)		
γ	[MHz]	– 213.5(1)		
p	[MHz]	– 24.62(1)		
p_D	[kHz]	2.738(5)		
p_H	[kHz]	$-70.1(5)\times10^{-6}$		
q	[MHz]	– 1.457 2(2) [b])		
q_D	[Hz]	15.70(3)		
$h_{3/2}(^1H)$ [c])	[MHz]	0.60(67)		
$b(^1H)$	[MHz]	– 13.0(15)		

[a]) The numbers in parentheses are 1 standard deviation of the least-squares fit, in units of the last quoted decimal place.
[b]) The sign of *q* was assumed to be negative.
[c]) $h_{3/2}(^1H) = a + (b+c)/2$.

Microwave data for $^{12}C_6{}^2H$ (C_6D)

Transition				ν	Ref.
spin Ω	rotational $J' - J''$	parity e/f [a])	hyperfine $F' - F''$	[MHz]	
State: electronic $\tilde{X}\,^2\Pi$; vibrational zero point level					
$\frac{3}{2}$	$6\frac{1}{2} \leftarrow 5\frac{1}{2}$	*e*	$7\frac{1}{2} \leftarrow 6\frac{1}{2}$	17 202.424(5) [b])	99Li
			$6\frac{1}{2} \leftarrow 5\frac{1}{2}$	17 202.443(5)	
			$5\frac{1}{2} \leftarrow 4\frac{1}{2}$	17 202.452(5)	

		f	$7\frac{1}{2} \leftarrow 6\frac{1}{2}$	17 203.495(5)	
			$6\frac{1}{2} \leftarrow 5\frac{1}{2}$	17 203.503(5)	
			$5\frac{1}{2} \leftarrow 4\frac{1}{2}$	17203.511(5)	
	$7\frac{1}{2} \leftarrow 6\frac{1}{2}$	e	$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	19 848.862(5)	
			$7\frac{1}{2} \leftarrow 6\frac{1}{2}$	19 848.878(5)	
			$6\frac{1}{2} \leftarrow 5\frac{1}{2}$	19 848.889(5)	
		f	$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	19 850.277(5)	
			$7\frac{1}{2} \leftarrow 6\frac{1}{2}$	19 850.292(5)	
			$6\frac{1}{2} \leftarrow 5\frac{1}{2}$	19 850.304(5)	
	$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	e	$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	22 495.278(2)	
			$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	22 495.293(2)	
			$7\frac{1}{2} \leftarrow 6\frac{1}{2}$	22 495.303(2)	
		f	$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	22 497.096(2)	
			$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	22 497.110(2)	
			$7\frac{1}{2} \leftarrow 6\frac{1}{2}$	22 497.120(2)	
	$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	e	$10\frac{1}{2} \leftarrow 9\frac{1}{2}$	25 141.668(2)	
			$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	25 141.682(2)	
			$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	25 141.695(2)	
		f	$10\frac{1}{2} \leftarrow 9\frac{1}{2}$	25 143.940(2)	
			$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	25 143.953(2)	
			$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	25 143.964(2)	
$\frac{3}{2}$	$53\frac{1}{2} \leftarrow 52\frac{1}{2}$	e	c)	141 565.117(15)	99Li
		f	c)	141 628.682(15)	
$\frac{1}{2}$		f	c)	142 484.522(15)	
		e	c)	142 554.673(15)	
$\frac{3}{2}$	$54\frac{1}{2} \leftarrow 53\frac{1}{2}$	e	c)	144 210.839(15)	
		f	c)	144 276.453(15)	
$\frac{1}{2}$		f	c)	145 145.990(15)	
		e	c)	145 217.542(15)	
$\frac{3}{2}$	$55\frac{1}{2} \leftarrow 54\frac{1}{2}$	e	c)	146 856.550(15)	
		f	c)	146 924.233(15)	
$\frac{1}{2}$		f	c)	147 807.355(15)	
		e	c)	147 880.310(15)	
$\frac{3}{2}$	$56\frac{1}{2} \leftarrow 55\frac{1}{2}$	e	c)	149 502.225(15)	
		f	c)	149 572.031(15)	
$\frac{1}{2}$		f	c)	150 468.618(15)	
		e	c)	150 542.993(15)	
$\frac{3}{2}$	$57\frac{1}{2} \leftarrow 56\frac{1}{2}$	e	c)	152 147.890(15)	
		f	c)	152 219.815(15)	
$\frac{1}{2}$		f	c)	153 129.787(15)	
		e	c)	153 205.605(15)	
$\frac{3}{2}$	$58\frac{1}{2} \leftarrow 57\frac{1}{2}$	e	c)	154 793.536(15)	
		f	c)	154 867.614(15)	
$\frac{1}{2}$		f	c)	155 790.833(15)	
		e	c)	155 868.123(15)	
$\frac{3}{2}$	$59\frac{1}{2} \leftarrow 58\frac{1}{2}$	e	c)	157 439.178(15)	
		f	c)	157 515.424(15)	

$\frac{1}{2}$		f	c)	158 451.835(15)
		e	c)	158 530.540(15)

a) States with parity equal to ± (–1) $^{J-0.5}$ are labeled *e* and *f* respectively.
b) The figures in parentheses are the authors' estimates of experimental uncertainty (1σ).
c) Deuteron hyperfine structure not resolved.

Molecular parameters for $^{12}C_6{}^2H$ (C_6D)

Parameter		Value	Method	Ref.
State: electronic $\tilde{X}\,^2\Pi$; vibrational zero point level				
B	[MHz]	1 327.853 74(5) a)	MW	99Li
D	[Hz]	36.04(1)		
A	[GHz]	– 453. 514(48)		
γ	[MHz]	– 226.1(1)		
p	[MHz]	– 21.32(10)		
p_D	[kHz]	1.97(1)		
q	[MHz]	– 1.374 1(6) b)		
q_D	[Hz]	15.2(1)		
$h_{3/2}(^2H)$ c)	[MHz]	0.12(26)		
$b(^2H)$	[MHz]	– 3.20(72)		

a) The numbers in parentheses are 1 standard deviation of the least-squares fit, in units of the last quoted decimal place.
b) The sign of *q* was assumed to be negative.
c) $h_{3/2}(^2H) = a + (b+c)/2$.

References for C_6H

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3.2.1.2.6 C_7H

Microwave data for $^{12}C_7{}^1H$

Transition				ν	
spin Ω	rotational $J' - J''$	parity e/f a)	hyperfine $F' - F''$	[MHz]	Ref.
State: electronic $\tilde{X}\,^2\Pi$; vibrational zero point level					
$\frac{1}{2}$	$4\frac{1}{2} \leftarrow 3\frac{1}{2}$	e	5 ← 4	7 869.429(5) b)	99McC
			4 ← 3	7 869.698(5)	
		f	5 ← 4	7 871.093(5)	
			4 ← 3	7 871.398(5)	
	$5\frac{1}{2} \leftarrow 4\frac{1}{2}$	e	6 ← 5	9 618.440(5)	
			5 ← 4	9 618.626(5)	
		f	6 ← 5	9 620.086(5)	
			5 ← 4	9 620.291(5)	
	$6\frac{1}{2} \leftarrow 5\frac{1}{2}$	e	7 ← 6	11 367.433(5)	
			6 ← 5	11 367.573(5)	
		f	7 ← 6	11 369.069(5)	
			6 ← 5	11 369.219(5)	
	$7\frac{1}{2} \leftarrow 6\frac{1}{2}$	e	8 ← 7	13116.414(5)	
			7 ← 6	13116.524(5)	
		f	8 ← 7	13118.045(5)	
			7 ← 6	13 118.162(5)	
	$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	e	9 ← 8	14 865.391(5)	

			8 ← 7	14 865.483(5)	
		f	9 ← 8	14 867.015(5)	
			8 ← 7	14 867.113(5)	
	$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	*e*	10 ← 9	16 614.362(5)	
			9 ← 8	16 614.438(5)	
		f	10 ← 9	16 615.986(5)	
			9 ← 8	16 616.066(5)	
	$10\frac{1}{2} \leftarrow 9\frac{1}{2}$	*e*	11 ← 10	18 363.327(5)	
			10 ← 9	18 363.394(5)	
		f	11 ← 10	18 364.950(5)	
			10 ← 9	18 365.022(5)	
$\frac{3}{2}$	$39\frac{1}{2} \leftarrow 38\frac{1}{2}$	*e.f*		69 238.956(27)	96Tr
$\frac{1}{2}$	$65\frac{1}{2} \leftarrow 64\frac{1}{2}$	*e*		114 545.484(17)	
		f		114 547.516(17)	
$\frac{1}{2}$	$68\frac{1}{2} \leftarrow 67\frac{1}{2}$	*e*		119 790.761(19)	
		f		119 792.818(23)	
$\frac{3}{2}$		*f*		120 061.581(19)	
		e		120 062.070(20)	
$\frac{1}{2}$	$69\frac{1}{2} \leftarrow 68\frac{1}{2}$	*e*		121 539.166(20)	
		f		121 541.235(21)	
$\frac{3}{2}$		*f*		121 813.828(26)	
		e		121 814.326(21)	
$\frac{1}{2}$	$70\frac{1}{2} \leftarrow 69\frac{1}{2}$	*e*		123 287.525(21)	
		f		123 289.623(19)	
$\frac{3}{2}$		*f*		123 566.041(19)	
		e		123 566.548(19)	
$\frac{1}{2}$	$71\frac{1}{2} \leftarrow 70\frac{1}{2}$	*e*		125 035.840(22)	
		f		125 037.980(19)	
$\frac{3}{2}$		*f*		125 318.202(25)	
		e		125 318.818(41)	
$\frac{1}{2}$	$72\frac{1}{2} \leftarrow 71\frac{1}{2}$	*e*		126 784.225(18)	
		f		126 786.370(20)	
$\frac{3}{2}$		*f*		127 070.366(25)	
		e		127 070.980(23)	
$\frac{1}{2}$	$73\frac{1}{2} \leftarrow 72\frac{1}{2}$	*e*		128 532.558(21)	
		f		128 534.714(20)	
$\frac{3}{2}$		*f*		128 822.590(21)	
		e		128 823.137(20)	
$\frac{1}{2}$	$74\frac{1}{2} \leftarrow 73\frac{1}{2}$	*e*		130 280.883(19)	
		f		130 283.006(19)	
$\frac{3}{2}$		*f*		130 574.674(32)	
		e		130 575(271(24)	
$\frac{1}{2}$	$91\frac{1}{2} \leftarrow 90\frac{1}{2}$	*e*		159 999.105(26)	
$\frac{3}{2}$		*f*		160 357.189(25)	
		e		160 358.125(28)	
$\frac{1}{2}$	$93\frac{1}{2} \leftarrow 92\frac{1}{2}$	*e*		163 497.467(19)	
$\frac{3}{2}$		*f*		163 860.550(26)	
		e		163 861.470(27)	
$\frac{1}{2}$	$95\frac{1}{2} \leftarrow 94\frac{1}{2}$	*e*		166 990.723(23)	
		f		166 993.258(17)	

$\frac{3}{2}$		*f*	167 363.752(23)
		e	167 364.706(29)
$\frac{1}{2}$	$96\frac{1}{2} \leftarrow 95\frac{1}{2}$	*e*	168 738.651(22)
		f	168 741.138(25)
$\frac{3}{2}$		*f*	169 115.337(27)
		e	166 116.259(26)
$\frac{1}{2}$	$108\frac{1}{2} \leftarrow 107\frac{1}{2}$	*e*	189 711,069(26)
$\frac{3}{2}$		*f*	190 131.863(26)
		e	190 133.014(30)
$\frac{3}{2}$	$111\frac{1}{2} \leftarrow 110\frac{1}{2}$	*f*	195 385.245(37)
		e	195 386.442(27)

[a]) States with parity equal to ± $(-1)^{J-0.5}$ are labeled *e* and *f* respectively.
[b]) The figures in parentheses are the authors' estimates of experimental uncertainty (1σ).

Molecular parameters for $^{12}C_7\,^1H$

Parameter		Value	Method	Ref.
State: electronic $\tilde{X}\,^2\Pi$; vibrational zero point level				
B	[MHz]	875.484 09(5) [a])	MW	99McC
D	[kHz]	0.011 290(3)		
A	[GHz]	784. 700(2100)		
γ	[MHz]	– 16.6(23)		
$p + 2q$	[MHz]	1.597(4)		
q	[MHz]	– 0.016 3(1)		
$h_{1/2}(^1H)$ [b])	[MHz]	10.2(20)		
$b(^1H)$	[MHz]	– 19.2(35)		
$d(^1H)$	[MHz]	6.51(51)		

[a]) The numbers in parentheses are 1 standard deviation of the least-squares fit, in units of the last quoted decimal place.
[b]) $h_{1/2}(^1H) = a - (b+c)/2$.

Microwave data for $^{12}C_7\,^2H$ (C_7D)

Transition			ν	Ref.
spin Ω	rotational $J' - J''$	parity e/f [a])	[MHz]	
State: electronic $\tilde{X}\,^2\Pi$; vibrational zero point level				
$\frac{1}{2}$	$4\frac{1}{2} \leftarrow 3\frac{1}{2}$	*e*	10 930.149(5) [b])	99McC
$\frac{3}{2}$	$70\frac{1}{2} \leftarrow 69\frac{1}{2}$	*f*	118 802.342(21)	
		e	118 802.801(20)	
$\frac{1}{2}$	$71\frac{1}{2} \leftarrow 70\frac{1}{2}$	*e*	120 225.537(17)	
		f	120 227.599(17)	
$\frac{3}{2}$		*f*	120 486.975(22)	
		e	120 487.552(23)	
$\frac{1}{2}$	$72\frac{1}{2} \leftarrow 71\frac{1}{2}$	*e*	121 906.623(20)	
		f	121 908.626(22)	
$\frac{1}{2}$	$73\frac{1}{2} \leftarrow 72\frac{1}{2}$	*e*	123 587.735(27)	
		f	123 589.830(21)	
$\frac{1}{2}$	$74\frac{1}{2} \leftarrow 73\frac{1}{2}$	*e*	125 268.794(33)	
		f	125 270.918(25)	
$\frac{3}{2}$		*f*	125 540.936(43)	
		e	125 541.477(35)	
$\frac{3}{2}$	$80\frac{1}{2} \leftarrow 79\frac{1}{2}$	*f*	135 648.176(29)	
		e	135 648.815(22)	

$\frac{1}{2}$	$84\frac{1}{2} \leftarrow 83\frac{1}{2}$	*e*	142 078.514(20)
		f	142 080.828(24)
$\frac{1}{2}$	$90\frac{1}{2} \leftarrow 89\frac{1}{2}$	*e*	152 163.417(17)
		f	152 165.904(23)
$\frac{3}{2}$		*f*	152 491.712(71)
		e	152 492.603(44)
$\frac{1}{2}$	$92\frac{1}{2} \leftarrow 91\frac{1}{2}$	*e*	155 524.973(31)
		f	155 527.389(27)
$\frac{3}{2}$		*f*	155 860.287(27)
		e	155 861.131(27)

[a]) States with parity equal to ± $(-1)^{J-0.5}$ are labeled *e* and *f* respectively.
[b]) The figures in parentheses are the authors' estimates of experimental uncertainty (1σ).

Molecular parameters for $^{12}C_7{}^2H$ (C_7D)

Parameter		Value	Method	Ref.
State: electronic $\tilde{X}\,^2\Pi$; vibrational zero point level				
B	[MHz]	841.761 61(13) [a])	MW	99McC
D	[kHz]	0.010 26(1)		
A	[GHz]	784.046(27)		
γ	[MHz]	– 15.91 [b])		
$p + 2q$	[MHz]	1.499(9)		
q	[MHz]	– 0.017 8(3)		

[a]) The numbers in parentheses are 1 standard deviation of the least-squares fit, in units of the last quoted decimal place.
[b]) Estimated from the value of γ for C_7H, scaled as *B*.

References for C_7H

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99McC McCarthy, M.C., Travers, M.J., Kovács, A., Gottlieb, C.A., Thaddeus, P. : Astrophys. J. Supp. **113** (1999) 105.

3.2.1.2.7 C_8H

Microwave data for $^{12}C_8{}^1H$

Transition				ν	Ref.
spin Ω	rotational $J' - J''$	parity e/f [a])	hyperfine $F' - F''$	[MHz]	
State: electronic $\tilde{X}\,^2\Pi$; vibrational zero point level					
$\frac{3}{2}$	$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	*e*	9 ← 8	9 973.397(2) [b])	99McC
			8 ← 7	9 973.379(2)	
		f	9 ← 8	9 973.397(2)	
			8 ← 7	9 973.419(2)	
	$10\frac{1}{2} \leftarrow 9\frac{1}{2}$	*e*	11 ← 10	12 320.020(2)	
			10 ← 9	12 320.040(2)	
		f	11 ← 10	12 320.079(2)	
			10 ← 9	12 320.100(2)	
	$11\frac{1}{2} \leftarrow 10\frac{1}{2}$	*e*	12 ← 11	13 493.349(2)	
			11 ← 10	13 493.367(2)	
		f	12 ← 11	13 493.422(2)	
			11 ← 10	13 493.440(2)	
	$12\frac{1}{2} \leftarrow 11\frac{1}{2}$	*e*	13 ← 12	14 666.676(2)	
			12 ← 11	14 666.694(2)	

		f	13 ← 12	14 666.762(2)	
			12 ← 11	14 666. 780(2)	
	$15\frac{1}{2} \leftarrow 14\frac{1}{2}$	*e*	16 ← 15	18 186.647(2)	
			15 ← 14	18 186.665(2)	
		f	16 ← 15	18 186.779(2)	
			15 ← 14	18 186.794(2)	
	$17\frac{1}{2} \leftarrow 16\frac{1}{2}$	*e*	18 ← 17	20 533.284(2)	
			17 ← 16	20 533.300(2)	
		f	18 ← 17	20 533.452(2)	
			17 ← 16	20 533.468(2)	
$\frac{3}{2}$	$26\frac{1}{2} \leftarrow 25\frac{1}{2}$	*e*	[c])	31 092.1 [d])	96Ce
	$27\frac{1}{2} \leftarrow 26\frac{1}{2}$	*f*	[c])	32 266.6 [d])	
	$30\frac{1}{2} \leftarrow 29\frac{1}{2}$	*f*	[c])	35 787.5 [d])	
	$31\frac{1}{2} \leftarrow 30\frac{1}{2}$	*f*	[c])	36 960.8 [d])	
	$34\frac{1}{2} \leftarrow 33\frac{1}{2}$	*f*	[c])	40 480 [d])	
	$35\frac{1}{2} \leftarrow 34\frac{1}{2}$	*f*	[c])	41 653 [d])	
	$42\frac{1}{2} \leftarrow 41\frac{1}{2}$	*e*	[c])	49 865.4 [d])	
	$63\frac{1}{2} \leftarrow 62\frac{1}{2}$	*f*	[c])	74 503.0(25) [d])	
	$68\frac{1}{2} \leftarrow 67\frac{1}{2}$	*e*	[c])	80 367.224(24)	96McC
	$70\frac{1}{2} \leftarrow 69\frac{1}{2}$	*e*	[c])	82 712.7(17) [d])	96Ce
$\frac{3}{2}$	$71\frac{1}{2} \leftarrow 70\frac{1}{2}$	*e*	[c])	83 886.508(24)	96McC
		f	[c])	83 889.245(22)	
$\frac{3}{2}$	$72\frac{1}{2} \leftarrow 71\frac{1}{2}$	*e*	[c])	85 059.531(18)	
		f	[c])	85 062.314(19)	
$\frac{3}{2}$	$73\frac{1}{2} \leftarrow 72\frac{1}{2}$	*e*	[c])	86 232.571(21)	
		f	[c])	86 235.410(21)	
$\frac{3}{2}$	$75\frac{1}{2} \leftarrow 74\frac{1}{2}$	*e*	[c])	88 578.640(22)	
		f	[c])	88 581.622(27)	
$\frac{3}{2}$	$76\frac{1}{2} \leftarrow 75\frac{1}{2}$	*e*	[c])	89 751.636(21)	
		f	[c])	89 754.746(20)	
$\frac{1}{2}$	$78\frac{1}{2} \leftarrow 77\frac{1}{2}$	*e*	[c])	92 279.781(21)	
		f	[c])	92 286.773(26)	
$\frac{1}{2}$	$79\frac{1}{2} \leftarrow 78\frac{1}{2}$	*e*	[c])	93 455.122(21)	
		f	[c])	93 462.038(21)	
$\frac{1}{2}$	$80\frac{1}{2} \leftarrow 79\frac{1}{2}$	*e*	[c])	94 630.469(21)	
		f	[c])	94 637.270(21)	
$\frac{3}{2}$	$81\frac{1}{2} \leftarrow 80\frac{1}{2}$	*e*	[c])	95 616.577(21)	
		f	[c])	95 620.109(23)	
$\frac{1}{2}$		*e*	[c])	95 805.803(19)	
		f	[c])	95 812.528(19)	
$\frac{3}{2}$	$82\frac{1}{2} \leftarrow 81\frac{1}{2}$	*e*	[c])	96 789.638(21)	
		f	[c])	96 793.161(18)	
$\frac{1}{2}$		*e*	[c])	96 981.193(22)	
		f	[c])	96 987.806(19)	
$\frac{3}{2}$	$83\frac{1}{2} \leftarrow 82\frac{1}{2}$	*e*	[c])	97 962.497(18)	
		f	[c])	97 966.175(18)	
$\frac{1}{2}$		*e*	[c])	98 156.478(18)	
		f	[c])	98 163.044(22)	
$\frac{3}{2}$	$84\frac{1}{2} \leftarrow 83\frac{1}{2}$	*e*	[c])	99 135.362(22)	

		f		c)	99 139.267(24)
½		e		c)	99 331.750(23)
		f		c)	99 338.311(17)

a) States with parity equal to ± $(-1)^{J-0.5}$ are labeled *e* and *f* respectively.
b) The figures in parentheses are the authors' estimates of experimental uncertainty (1σ).
c) Proton hyperfine structure not resolved.
d) Observations made by radioastronomy (less accurate than the laboratory measurements). Calculated values for these transition frequencies are available in 97McC.

Molecular parameters for $^{12}C_8\,^1H$

Parameter		Value	Method	Ref.
State: electronic $\tilde{X}\,^2\Pi$; vibrational zero point level				
B	[MHz]	597.263 83(3) a)	MW	99McC
D	[Hz]	4.73(1)		
A	[GHz]	– 579.980(24)		
p	[MHz]	10.438(15)		
q	[MHz]	– 0.084 4(2) b)		
$h_{3/2}(^1H)$ c)	[MHz]	0.42(70)		
$b(^1H)$	[MHz]	– 13.7(16)		

a) The numbers in parentheses are 1 standard deviation of the least-squares fit, in units of the last quoted decimal place.
b) The sign of *q* was assumed to be negative.
c) $h_{3/2}(^1H) = a + (b+c)/2$.

References for C_8H

96Ce Cernicharo, J., Guélin, M. : Astron. Astrophys. **309** (1996) L27.
96McC McCarthy, M.C., Travers, M.J., Kovács, A., Gottlieb, C.A., Thaddeus, P. : Astron. Astrophys. **309** (1996) L31.
97McC McCarthy, M.C., Travers, M.J., Kovács, A., Gottlieb, C.A., Thaddeus, P. : Astrophys. J. Supp.Ser, **113** (1997) 105.
99McC McCarthy, M.C., Chen, W., Apponi, A.P., Gottlieb, C.A., Thaddeus, P. : Astrophys. J. **520** (1999) 158.

3.2.1.2.8 C_9H

Microwave data for $^{12}C_9\,^1H$

Transition				ν	Ref.
spin Ω	rotational J′ – J″	parity e/f a)	hyperfine F′ – F″	[MHz]	
State: electronic $\tilde{X}\,^2\Pi$; vibrational zero point level					
½	6½ ← 5½	e	7 ← 6	5 368.954(2) b)	96McC
			6 ← 5	5 369.030(2)	
		f	7 ← 6	5 369.743(2)	
			6 ← 5	5 369.826(2)	
	7½ ← 6½	e	8 ← 7	6 195.019(2)	
			7 ← 6	6 195.081(2)	
		f	8 ← 7	6 195.808(2)	
			7 ← 6	6 195.870(2)	
	8½ ← 7½	e	9 ← 8	7 021.085(2)	
			8 ← 7	7 021.137(2)	
		f	9 ← 8	7 021.867(2)	
			8 ← 7	7 021.918(2)	
	11½ ← 10½	e	12 ←11	9 499.267(2)	
			11 ← 10	9 499.295(2)	
		f	12 ←11	9 500.045(2)	
			11 ← 10	9 500.075(2)	

$13\frac{1}{2} \leftarrow 12\frac{1}{2}$	*e*	14 ← 13	11 151.382(2)
		13 ← 12	11 151.406(2)
	f	14 ← 13	11 152.160(2)
		13 ← 12	11 152.185(2)
$14\frac{1}{2} \leftarrow 13\frac{1}{2}$	*e*	15 ← 14	11 977.437(2)
		14 ← 13	11 977.459(2)
	f	15 ← 14	11 978.214(2)
		14 ← 13	11 978.236(2)
$15\frac{1}{2} \leftarrow 14\frac{1}{2}$	*e*	16 ← 15	12 803.492(2)
		15 ← 14	12 803.513(2)
	f	16 ← 15	12 804.270(2)
		15 ← 14	12 804.288(2)
$16\frac{1}{2} \leftarrow 15\frac{1}{2}$	*e*	17 ← 16	13 629.546(2)
		16 ← 15	13 629.566(2)
	f	17 ← 16	13 630.322(2)
		16 ← 15	13 630.314(2)
$17\frac{1}{2} \leftarrow 16\frac{1}{2}$	*e*	18 ← 17	14 455.600(2)
		17 ← 16	14 455.617(2)
	f	18 ← 17	14 456.377(2)
		17 ← 16	14 456.394(2)
$18\frac{1}{2} \leftarrow 17\frac{1}{2}$	*e*	19 ← 18	15 281.653(2)
		18 ← 17	15 281.668(2)
	f	19 ← 18	15 282.429(2)
		18 ← 17	15 282.447(2)

[a]) States with parity equal to ± $(-1)^{J-0.5}$ are labeled *e* and *f* respectively.
[b]) The figures in parentheses are the authors' estimates of experimental uncertainty (1σ).

Molecular parameters for $^{12}C_9\,^1H$

Parameter		Value	Method	Ref.
State: electronic $\tilde{X}\,^2\Pi$; vibrational zero point level				
B	[MHz]	413.257 59(3) [a])	MW	96McC
D	[kHz]	0.001 92 (6)		
A	[GHz]	750. 0 [b])		
γ	[MHz]	0.0 [c])		
$p + 2q$	[MHz]	0.774 1(9)		
$h_{1/2}(^1H)$ [d])	[MHz]	5.99(92)		
$b(^1H)$	[MHz]	– 13.7(16)		
$d(^1H)$	[MHz]	2.94(34)		

[a]) The numbers in parentheses are 1 standard deviation of the least-squares fit, in units of the last quoted decimal place.
[b]) Estimated from C_7H.
[c]) Constrained to the value in the least-squares fit.
[d]) $h_{1/2}(^1H) = a - (b+c)/2$.

References for C_9H

96McC McCarthy, M.C., Travers, M.J., Kalmus, P., Gottlieb, C.A., Thaddeus, P. : Astrophys. J. **467**(1996) L125.

3.2.1.2.9 $C_{10}H$

Microwave data for $^{12}C_{10}{}^{1}H$

Transition			ν	Ref.
spin Ω	rotational J′ – J″	parity e/f [a])	[MHz]	
State: electronic $\tilde{X}\,^2\Pi$; vibrational zero point level				
$\frac{3}{2}$	$11\frac{1}{2} \leftarrow 10\frac{1}{2}$	e,f	6 928.943(4) [b])	98Go
	$12\frac{1}{2} \leftarrow 11\frac{1}{2}$	e,f	7 531.461(4)	
	$13\frac{1}{2} \leftarrow 12\frac{1}{2}$	e,f	8 133.975(4)	
	$14\frac{1}{2} \leftarrow 13\frac{1}{2}$	e,f	8 736.490(4)	
	$15\frac{1}{2} \leftarrow 14\frac{1}{2}$	e,f	9 339.006(4)	
	$16\frac{1}{2} \leftarrow 15\frac{1}{2}$	e,f	9 941.520(4)	
	$17\frac{1}{2} \leftarrow 16\frac{1}{2}$	e,f	10 544.037(4)	
	$19\frac{1}{2} \leftarrow 18\frac{1}{2}$	e	11 749.053(4)	
		f	11 749.071(4)	
	$20\frac{1}{2} \leftarrow 19\frac{1}{2}$	e	12 351.566(4)	
		f	12 351.588(4)	
	$21\frac{1}{2} \leftarrow 20\frac{1}{2}$	e	12 954.075(4)	
		f	12 954.101(4)	

[a]) States with parity equal to ± $(-1)^{J-0.5}$ are labeled *e* and *f* respectively.
[b]) The figures in parentheses are the authors' estimates of experimental uncertainty (1σ).

Molecular parameters for $^{12}C_{10}{}^{1}H$

Parameter		Value	Method	Ref.
State: electronic $\tilde{X}\,^2\Pi$; vibrational zero point level				
B	[MHz]	301.409 92(10) [a])	MW	98Go
D	[Hz]	0.88(13)		
A	[GHz]	– 600 [b])		
$p + 2q$	[MHz]	10.438(15)		
q	[MHz]	– 0.013(2) [c])		

[a]) The numbers in parentheses are 1 standard deviation of the least-squares fit, in units of the last quoted decimal place.
[b]) Value estimated from that of C_8H (97McC).
[c]) The sign of *q* was assumed to be negative.

References for $C_{10}H$

98Go Gottlieb, C.A., McCarthy, Travers, M.J., Grabow, J.-U., Thaddeus, P. : J. Chem. Phys. **109** (1998) 5433.

3.2.1.2.10 $C_{11}H$

Microwave data for $^{12}C_{11}{}^{1}H$

Transition				ν	Ref.
spin Ω	rotational J′ – J″	parity e/f [a])	hyperfine F′ – F″	[MHz]	
State: electronic $\tilde{X}\,^2\Pi$; vibrational zero point level					
$\frac{1}{2}$	$13\frac{1}{2} \leftarrow 12\frac{1}{2}$	e	14 ← 13	6 124.228(4) [b])	97aMcC
			13 ← 12	6 124.244(4)	
		f	14 ← 13	6 124.654(4)	
			13 ← 12	6 124.668(4)	
	$14\frac{1}{2} \leftarrow 13\frac{1}{2}$	e	15 ← 14	6 577.890(4)	
			14 ← 13	6 577.900(4)	

	f	$15 \leftarrow 14$	6 578.316(4)
		$14 \leftarrow 13$	6 578.330(4)
$15\frac{1}{2} \leftarrow 14\frac{1}{2}$	*e*	$16 \leftarrow 15$	7 031.552(4)
		$15 \leftarrow 14$	7 031.565(4)
	f	$16 \leftarrow 15$	7 031.978(4)
		$15 \leftarrow 14$	7 031.988(4)
$16\frac{1}{2} \leftarrow 15\frac{1}{2}$	*e*	$17 \leftarrow 16$	7 485.212(4)
		$16 \leftarrow 15$	7 485.223(4)
	f	[c])	7 485.644(4)
$19\frac{1}{2} \leftarrow 18\frac{1}{2}$	*e*	[c])	8 846.202(4)
$20\frac{1}{2} \leftarrow 19\frac{1}{2}$	*e*	$21 \leftarrow 20$	9 299.857(4)
		$20 \leftarrow 19$	9 299.868(4)
	f	[c])	9 300.291(4)
$21\frac{1}{2} \leftarrow 20\frac{1}{2}$	*e*	[c])	9 753.520(4)
	f	[c])	9 753.950(4)
$22\frac{1}{2} \leftarrow 21\frac{1}{2}$	*e*	[c])	10 207.187(4)
	f	[c])	10 207.605(4)
$23\frac{1}{2} \leftarrow 22\frac{1}{2}$	*e*	[c])	10 660.841(4)
	f	[c])	10 660.265(4)
$24\frac{1}{2} \leftarrow 23\frac{1}{2}$	*e*	[c])	11 114.504(4)
	f	[c])	11 114.928(4)
$25\frac{1}{2} \leftarrow 24\frac{1}{2}$	*e*	[c])	11 568.164(4)
	f	[c])	11 568.590(4)
$26\frac{1}{2} \leftarrow 25\frac{1}{2}$	*e*	[c])	12 021.818(4)
	f	[c])	12 022.245(4)

[a]) States with parity equal to $\pm(-1)^{J-0.5}$ are labeled *e* and *f* respectively.
[b]) The figures in parentheses are the authors' estimates of experimental uncertainty (1σ).

Molecular parameters for $^{12}C_{11}{}^{1}H$

Parameter		Value	Method	Ref.
State: electronic $\tilde{X}\,^2\Pi$; vibrational zero point level				
B	[MHz]	226.900 25(3) [a])	MW	97aMcC
D	[Hz]	0.543(36)		
A	[GHz]	750. 0 [b])		
γ	[MHz]	0.0 [c])		
$p + 2q$	[MHz]	0 425 9(8)		
$h_{1/2}(^1H)$ [d])	[MHz]	4.87(42)		

[a]) The numbers in parentheses are 1 standard deviation of the least-squares fit, in units of the last quoted decimal place.
[b]) Estimated from C_7H (97bMcC).
[c]) Constrained to the value in the least-squares fit.
[d]) $h_{1/2}(^1H) = a - (b+c)/2$.

References for $C_{11}H$

97aMcC McCarthy, M.C., Travers, M.J., Kalmus, P., Gottlieb, C.A., Thaddeus, P. : Chem. Phys. Lett. **264** (1997) 252.

97bMcC McCarthy, M.C., Travers, M.J., Kovács, A., Gottlieb, C.A., Thaddeus, P. : Astrophys. J. Supp. Ser, **113** (1997) 105.

3.2.1.2.11 $C_{12}H$

Microwave data for $^{12}C_{12}{}^{1}H$

Transition spin Ω	rotational $J' - J''$	parity e/f [a])	ν [MHz]	Ref.
State: electronic $\tilde{X}\,^2\Pi$; vibrational zero point level				
$\frac{3}{2}$	$20\frac{1}{2} \leftarrow 19\frac{1}{2}$	*e,f*	7 164.044(4) [b])	98Go
	$23\frac{1}{2} \leftarrow 22\frac{1}{2}$	*e,f*	8 212.437(4)	
	$24\frac{1}{2} \leftarrow 23\frac{1}{2}$	*e,f*	8 561.901(4)	
	$26\frac{1}{2} \leftarrow 25\frac{1}{2}$	*e,f*	9 260.828(4)	
	$27\frac{1}{2} \leftarrow 26\frac{1}{2}$	*e,f*	9 610.294(4)	
	$28\frac{1}{2} \leftarrow 27\frac{1}{2}$	*e,f*	9 959.756(4)	
	$29\frac{1}{2} \leftarrow 28\frac{1}{2}$	*e,f*	10 309.220(4)	
	$30\frac{1}{2} \leftarrow 29\frac{1}{2}$	*e,f*	10 658.683(4)	
	$31\frac{1}{2} \leftarrow 30\frac{1}{2}$	*e,f*	11 008.145(4)	
	$32\frac{1}{2} \leftarrow 31\frac{1}{2}$	*e,f*	11 357.608(4)	
	$33\frac{1}{2} \leftarrow 32\frac{1}{2}$	*e,f*	11 707.072(4)	
	$35\frac{1}{2} \leftarrow 34\frac{1}{2}$	*e,f*	12 405.997(4)	
	$37\frac{1}{2} \leftarrow 36\frac{1}{2}$	*e,f*	13 104.920(4)	
	$39\frac{1}{2} \leftarrow 38\frac{1}{2}$	*e,f*	13 803.840(4)	
	$40\frac{1}{2} \leftarrow 39\frac{1}{2}$	*e,f*	14 153.301(4)	
	$43\frac{1}{2} \leftarrow 42\frac{1}{2}$	*e*	15 201.675(4)	
		f	15 201.691(4)	
	$44\frac{1}{2} \leftarrow 43\frac{1}{2}$	*e*	15 551.136(4)	
		f	15 551.152(4)	
	$45\frac{1}{2} \leftarrow 44\frac{1}{2}$	*e*	15 900.594(4)	
		f	15 900.612(4)	
	$46\frac{1}{2} \leftarrow 45\frac{1}{2}$	*e*	16 250.062(4)	
		f	16 250.076(4)	

[a]) States with parity equal to $\pm (-1)^{J-0.5}$ are labeled *e* and *f* respectively.
[b]) The figures in parentheses are the authors' estimates of experimental uncertainty (1σ).

Molecular parameters for $^{12}C_{12}{}^{1}H$

Parameter		Value	Method	Ref.
State: electronic $\tilde{X}\,^2\Pi$; vibrational zero point level				
B	[MHz]	174.783 87(10) [a])	MW	98Go
D	[Hz]	0.261(3)		
A	[GHz]	– 600 [b])		
q	[MHz]	– 0.0023(2) [c])		

[a]) The numbers in parentheses are 1 standard deviation of the least-squares fit, in units of the last quoted decimal place.
[b]) Value estimated from that of C_8H (97McC).
[c]) The sign of q was assumed to be negative, the same as C_8H.

References for $C_{12}H$

97McC McCarthy, M.C., Travers, M.J., Kovács, A., Gottlieb, C.A., Thaddeus, P. : Astrophys. J. Supp. Ser, **113** (1997) 105.

98Go Gottlieb, C.A., McCarthy, Travers, M.J., Grabow, J.-U., Thaddeus, P. : J. Chem. Phys. **109** (1998) 5433.

3.2.1.2.12 $C_{13}H$

Microwave data for $^{12}C_{13}{}^{1}H$

Transition			ν [MHz]	Ref.
spin Ω	rotational $J' - J''$	parity e/f [a])		
State: electronic $\tilde{X}\,^2\Pi$; vibrational zero point level				
$\frac{1}{2}$	$21\frac{1}{2} \leftarrow 20\frac{1}{2}$	*e*	5 920.318(4) [b])	98Go
		f	5 920.570(4)	
	$23\frac{1}{2} \leftarrow 22\frac{1}{2}$	*e*	6 471.049(4)	
		f	6 471.309(4)	
	$24\frac{1}{2} \leftarrow 23\frac{1}{2}$	*e*	6 746.418(4)	
		f	6 476.677(4)	
	$25\frac{1}{2} \leftarrow 24\frac{1}{2}$	*e*	7 021.790(4)	
		f	7 022.044(4)	
	$26\frac{1}{2} \leftarrow 25\frac{1}{2}$	*e*	7 297.157(4)	
		f	7 297.415(4)	
	$27\frac{1}{2} \leftarrow 26\frac{1}{2}$	*e*	7 572.527(4)	
		f	7 572.781(4)	
	$28\frac{1}{2} \leftarrow 27\frac{1}{2}$	*e*	[c])	
		f	7848.150(4)	
	$29\frac{1}{2} \leftarrow 28\frac{1}{2}$	*e*	8123.263(4)	
		f	8123.518(4)	
	$30\frac{1}{2} \leftarrow 29\frac{1}{2}$	*e*	8 398.630(4)	
		f	8 398.882(4)	
	$31\frac{1}{2} \leftarrow 30\frac{1}{2}$	*e*	[c])	
		f	8 674.254(4)	

[a]) States with parity equal to $\pm(-1)^{J-0.5}$ are labeled *e* and *f* respectively.
[b]) The figures in parentheses are the authors' estimates of experimental uncertainty (1σ).
[c]) Lower (*e*) component of $C_{13}H$ coincides with upper component of C_9H.

Molecular parameters for $^{12}C_{13}{}^{1}H$

Parameter		Value	Method	Ref.
State: electronic $\tilde{X}\,^2\Pi$; vibrational zero point level				
B	[MHz]	137.710 19(3) [a])	MW	98Go
D	[Hz]	0.187(20)		
A	[GHz]	750. 0 [b])		
γ	[MHz]	0.0 [c])		
$p + 2q$	[MHz]	0 256(1)		

[a]) The numbers in parentheses are 1 standard deviation of the least-squares fit, in units of the last quoted decimal place.
[b]) Estimated from C_7H (97McC).
[c]) Constrained to the value in the least-squares fit.

References for $C_{13}H$

97McC McCarthy, M.C., Travers, M.J., Kovács, A., Gottlieb, C.A., Thaddeus, P. : Astrophys. J. Supp. Ser, **113** (1997) 105.

98Go Gottlieb, C.A., McCarthy, Travers, M.J., Grabow, J.-U., Thaddeus, P. : J. Chem.Phys. **109** (1998) 5433.

3.2.1.2.13 $C_{14}H$

Microwave data for $^{12}C_{14}{}^{1}H$

Transition			ν	Ref.
spin Ω	rotational $J' - J''$	parity e/f [a])	[MHz]	
State: electronic $\tilde{X}\,^2\Pi$; vibrational zero point level				
$\frac{3}{2}$	$26\frac{1}{2} \leftarrow 25\frac{1}{2}$	*e,f*	5 841.731(4) [b])	98Go
	$27\frac{1}{2} \leftarrow 26\frac{1}{2}$	*e,f*	6 062.168(4)	
	$28\frac{1}{2} \leftarrow 27\frac{1}{2}$	*e,f*	6 282.612(4)	
	$29\frac{1}{2} \leftarrow 28\frac{1}{2}$	*e,f*	6 503.053(4)	
	$33\frac{1}{2} \leftarrow 32\frac{1}{2}$	*e,f*	7 384.820(4)	
	$34\frac{1}{2} \leftarrow 33\frac{1}{2}$	*e,f*	7 605.264(4)	
	$35\frac{1}{2} \leftarrow 34\frac{1}{2}$	*e,f*	7 825.704(4)	
	$36\frac{1}{2} \leftarrow 35\frac{1}{2}$	*e,f*	8 046.145(4)	
	$37\frac{1}{2} \leftarrow 36\frac{1}{2}$	*e,f*	8 266.584(4)	
	$38\frac{1}{2} \leftarrow 37\frac{1}{2}$	*e,f*	8 487.027(4)	

[a]) States with parity equal to $\pm(-1)^{J-0.5}$ are labeled *e* and *f* respectively.
[b]) The figures in parentheses are the authors' estimates of experimental uncertainty (1σ).

Molecular parameters for $^{12}C_{14}{}^{1}H$

Parameter		Value	Method	Ref.
State: electronic $\tilde{X}\,^2\Pi$; vibrational zero point level				
B	[MHz]	110.241 68(2) [a])	MW	98Go
D	[Hz]	0.102(9)		
A	[GHz]	– 600 [b])		
q	[MHz]	[c])		

[a]) The numbers in parentheses are 1 standard deviation of the least-squares fit, in units of the last quoted decimal place.
[b]) Value estimated from that of C_8H (97McC).
[c]) The parameter q was not determined because the parity doubling was not resolved.

References for $C_{14}H$

97McC McCarthy, M.C., Travers, M.J., Kovács, A., Gottlieb, C.A., Thaddeus, P. : Astrophys. J. Supp. Ser. **113** (1997) 105.

98Go Gottlieb, C.A., McCarthy, Travers, M.J., Grabow, J.-U., Thaddeus, P. : J.Chem. Phys. **109** (1998) 5433.

3.2.1.2.14 CCN

Microwave data for $^{12}C^{12}C^{14}N$

Transition				ν	Ref.
spin Ω	rotational $J' - J''$	parity e/f [a])	hyperfine $F' - F''$	[MHz]	
State: electronic $\tilde{X}\,^2\Pi$; vibrational zero point level					
$\frac{1}{2}$	$1\frac{1}{2} \leftarrow \frac{1}{2}$	*f*	$\frac{1}{2} \leftarrow \frac{1}{2}$	35 486.586 6(8) [b])	95Oh
			$1\frac{1}{2} \leftarrow \frac{1}{2}$	35 510.659 9(8)	
			$\frac{1}{2} \leftarrow 1\frac{1}{2}$	35 403.858 0(8)	
			$1\frac{1}{2} \leftarrow 1\frac{1}{2}$	35 427.931 7(8)	
			$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	35 472.588 7(8)	

e	$\frac{1}{2} \leftarrow \frac{1}{2}$	35 442.943 9(8)
	$1\frac{1}{2} \leftarrow \frac{1}{2}$	35 429.386 8(8)
	$\frac{1}{2} \leftarrow 1\frac{1}{2}$	35 453.776 4(8)
	$1\frac{1}{2} \leftarrow 1\frac{1}{2}$	35 440.232 5(8)
	$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	35 422.683 7(8)

[a]) States with parity equal to $\pm(-1)^{J-0.5}$ are labeled *e* and *f* respectively.
[b]) The figures in parentheses are the authors' estimates of experimental uncertainty (1σ).

Molecular parameters for $^{12}C^{12}C^{14}N$

Parameter		Value	Method	Ref.
State: electronic $\tilde{X}\,^2\Pi$; vibrational zero point level				
B	[MHz]	11 938.583 871(145) [a])	MW	95Oh
D	[kHz]	6.613 [b])	Opt	82Ka
A	[GHz]	1 210.559 [b])		82Ka
γ	[MHz]	– 112.63 [b])		82Ka
p	[MHz]	30.346 06(73)	MW	95Oh
q	[MHz]	7.132 [b])	Opt	82Ka
$h_{1/2}(^{14}N)$ [c])	[MHz]	35.961 80(75)	MW	95Oh
$b(^{14}N)$	[MHz]	19.754(31)		
$d(^{14}N)$	[MHz]	46.767 40(70)		
eQq_0	[MHz]	– 4.822 13(186)		
eQq_2	[MHz]	– 9.190(87)		

[a]) The numbers in parentheses are 1 standard deviation of the least-squares fit, in units of the last quoted decimal place.
[b]) Parameter constrained to this value from 82Ka in the least-squares fit.
[c]) $h_{1/2}(^{14}N) = a - (b+c)/2$.

References for CCN

82Ka Kakimoto, M., Kasuya, T. : J. Mol. Spectrosc. **94** (1982) 380.
95Oh Ohshima, Y., Endo, Y. : J. Mol. Spectrosc. **172** (1995) 225.

3.2.1.2.15 CCCN

Microwave data for $^{13}C^{12}C^{12}C^{14}N$

Transition rotational $N' - N''$	fine structure $J' - J''$	Hyperfine [a]) $F' - F''$	ν [MHz]	Ref.
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (0,0,0,0,0)				
$18 \leftarrow 17$	$18\frac{1}{2} \leftarrow 17\frac{1}{2}$	$19 \leftarrow 18$	171 738.524(22) [b])	95McC
		$18 \leftarrow 17$	171 744.850(22)	
	$17\frac{1}{2} \leftarrow 16\frac{1}{2}$	$18 \leftarrow 17$	171 750.381(28)	
		$17 \leftarrow 16$	171 756.587(26)	
$19 \leftarrow 18$	$19\frac{1}{2} \leftarrow 18\frac{1}{2}$	$20 \leftarrow 19$	181 278.136(23)	
		$19 \leftarrow 18$	181 284.284(22)	
	$18\frac{1}{2} \leftarrow 17\frac{1}{2}$	$19 \leftarrow 18$	181 290.062(24)	
		$18 \leftarrow 17$	181 296.147(25)	
$26 \leftarrow 25$	$26\frac{1}{2} \leftarrow 25\frac{1}{2}$	$27 \leftarrow 26$	248 045.278(46)	
		$26 \leftarrow 25$	248 050.481(32)	
	$25\frac{1}{2} \leftarrow 24\frac{1}{2}$	$26 \leftarrow 25$	248 057.990(29)	
		$25 \leftarrow 24$	248 063.208(51)	
$27 \leftarrow 26$	$27\frac{1}{2} \leftarrow 26\frac{1}{2}$	$28 \leftarrow 27$	257 581.796(19)	

		27 ← 26	257 586.852(17)	
	$26\frac{1}{2} \leftarrow 25\frac{1}{2}$	27 ← 26	257 594.736(17)	
		26 ← 25	257 599.829(21)	
29 ← 28	$29\frac{1}{2} \leftarrow 28\frac{1}{2}$	30 ← 29	276 653.521(38)	
		29 ← 28	276 658.376(26)	
	$28\frac{1}{2} \leftarrow 27\frac{1}{2}$	29 ← 28	276 666.681(33)	
		28 ← 27	276 671.556(86)	

[a]) Coupling scheme: $\boldsymbol{J} = \boldsymbol{N} + \boldsymbol{S}$; $\boldsymbol{F} = \boldsymbol{J} + \boldsymbol{I}_1$ where $\boldsymbol{I}_1$ is the ^{13}C nuclear spin. ^{14}N hyperfine structure is not resolved.
[b]) The figures in parenthesis are the authors' estimate of the experimental uncertainty, in units of the last quoted decimal place.

Molecular parameters for $^{13}C^{12}C^{12}C^{14}N$

Parameter		Value	Method	Ref.
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (0,0,0,0,0)				
B	[MHz]	4 771.219 3(4) [a])	MW	95McC
D	[kHz]	0.699 0(3)		
γ	[MHz]	– 18.03(2)		
$b_F(^{13}C)$	[MHz]	999(3)		
$c(^{13}C)$	[MHz]	0.0 [b])		

[a]) The numbers in parenthesis is 1 standard deviation of the least-squares fit, in units of the last quoted decimal place.
[b]) The parameter $c(^{13}C)$ is constrained to zero because it was not determinable from the $\Delta F = \Delta N$ millimeter-wave transitions with largish N-values.

Microwave data for $^{12}C^{13}C^{12}C^{14}N$

Transition			ν [MHz]	Ref.
rotational $N' - N''$	fine structure $J' - J''$	Hyperfine [a]) $F' - F''$		
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (0,0,0,0,0)				
11 ← 10	$11\frac{1}{2} \leftarrow 10\frac{1}{2}$	12 ← 11	108 242.334(33) [b])	95McC
		11 ← 10	108 245.108(26)	
	$10\frac{1}{2} \leftarrow 9\frac{1}{2}$	11 ← 10	108 258.204(26)	
		10 ← 9	108 260.988(27)	
16 ← 15	$16\frac{1}{2} \leftarrow 15\frac{1}{2}$	17 ← 16	157 441.187(30)	
		16 ← 15	157 442.857(32)	
	$15\frac{1}{2} \leftarrow 14\frac{1}{2}$	16 ← 15	157 458.159(32)	
		15 ← 14	157 459.824(33)	
17 ← 16	$17\frac{1}{2} \leftarrow 16\frac{1}{2}$	18 ← 17	167 280.152(26)	
		17 ← 16	167 281.697(24)	
	$16\frac{1}{2} \leftarrow 15\frac{1}{2}$	17 ← 16	167 297.303(24)	
		16 ← 15	167 298.808(25)	
18 ← 17	$18\frac{1}{2} \leftarrow 17\frac{1}{2}$	19 ← 18	177 118.855(25)	
		18 ← 17	177 120.246(26)	
	$17\frac{1}{2} \leftarrow 16\frac{1}{2}$	18 ← 17	177 136.078(22)	
		17 ← 16	177 137.490(26)	
19 ← 18	$19\frac{1}{2} \leftarrow 18\frac{1}{2}$	20 ← 19	186 957.168(27)	
		19 ← 18	186 958.481(24)	
	$18\frac{1}{2} \leftarrow 17\frac{1}{2}$	19 ← 18	186 974.479(23)	
		18 ← 17	186 975.825(27)	
26 ← 25	$26\frac{1}{2} \leftarrow 25\frac{1}{2}$	27 ← 26	255 815.202	
		26 ← 25	255 815.793	

	$25\frac{1}{2} \leftarrow 24\frac{1}{2}$	$26 \leftarrow 25$	255 832.918	
		$25 \leftarrow 24$	255 833.571	
$27 \leftarrow 26$	$27\frac{1}{2} \leftarrow 26\frac{1}{2}$	$28 \leftarrow 27$	265 650.826 [c])	
		$27 \leftarrow 26$	265 650.826 [c])	
	$26\frac{1}{2} \leftarrow 25\frac{1}{2}$	$27 \leftarrow 26$	265 668.514 [c])	
		$26 \leftarrow 25$	265 668.514 [c])	

[a]) Coupling scheme: $\boldsymbol{J} = \boldsymbol{N} + \boldsymbol{S}$; $\boldsymbol{F} = \boldsymbol{J} + \boldsymbol{I}_1$ where $\boldsymbol{I}_1$ is the ^{13}C nuclear spin. ^{14}N hyperfine structure is not resolved.
[b]) The figures in parenthesis are the authors' estimate of the experimental uncertainty, in units of the last quoted decimal place.
[c]) Blended lines.

Molecular parameters for $^{12}C^{13}C^{12}C^{14}N$

Parameter		Value	Method	Ref.
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (0,0,0,0,0)				
B	[MHz]	4 920.711 1(8) [a])	MW	95McC
D	[kHz]	0.747 8(12)		
γ	[MHz]	− 18.64(2)		
$b_F(^{13}C)$	[MHz]	199(1)		
$c(^{13}C)$	[MHz]	0.0 [b])		

[a]) The numbers in parentheses are 1 standard deviation of the least-squares fit, in units of the last quoted decimal place.
[b]) The parameter $c(^{13}C)$ is constrained to zero because it was not determinable from the $\Delta F = \Delta N$ millimeter-wave transitions with largish N-values.

Microwave data for $^{12}C^{12}C^{13}C^{14}N$

Transition		ν	Ref.
rotational $N' - N''$	fine structure $J' - J''$ [a])	[MHz]	
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (0,0,0,0,0)			
$11 \leftarrow 10$	$11\frac{1}{2} \leftarrow 10\frac{1}{2}$	108 426.168(27) [b])	95McC
	$10\frac{1}{2} \leftarrow 9\frac{1}{2}$	108 444.688(27)	
$17 \leftarrow 16$	$17\frac{1}{2} \leftarrow 16\frac{1}{2}$	167 564.136(17)	
	$16\frac{1}{2} \leftarrow 15\frac{1}{2}$	167 582.742(17)	
$18 \leftarrow 17$	$18\frac{1}{2} \leftarrow 17\frac{1}{2}$	177 419.526(21)	
	$17\frac{1}{2} \leftarrow 16\frac{1}{2}$	177 438.097(21)	
$24 \leftarrow 23$	$24\frac{1}{2} \leftarrow 23\frac{1}{2}$	236 544.274(53)	
	$23\frac{1}{2} \leftarrow 22\frac{1}{2}$	236 562.923(37)	
$26 \leftarrow 25$	$26\frac{1}{2} \leftarrow 25\frac{1}{2}$	256 249.360(43)	
	$25\frac{1}{2} \leftarrow 24\frac{1}{2}$	256 267.932(36)	
$27 \leftarrow 26$	$27\frac{1}{2} \leftarrow 26\frac{1}{2}$	266 101.099(37)	
	$26\frac{1}{2} \leftarrow 25\frac{1}{2}$	266 119.761(43)	

[a]) Nuclear hyperfine structure not resolved.
[b]) The figures in parenthesis are the authors' estimate of the experimental uncertainty, in units of the last quoted decimal place.

Molecular parameters for $^{12}C^{12}C^{13}C^{14}N$

Parameter		Value	Method	Ref.
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (0,0,0,0,0)				
B	[MHz]	4 929.063 9(3) [a])	MW	95McC
D	[kHz]	0.749 6 (4)		
γ	[MHz]	– 18.59(1)		
$b_F(^{13}C)$	[MHz]	≤ 60		
$c(^{13}C)$	[MHz]	0.0 [b])		

[a]) The numbers in parentheses are 1 standard deviation of the least-squares fit, in units of the last quoted decimal place.
[b]) The parameter $c(^{13}C)$ is constrained to zero because it was not determinable from the $\Delta F = \Delta N$ millimeter-wave transitions with largish N-values.

Microwave data for $^{12}C^{12}C^{12}C^{15}N$

Transition		ν	Ref.
rotational $N' - N''$	fine structure $J' - J''$ [a])	[MHz]	
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (0,0,0,0,0)			
9 ← 8	$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	86 410.937(18) [b])	95McC
	$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	86 429.106(17)	
10 ← 9	$10\frac{1}{2} \leftarrow 9\frac{1}{2}$	96 012.610(17)	
	$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	96 030.791(16)	
17 ← 16	$17\frac{1}{2} \leftarrow 16\frac{1}{2}$	163 218.734(16)	
	$16\frac{1}{2} \leftarrow 15\frac{1}{2}$	163 236.918(16)	
18 ← 17	$18\frac{1}{2} \leftarrow 17\frac{1}{2}$	172 818.578(16)	
	$17\frac{1}{2} \leftarrow 16\frac{1}{2}$	172 836.767(16)	
19 ← 18	$19\frac{1}{2} \leftarrow 18\frac{1}{2}$	182 418.129(16)	
	$18\frac{1}{2} \leftarrow 17\frac{1}{2}$	182 436.325(16)	
27 ← 26	$27\frac{1}{2} \leftarrow 26\frac{1}{2}$	259 201.528(16)	
	$26\frac{1}{2} \leftarrow 25\frac{1}{2}$	259 219.750(16)	
28 ← 27	$28\frac{1}{2} \leftarrow 27\frac{1}{2}$	268 797.552(16)	
	$27\frac{1}{2} \leftarrow 26\frac{1}{2}$	268 815.772(16)	

[a]) Nuclear hyperfine structure not resolved.
[b]) The figures in parenthesis are the authors' estimate of the experimental uncertainty, in units of the last quoted decimal place.

Molecular parameters for $^{12}C^{12}C^{12}C^{15}N$

Parameter		Value	Method	Ref.
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (0,0,0,0,0)				
B	[MHz]	4 801.226 4(2) [a])	MW	95McC
D	[kHz]	0.706 2(2)		
γ	[MHz]	– 18.195(6)		

[a])The numbers in parentheses are 1 standard deviation of the least-squares fit, in units of the last quoted decimal place.

References for CCCN

95McC McCarthy, M.C., Gottlieb, C.A., Thaddeus, P., Horn, M., Botschwina, P. : J. Chem. Phys. **103** (1995) 7820.

3.2.1.2.16 C_5N

Microwave data for $^{12}C_5{}^{14}N$

Transition			ν [MHz]	Ref.
rotational $N'-N''$	fine structure $J'-J''$	hyperfine $F'-F''$		
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational zero point level				
2 ← 1	$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	$1\frac{1}{2} \leftarrow 1\frac{1}{2}$	5 607.720 9	97Ka
		$2\frac{1}{2} \leftarrow 2\frac{1}{2}$	5 604.249 0	
		$1\frac{1}{2} \leftarrow \frac{1}{2}$	5 607.039 1	
		$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	5 607.055 8	
		$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	5 607.137 7	
	$1\frac{1}{2} \leftarrow \frac{1}{2}$	$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	5 617.782 0	
		$1\frac{1}{2} \leftarrow \frac{1}{2}$	5 615.323.1	
		$1\frac{1}{2} \leftarrow 1\frac{1}{2}$	5 618.734 2	
		$\frac{1}{2} \leftarrow \frac{1}{2}$	5 618.426 6	
3 ← 2	$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	8 413.095 7	
		$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	8 413.159 8	
		$4\frac{1}{2} \leftarrow 3\frac{1}{2}$	8 413.209 8	
	$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	$1\frac{1}{2} \leftarrow \frac{1}{2}$	8 423.389 2	
		$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	8 423.413 3	
		$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	8 413.888 0	
4 ← 3	$4\frac{1}{2} \leftarrow 3\frac{1}{2}$	$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	11 219.230 0	
		$4\frac{1}{2} \leftarrow 3\frac{1}{2}$	11 219.292 8	
		$5\frac{1}{2} \leftarrow 4\frac{1}{2}$	11 219.324 3	
	$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	11 229.809 0	
		$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	11 229.809 0	
		$4\frac{1}{2} \leftarrow 3\frac{1}{2}$	11 230.021 5	
5 ← 4	$5\frac{1}{2} \leftarrow 4\frac{1}{2}$	$4\frac{1}{2} \leftarrow 3\frac{1}{2}$	14 025.377 0	
		$5\frac{1}{2} \leftarrow 4\frac{1}{2}$	14 025.446 1	
		$6\frac{1}{2} \leftarrow 5\frac{1}{2}$	14 025.446 1	
	$4\frac{1}{2} \leftarrow 3\frac{1}{2}$	$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	14 036.042 8	
		$4\frac{1}{2} \leftarrow 3\frac{1}{2}$	14 036.042 8	
		$5\frac{1}{2} \leftarrow 4\frac{1}{2}$	14 036.158 5	
6 ← 5	$6\frac{1}{2} \leftarrow 5\frac{1}{2}$	$5\frac{1}{2} \leftarrow 4\frac{1}{2}$	16 831.520 2	
		$6\frac{1}{2} \leftarrow 5\frac{1}{2}$	16 831.581 6	
		$7\frac{1}{2} \leftarrow 6\frac{1}{2}$	16 831.581 6	
		$4\frac{1}{2} \leftarrow 3\frac{1}{2}$	16 842.218 9	
		$5\frac{1}{2} \leftarrow 4\frac{1}{2}$	16 842.218 9	
		$6\frac{1}{2} \leftarrow 5\frac{1}{2}$	16 842.305 3	
9 ← 8	$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	[a])	25 249.938(4) [b])	98 Gu
	$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	[a])	25 260.649(4)	
32 ← 31	$32\frac{1}{2} \leftarrow 31\frac{1}{2}$	[a])	89 785.6(4)	
	$31\frac{1}{2} \leftarrow 30\frac{1}{2}$	[a])	89 797.0(3)	

[a]) N hyperfine structure not resolved.

[b]) The figures in parentheses are the authors' estimates of experimental uncertainty (1σ).

Molecular parameters for $^{12}C_5{}^{14}N$

Parameter		Value	Method	Ref.
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational zero point level				
B	[MHz]	1 403.079 91(54) [a])	MW	97Ka
D	[kHz]	0.050(10)		
γ	[MHz]	– 10747 2(35)		
b	[MHz]	1.583(13)		
c	[MHz]	– 3.613(25)		
eQq_0	[MHz]	– 4.341(17)		

[a]) The numbers in parentheses are 1 standard deviation of the least-squares fit, in units of the last quoted decimal place.

References for C_5N

97Ka Kasai, Y., Sumiyoshi, Y., Endo, Y., Kawaguchi, K. : Astrophys. J. **477** (1997) L65.

98Gu Guélin, M., Neininger, N., Cernicharo, J. : Astron. Astrophys **335** (1998) L1.

3.2.1.2.17 C_2O

Microwave data for $^{12}C_2{}^{16}O$

Transition: rotational $N' - N''$	Transition: fine structure $J' - J''$	ν [MHz]	Ref.
State: electronic $\tilde{X}\,^3\Sigma^-$; vibrational (0,0,0)			
1 ← 0	0 ← 1	9 647.567	95Oh
	2 ← 1	22 258.175	
2 ← 1	2 ← 1	46 182.189	85Ya
	3 ← 2	45 826.706	
3 ← 2	2 ← 1	70 105.960	
	3 ← 2	69 272.927	
	4 ← 3	69 069.476	
4 ← 3	3 ← 2	92 718.800	
	4 ← 3	92 363.286	
	5 ← 4	92 227.853	
5 ← 4	4 ← 3	115 656.566	
	5 ← 4	115 453.024	
	6 ← 5	115 354.035	
6 ← 5	5 ← 4	138 677.586	
	6 ← 5	138 542.092	
	7 ← 6	138 464.858	
7 ← 6	6 ← 5	161 729.433	
	7 ← 6	161 630.306	
	8 ← 7	161 567.126	
8 ← 7	7 ← 6	184 794.969	
	8 ← 7	184 717.580	
	9 ← 8	184 664.004	

Molecular parameters for $^{12}C_2{}^{16}O$

Parameter		Value	Method	Ref.
State: electronic $\tilde{X}\,^3\Sigma^-$; vibrational (0,0,0)				
B	[MHz]	11 545.597 0(7) [a])	MW	95Oh
D	[kHz]	5.819(8)		
λ	[MHz]	11 496.870(9)		
λ_D	[kHz]	– 5.4(6)		
γ	[MHz]	– 17.820(3)		

[a]) The numbers in parentheses are 1 standard deviation of the least-squares fit, in units of the last quoted decimal place.

References for C_2O

85Ya Yamada, C., Saito, S., Kanamori, H., Hirota, E. : Astrophys. J. **290** (1985) L65.
95Oh Ohshima, Y., Endo, Y., Ogata, T.: J. Chem. Phys. **102** (1995) 1493.

3.2.1.2.18 C_4O

Microwave data for $^{12}C_4{}^{16}O$

Transition		ν	Ref.
rotational $N' - N''$	fine structure $J' - J''$	[MHz]	
State: electronic $\tilde{X}\,^3\Sigma^-$; vibrational zero point level			
1 ← 0	2 ← 1	6 033.511	95Oh
2 ← 1	1 ← 0	25 487.747	
	2 ← 1	9 405.052	
	3 ← 2	10 152.516	
3 ← 2	2 ← 1	12 776.575	
	3 ← 2	14 107.563	
	4 ← 3	14 570.267	
4 ← 3	3 ← 2	18 062.594	
	4 ← 3	18 810.072	
	5 ← 4	19 119.800	
5 ← 4	4 ← 3	23 049.847	
	5 ← 4	23 512.570	
	6 ← 5	23 732.453	

Molecular parameters for $^{12}C_4{}^{16}O$

Parameter		Value	Method	Ref.
State: electronic $\tilde{X}\,^3\Sigma^-$; vibrational zero point level				
B	[MHz]	2 351.262 5(2) [a])	MW	95Oh
D	[kHz]	0.128(6)		
λ	[MHz]	11 680.181(12)		
λ_D	[kHz]	1.13(18)		
γ	[MHz]	– 4.755 9(8)		

[a]) The numbers in parentheses are 1 standard deviation of the least-squares fit, in units of the last quoted decimal place.

References for C_4O

95Oh Ohshima, Y., Endo, Y., Ogata, T.: J. Chem. Phys. **102** (1995) 1493.

3.2.1.2.19 C_6O

Microwave data for $^{12}C_6{}^{16}O$

Transition rotational $N' - N''$	fine structure $J' - J''$	ν [MHz]	Ref.
State: electronic $\tilde{X}\,^3\Sigma^-$; vibrational zero point level			
2 ← 1	3 ← 2	4 596.212	95Oh
3 ← 2	3 ← 2	5 098.544	
	4 ← 3	6 149.874	
4 ← 3	3 ← 2	5 600.866	
	4 ← 3	6 798.061	
	5 ← 4	7 718.496	
5 ← 4	4 ← 3	7 446.229	
	5 ← 4	8 497.574	
	6 ← 5	9 302.524	
6 ← 5	5 ← 4	9 276.632	
	6 ← 5	10 197.083	
	7 ← 6	10 901.418	
7 ← 6	6 ← 5	11 091.621	
	7 ← 6	11 896.595	
	8 ← 7	12 514.009	
8 ← 7	7 ← 6	12 891.743	
	8 ← 7	13 596.102	
	9 ← 8	14 138.823	
9 ← 8	8 ← 7	14 678.164	
	9 ← 8	15 295.613	
	10 ← 9	15 774.299	
10 ← 9	9 ← 8	16 452.366	
	10 ← 9	16 995.120	
	11 ← 10	17 418.940	

Molecular parameters for $^{12}C_6{}^{16}O$

Parameter		Value	Method	Ref.
State: electronic $\tilde{X}\,^3\Sigma^-$; vibrational zero point level				
B	[MHz]	849.757 09(7) [a])	MW	95Oh
D	[kHz]	0.009 3(5)		
λ	[MHz]	17 352.74(10)		
λ_D	[kHz]	0.98(5)		
γ	[MHz]	– 1.043(4)		

[a]) The numbers in parentheses are 1 standard deviation of the least-squares fit, in units of the last quoted decimal place.

References for C_6O

95Oh Ohshima, Y., Endo, Y., Ogata, T.: J. Chem. Phys. **102** (1995) 1493.

3.2.1.2.20 C_8O

Microwave data for $^{12}C_8{}^{16}O$

Transition rotational $N' - N''$	Transition fine structure $J' - J''$	ν [MHz]	Ref.
State: electronic $\tilde{X}\,^3\Sigma^-$; vibrational zero point level			
5 ← 4	6 ← 5	4 694.628	95Oh
6 ← 5	7 ← 6	5 477.536	
7 ← 6	8 ← 7	6 260.659	
8 ← 7	8 ← 7	6 410.278	
	9 ← 8	7 044.011	
9 ← 8	8 ← 7	6 559.864	
	9 ← 8	7 211.563	
	10 ← 9	7 827.627	
10 ← 9	9 ← 8	7 379.066	
	10 ← 9	8 012.846	
	11 ← 10	8 611.521	
11 ← 10	10 ← 9	8 198 024	
	11 ← 10	8 814.135	
	12 ← 11	9 395.717	
12 ← 11	11 ← 10	9 016.681	
	12 ← 11	9 615.413	
	13 ← 12	10 180.232	
13 ← 12	12 ← 11	9 835.043	
	13 ← 12	10 416.695	
	14 ← 13	10 965.076	
14 ← 13	13 ← 12	10 653.091	
	14 ← 13	11 217.977	
	15 ← 14	11 750.268	
15 ← 14	14 ← 13	11 470.799	
	15 ← 14	12 019.257	
	16 ← 15	12 535.822	
16 ← 15	15 ← 14	12 288.173	
	16 ← 15	12 820.545	
	17 ← 16	13 321.738	
17 ← 16	18 ← 17	14 108.037	

Molecular parameters for $^{12}C_8{}^{16}O$

Parameter		Value	Method	Ref.
State: electronic $\tilde{X}\,^3\Sigma^-$; vibrational zero point level				
B	[MHz]	400.641 83(8) [a])	MW	95Oh
D	[kHz]	0.001 6 (2)		
λ	[MHz]	34 096.(7)		
λ_D	[kHz]	1.32(5)		
γ	[MHz]	0.46(8)		

[a]) The numbers in parentheses are 1 standard deviation of the least-squares fit, in units of the last quoted decimal place.

References for C_8O

95Oh Ohshima, Y., Endo, Y., Ogata, T.: J. Chem. Phys. **102** (1995) 1493.

3.2.1.2.21 C_2S

Microwave data for $^{12}C_2{}^{32}S$

Transition		ν	Ref.
rotational $N' - N''$	fine structure $J' - J''$	[MHz]	
State: electronic $\tilde{X}\,^3\Sigma^-$; vibrational (0,0,0)			
0 ← 1	1 ← 0	11 119.446(4) [a])	92Lo
1 ← 0	2 ← 1	22 344.029(4)	

[a]) The figures in parentheses are the authors' estimates of experimental uncertainty (1σ).

Microwave data for $^{13}C^{12}C^{32}S$

Transition			ν	Ref.
rotational $N' - N''$	fine structure $J' - J''$	hyperfine $F' - F''$	[MHz]	
State: electronic $\tilde{X}\,^3\Sigma^-$; vibrational (0,0,0)				
0 ← 1	1 ← 0	$1\frac{1}{2} \leftarrow \frac{1}{2}$	10 706.913(4) [a])	97Ik
		$\frac{1}{2} \leftarrow \frac{1}{2}$	10 699.954(4)	
1 ← 0	2 ← 1	$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	21 498.660(4)	
		$1\frac{1}{2} \leftarrow \frac{1}{2}$	21 494.411(4)	
2 ← 1	3 ← 2	$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	32 443.951(4)	
		$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	32 440.114(4)	
3 ← 2	4 ← 3	$4\frac{1}{2} \leftarrow 3\frac{1}{2}$	43 577.761(4)	
		$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	43 574.443(4)	
9 ← 8	8 ← 7	$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	108 136.386(4)	
		$7\frac{1}{2} \leftarrow 6\frac{1}{2}$	108 137.577(4)	
	9 ← 8	[b])	111 381.287(4)	
	10 ← 9	$10\frac{1}{2} \leftarrow 9\frac{1}{2}$	113 765.975(4)	
		$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	113 764.988(4)	
10 ← 9	9 ← 8	$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	120 983.417(4)	
	10 ← 9	[b])	123 755.760(4)	
11 ← 10	10 ← 9	$10\frac{1}{2} \leftarrow 9\frac{1}{2}$	133 744.203(4)	
		$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	133 745.175(4)	
	12 ← 11	$12\frac{1}{2} \leftarrow 11\frac{1}{2}$	137 932.979(4)	
		$11\frac{1}{2} \leftarrow 10\frac{1}{2}$	137 932.225(4)	
18 ← 17	18 ← 17	[b])	222 735.062(4)	
	19 ← 18	[b])	223 550.258(4)	
19 ← 18	18 ← 17	[b])	234 203.136(4)	
	19 ← 18	[b])	235 104.797(4)	
	20 ← 19	[b])	235 846.178(4)	
20 ← 19	19 ← 18	[b])	246 656.732(4)	
	20 ← 19	[b])	247 473.824(4)	
	21 ← 20	[b])	248 150.593(4)	
22 ← 21	22 ← 21	[b])	272 209.575(4)	
	23 ← 22	[b])	272 779.103(4)	
23 ← 22	22 ← 21	[b])	283 954.220(4)	
	23 ← 22	[b])	284 576.207(4)	

[a]) The figures in parentheses are the authors' estimates of experimental uncertainty (1σ).
[b]) ^{13}C hyperfine structure not resolved.

Molecular parameters for $^{13}C^{12}C^{32}S$

Parameter		Value	Method	Ref.
State: electronic $\tilde{X}\,^3\Sigma^-$; vibrational (0,0,0)				
B	[MHz]	6 188.086 78(42) [a]	MW	97Ik
D	[kHz]	1.572 09(50)		
λ	[MHz]	97 203.92(49)		
λ_D	[kHz]	24.56(32)		
γ	[MHz]	– 14.058(27)		
γ_D	[kHz]	0.035 8(194)		
$b(^{13}C)$	[MHz]	35.185(78)		
$c(^{13}C)$	[MHz]	– 49.31(197)		

[a]) The numbers in parentheses are 1 standard deviation of the least-squares fit, in units of the last quoted decimal place.

Microwave data for $^{12}C^{13}C^{32}S$

Transition			ν	Ref.
rotational $N'-N''$	fine structure $J'-J''$	hyperfine $F'-F''$	[MHz]	
State: electronic $\tilde{X}\,^3\Sigma^-$; vibrational (0,0,0)				
0 ← 1	1 ← 0	$1\frac{1}{2} \leftarrow \frac{1}{2}$	11 075.301(4) [a]	97Ik
		$\frac{1}{2} \leftarrow \frac{1}{2}$	11 078.411(4)	
1 ← 0	2 ← 1	$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	22 254.730(4)	
		$1\frac{1}{2} \leftarrow \frac{1}{2}$	22 256.609(4)	
2 ← 1	3 ← 2	$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	33 613.548(4)	
		$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	33 615.174(4)	
9 ← 8	8 ← 7	$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	112 848.719(4)	
		$7\frac{1}{2} \leftarrow 6\frac{1}{2}$	112 847.677(4)	
	9 ← 8	[b])	116 040.764(4)	
	10 ← 9	$10\frac{1}{2} \leftarrow 9\frac{1}{2}$	118 368.541(4)	
10 ← 9	10 ← 9	[b])	128 932.847(4)	
	11 ← 10	[b])	130 944.007(4)	
11 ← 10	10 ← 9	$10\frac{1}{2} \leftarrow 9\frac{1}{2}$	139 495.876(4)	
		$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	139 495.204(4)	
18 ← 17	17 ← 16	[b])	231 089.099(4)	
	18 ← 17	[b])	232 051.491(4)	
	19 ← 18	[b])	232 834.729(4)	
19 ← 18	18 ← 17	[b])	244 070.929(4)	
	20 ← 19	[b])	245 650.120(4)	
20 ← 19	20 ← 19	[b])	257 824.587(4)	
	21 ← 20	[b])	258 473.673(4)	
22 ← 21	21 ← 20	[b])	282 942.927(4)	
	22 ← 21	[b])	283 594.371(4)	
	23 ← 22	[b])	284 139.810(4)	

[a]) The figures in parentheses are the authors' estimates of experimental uncertainty (1σ).
[b]) ^{13}C hyperfine structure not resolved.

Molecular parameters for $^{12}C^{13}C^{32}S$

Parameter		Value	Method	Ref.
State: electronic $\tilde{X}\,^3\Sigma^-$; vibrational (0,0,0)				
B	[MHz]	6 446.965 95(51) [a])	MW	97Ik
D	[kHz]	1.712 41(68)		
λ	[MHz]	97 266.64(56)		
λ_D	[kHz]	28.20(39)		
γ	[MHz]	– 14.622(33)		
γ_D	[kHz]	0.032(26)		
$b(^{13}C)$	[MHz]	– 13.835(80)		
$c(^{13}C)$	[MHz]	– 15.8(20)		

[a]) The numbers in parentheses are 1 standard deviation of the least-squares fit, in units of the last quoted decimal place.

Microwave data for $^{13}C^{13}C^{32}S$

Transition				ν [MHz]	Ref.
rotational $N' - N''$	fine structure $J' - J''$	Hyperfine [a])			
		$F_1' - F_1''$	$F' - F''$		
State: electronic $\tilde{X}\,^3\Sigma^-$; vibrational (0,0,0)					
$0 \leftarrow 1$	$1 \leftarrow 0$	$1\frac{1}{2} \leftarrow \frac{1}{2}$	$2 \leftarrow 1$	10 670.103(4) [b])	97Ik
			$1 \leftarrow 1$	10 672.825(4)	
			$1 \leftarrow 0$	10 672.825(4)	
		$\frac{1}{2} \leftarrow \frac{1}{2}$	$1 \leftarrow 1$	10 663.402(4)	
			$1 \leftarrow 0$	10 663.402(4)	
$1 \leftarrow 0$	$2 \leftarrow 1$	$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	$3 \leftarrow 2$	21 424.581(4)	
			$2 \leftarrow 1$	21 426.484(4)	
		$1\frac{1}{2} \leftarrow \frac{1}{2}$	$2 \leftarrow 1$	21 420.246(4)	
			$1 \leftarrow 0$	21 422.148(4)	
		$1\frac{1}{2} \leftarrow 1\frac{1}{2}$	$2 \leftarrow 2$	21 413.554(4)	
			$1 \leftarrow 1$	21 415.467(4)	
		$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	$2 \leftarrow 2$	21 429.203(4)	
		$1\frac{1}{2} \leftarrow \frac{1}{2}$	$1 \leftarrow 1$	21 424.874(4)	
$2 \leftarrow 1$	$3 \leftarrow 2$	$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	$4 \leftarrow 3$	32 330.145(4)	
			$3 \leftarrow 2$	32 331.775(4)	
		$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	$3 \leftarrow 2$	32 326.351(4)	
			$2 \leftarrow 1$	32 327.981(4)	

[a]) Coupling scheme: $\boldsymbol{J} = \boldsymbol{N} + \boldsymbol{S}$; $\boldsymbol{F}_1 = \boldsymbol{J} + \boldsymbol{I}_1$; $\boldsymbol{F} = \boldsymbol{F}_1 + \boldsymbol{I}_2$ where $\boldsymbol{I}_1$ is the $^{13}C_\alpha$ nuclear spin and $\boldsymbol{I}_2$ is the $^{13}C_\beta$ nuclear spin.
[b]) The figures in parentheses are the authors' estimates of experimental uncertainty (1σ).

Molecular parameters for $^{13}C^{13}C^{32}S$

Parameter		Value	Method	Ref.
State: electronic $\tilde{X}\,^3\Sigma^-$; vibrational (0,0,0)				
B	[MHz]	6 162.948 7(37) [a])	MW	97Ik
D	[kHz]	1.556 54 [b])		
λ	[MHz]	97 235.48(36)		
λ_D	[kHz]	25.76 [b])		
γ	[MHz]	– 13.943 [b])		
γ_D	[kHz]	0.0 [b])		
$b(^{13}C_\alpha)$	[MHz]	35.185 5(89)		
$c(^{13}C_\alpha)$	[MHz]	– 49.3 [b])		
$b(^{13}C_\beta)$	[MHz]	– 13.829 3(91)		
$c(^{13}C_\beta)$	[MHz]	– 15.8 [b])		

[a]) The numbers in parentheses are 1 standard deviation of the least-squares fit, in units of the last quoted decimal place.
[b]) Parameter constrained to this value in the least-squares fit.

References for C_2S

92Lo Lovas, F.J., Suenram, R.D., Ogata, T., Yamamoto, S. : Astrophys. J. **399** (1992) 325.
97Ik Ikeda, M., Sekimoto, Y., Yamamoto, S. : J. Mol. Spectrosc. **185** (1997) 21.

3.2.1.2.22 C_4S

Microwave data for $^{12}C_4{}^{32}S$

Transition		ν	
rotational $N' – N''$	fine structure $J' – J''$	[MHz]	Ref.
State: electronic $\tilde{X}\,^3\Sigma^-$; vibrational zero-point level			
1 ← 0	2 ← 1	5 912.174(4) [a])	93Hi
2 ← 1	3 ← 2	8 868.707(4)	
3 ← 2	4 ← 3	11 825.772(4)	
4 ← 3	5 ← 4	14 783.540(4)	
5 ← 4	6 ← 5	17 742.167(4)	
6 ← 5	7 ← 6	20 701.804(4)	
7 ← 6	8 ← 7	23 662.506(4)	

[a]) The figures in parentheses are the authors' estimates of experimental uncertainty (1σ).

Molecular parameters for $^{12}C_4{}^{32}S$

Parameter		Value	Method	Ref.
State: electronic $\tilde{X}\,^3\Sigma^-$; vibrational zero-point level				
B	[MHz]	1 519.165(2) [a])	MW	93Hi
D	[kHz]	56 [b])		
λ	[MHz]	113 603(5)		
γ	[MHz]	0.0 [b])		

[a]) The numbers in parentheses are 1 standard deviation of the least-squares fit, in units of the last quoted decimal place.
[b]) Parameter constrained to this value in the least-squares fit.

References for C_4S

93Hi Hirahara, Y., Ohshima, Y., Endo, Y. : Astrophys. J. **408** (1993) L113.

3.2.1.2.23 HCCN

Microwave data for $^{1}H^{12}C^{12}C^{14}N$

Transition: rotational $N' - N''$	Transition: fine structure $J' - J''$	Transition: Hyperfine [a]) $F_1' - F_1''$	Transition: Hyperfine [a]) $F' - F''$	ν [MHz]	Ref.
State: electronic $\tilde{X}\,^3\Sigma^-$; vibrational (0,0,0,0,0)					
$1 \leftarrow 0$	$0 \leftarrow 1$	$\frac{1}{2} \leftarrow 1\frac{1}{2}$	$1\frac{1}{2} \leftarrow 2\frac{1}{2}$	6 746.144	93En
			$1\frac{1}{2} \leftarrow 1\frac{1}{2}$	6 769.532	
			$\frac{1}{2} \leftarrow 1\frac{1}{2}$	6 769.450	
			$\frac{1}{2} \leftarrow \frac{1}{2}$	6 781.325	
		$\frac{1}{2} \leftarrow \frac{1}{2}$	$1\frac{1}{2} \leftarrow 1\frac{1}{2}$	6 686.830	
			$\frac{1}{2} \leftarrow 1\frac{1}{2}$	6 686.762	
			$1\frac{1}{2} \leftarrow \frac{1}{2}$	6 713.791	
	$2 \leftarrow 1$	$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	21 222.968	
			$2\frac{1}{2} \leftarrow 2\frac{1}{2}$	21 199.230	
		$1\frac{1}{2} \leftarrow 1\frac{1}{2}$	$2\frac{1}{2} \leftarrow 2\frac{1}{2}$	21 279.424	
		$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	21 222.622	
			$1\frac{1}{2} \leftarrow 1\frac{1}{2}$	21 208.130	
		$1\frac{1}{2} \leftarrow 1\frac{1}{2}$	$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	21 302.812	
			$1\frac{1}{2} \leftarrow 1\frac{1}{2}$	21 277.895	
			$\frac{1}{2} \leftarrow 1\frac{1}{2}$	21 264.580	
		$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	$1\frac{1}{2} \leftarrow \frac{1}{2}$	21 220.018	
		$1\frac{1}{2} \leftarrow 1\frac{1}{2}$	$1\frac{1}{2} \leftarrow \frac{1}{2}$	21 289.765	
			$\frac{1}{2} \leftarrow \frac{1}{2}$	21 276.450	
		$1\frac{1}{2} \leftarrow \frac{1}{2}$	$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	21 220.108	
			$1\frac{1}{2} \leftarrow 1\frac{1}{2}$	21 195.191	
			$1\frac{1}{2} \leftarrow \frac{1}{2}$	21 222.160	
			$\frac{1}{2} \leftarrow \frac{1}{2}$	21 208.840	
$5 \leftarrow 4$	$4 \leftarrow 3$	[c])	[c])	110 046.222	84Sai
$6 \leftarrow 5$	$5 \leftarrow 4$	[c])	[c])	131 956.227	
	$6 \leftarrow 5$	[c])	[c])	131 833.305	
	$7 \leftarrow 6$	[c])	[c])	131 762.851	
$7 \leftarrow 6$	$6 \leftarrow 5$	[c])	[c])	153 894.083(20) [b])	95McC
	$7 \leftarrow 6$	[c])	[c])	153 804.033(21)	
	$8 \leftarrow 7$	[c])	[c])	153 746.186(20)	
$8 \leftarrow 7$	$7 \leftarrow 6$	[c])	[c])	175 844.436(20)	
	$8 \leftarrow 7$	[c])	[c])	175 774.042(20)	
	$9 \leftarrow 8$	[c])	[c])	175 724.839(20)	
$9 \leftarrow 8$	$8 \leftarrow 7$	[c])	[c])	197 800.949(20)	
	$9 \leftarrow 8$	[c])	[c])	197 743.235(20)	
	$10 \leftarrow 9$	[c])	[c])	197 700.229(20)	
$11 \leftarrow 10$	$10 \leftarrow 9$	[c])	[c])	241 721.721(28)	
	$11 \leftarrow 10$	[c])	[c])	241 678.864(21)	
	$12 \leftarrow 11$	[c])	[c])	241 643.862(20)	
$12 \leftarrow 11$	$11 \leftarrow 10$	[c])	[c])	263 683.362(20)	
	$12 \leftarrow 11$	[c])	[c])	263 645.074(21)	
	$13 \leftarrow 12$	[c])	[c])	263 612.732(20)	

13 ← 12	12 ← 11	[c])	[c])	285 644.872(20)
	13 ← 12	[c])	[c])	285 610.199 [d])
	14 ← 13	[c])	[c])	285 579.866(20)
15 ← 14	14 ← 13	[c])	[c])	329 566.060(20)
	15 ← 14	[c])	[c])	329 536.100(21)
	16 ← 15	[c])	[c])	329 508.958(20)
16 ← 15	15 ← 14	[c])	[c])	351 525.028(22)
	16 ← 15	[c])	[c])	351 496.907(21)
	17 ← 16	[c])	[c])	351 470.912(20)
17 ← 16	16 ← 15	[c])	[c])	373 482.897(22)
	17 ← 16	[c])	[c])	373 456.104(21)
	18 ← 17	[c])	[c])	373 431.074(20)
18 ← 17	17 ← 16	[c])	[c])	395 439.123(20)
	18 ← 17	[c])	[c])	395 413.622(23)
	19 ← 18	[c])	[c])	395 389.451(20)

[a]) Coupling scheme: $\boldsymbol{J} = \boldsymbol{N} + \boldsymbol{S}$; $\boldsymbol{F}_1 = \boldsymbol{J} + \boldsymbol{I}_1$; $\boldsymbol{F} = \boldsymbol{F}_1 + \boldsymbol{I}_2$ where $\boldsymbol{I}_1$ is the ^{1}H nuclear spin and $\boldsymbol{I}_2$ is the ^{14}N nuclear spin. This scheme is different from that adopted by Endo *et al.* [93En].

[b]) The figures in parentheses are the authors' estimates of experimental uncertainty (1σ).

[c]) ^{14}N and ^{1}H hyperfine structure not resolved.

[d]) Blended line.

Microwave data for $^1H^{12}C^{12}C^{14}N$

Transition			ν [MHz]	Ref.
rotational $N' - N''$	parity	fine structure $J' - J''$		
State: electronic $\tilde{X}\,^3\Sigma^-$; vibrational (0,0,0,0,1^1)				
5← 4	+ ← −	6← 5	109 458.916(26) [a])	95McC
		4← 3	109 475.559(27)	
	− ← +	6← 5	109 880.665(23)	
		5← 4	110 506.607(23)	
		4← 3	109 795.338(23)	
7← 6	+ ← −	8← 7	153 435.756(20)	
		7← 6	153 710.864(21)	
		6← 5	153 530.900(23)	
	− ← +	8← 7	154 013.297(21)	
		7← 6	154 267.679(21)	
		6← 5	154 065.335(27)	
8← 7	− ← +	9← 8	175 394.595(20)	
		8← 7	175 590.858(20)	
		7← 6	175 486.885(20)	
	+ ← −	9← 8	176 051.160(20)	
		8← 7	176 232.257(20)	
		7← 6	176 112.219(20)	
9← 8	+ ← −	10← 9	197 344.217(20)	
		9← 8	197 491.533(20)	
		8← 7	197 430.082(20)	
	− ← +	10← 9	198 080.413(20)	
		9← 8	198 216.149(20)	
		8← 7	198 142.697(20)	
11← 10	+ ← −	12← 11	241 227.376(20)	
		11← 10	241 320.356(26)	
		10← 9	241 300.410(22)	
	− ← +	12← 11	242 123.578(20)	

		11← 10	242 209.289(26)	
		10← 9	242 181.954(28)	
12← 11	− ← +	13← 12	263 163.610(20)	
		12← 11	263 240.772(22)	
		11← 10	263 231.355(20)	
	+ ← −	13← 12	264 140.047(20)	
		12← 11	264 211.316(21)	
		11← 10	264 195.847(20)	
13← 12	+ ← −	14← 13	285 097.131(20)	
		13← 12	285 162.719(21)	
		12← 11	285 160.417(20)	
	− ← +	14← 13	286 153.921(20)	
		13← 12	286 214.666(21)	
		12← 11	286 207.345(20)	
15 ← 14	+ ← −	16← 15	328 957.339(22)	
		15← 14	329 007.612(34)	
		14← 13	329 013.742(22)	
	− ← +	16← 15	330 175.029(21)	
16 ← 15	− ← +	17← 16	350 884.230(20)	
		16← 15	350 929.250(23)	
		15← 14	350 937.924(20)	
	+ ← −	17← 16	352 182.470(20)	
17 ← 16	+ ← −	18 ← 17	372 809.086(20)	
		17← 16	372 849.920(22)	
		16← 15	372 860.463(20)	
	− ← +	18 ← 17	374 187.913(20)	
		17← 16	374 225.892(24)	
		16← 15	374 233.885(20)	
18 ← 17	− ← +	19 ← 18	394 731.966(20)	
		17← 16	394 781.243(20)	
	+ ← −	19 ← 18	396 191.071(21)	
		18 ← 17	396 226.374(26)	
		17← 16	396 235.937(21)	

[a]) The figures in parentheses are the authors' estimates of experimental uncertainty (1σ).

Microwave data for $^{1}H^{12}C^{12}C^{14}N$

Transition			ν [MHz]	Ref.
rotational $N' - N''$	fine structure $J' - J''$	Parity [a])		
State: electronic $\tilde{X}\,^3\Sigma^-$; vibrational (0,0,0,0,2^2)				
7← 6	7← 6	+ ← −	154 424.940 [b])	95McC
		− ← +	154 424.940 [b])	
8← 7	9← 8	− ← +	175 599.370 [b])	
		+ ← −	175 599.370 [b])	
	8← 7	− ← +	176 194.497 [b])	
		+ ← −	176 194.497 [b])	
9← 8	10← 9	+ ← −	197 615.574 [b])	
		− ← +	197 615.574 [b])	
	9← 8	+ ← −	198 044.238 [b])	
		− ← +	198 044.238 [b])	
11← 10	12← 11	+ ← −	241 606.101(21) [c])	
		− ← +	241 607.334(21)	
	11← 10	+ ← −	241 854.243(23)	

		− ← +	241 855.155(26)	
	10← 9	+ ← −	241 638.738(22)	
		− ← +	241 640.000(22)	
12← 11	13← 12	− ← +	263 589.377(24)	
		+ ← −	263 590.961(24)	
	11← 10	− ← +	263 627.634(23)	
		+ ← −	263 629.240(23)	
13← 12	14← 13	+ ← −	285 567.452(23)	
		− ← +	285 569.329((23)	
	13← 12	+ ← −	285 727.562(47)	
		− ← +	285 729.315(28)	
	12← 11	+ ← −	285 608.445(23)	
		− ← +	285 610.199 [b])	
15 ← 14	16 ← 15	− ← +	329 514.666(22)	
	15 ← 14	+ ← −	329 623.986(30)	
		− ← +	329 626.562(31)	
	14← 13	+ ← −	329 554.574(34)	
		− ← +	329 557.574(28)	
16 ← 15	17 ← 16	− ← +	351 479.269(23)	
		+ ← −	351 482.671(23)	
17 ← 16	18 ← 17	+ ← −	373 443.914(21)	
		− ← +	373 448.069(21)	
	17 ← 16	+ ← −	373 527.405(36)	
		− ← +	373 531.246(39)	
	16 ← 15	+ ← −	373 486.130(22)	
		− ← +	373 490.473(21)	
18 ← 17	19 ← 18	− ← +	395 405.869(23)	
		+ ← −	395 410.717(23)	

[a]) The relative parity was assumed to be as shown.
[b]) Blended line.
[c]) The figures in parentheses are the authors' estimates of experimental uncertainty (1σ).

Microwave data for $^{1}H^{12}C^{12}C^{14}N$

Transition			ν [MHz]	Ref.
rotational $N' - N''$	fine structure $J' - J''$	Parity		
State: electronic $\tilde{X}\,^3\Sigma^-$; vibrational (0,0,0,0,3[3])				
8← 7	8← 7	[a])	176 703.920(23) [b])	95McC
9← 8	9← 8	[a])	198 410.796`(22)	
11← 10	12← 11	[a])	241 568.730(23)	
	11← 10	[a])	242 073.032(28)	
	10← 9	[a])	241 550.930(34)	
12← 11	13← 12	[a])	263 570.698(34)	
	12← 11	[a])	263 965.675(35)	
	11← 10	[a])	263 572.664(53)	
13← 12	14← 13	[a])	285 563.162(28)	
	13← 12	[a])	285 879.395(24)	
15 ← 14	16 ← 15	[a])	329 528.755(24)	
16 ← 15	17 ← 16	[a])	351 504.337(51)	
	16 ← 15	[a])	351 684.444(43)	
	15 ← 14	[a])	351 534.685(45)	
17 ← 16	18 ← 17	[a])	373 476.202(31)	
	17 ← 16	[a])	373 629.660(31)	

	16 ← 15	[a])	373 508.702 [c])	
18 ← 17	19 ← 18	[a])	395 444.595(34)	
	18 ← 17	[a])	395 577.139(41)	

[a]) Parity doubling not resolved.
[b]) The figures in parentheses are the authors' estimates of experimental uncertainty (1σ).
[c]) Blended line.

Microwave data for $^{1}H^{12}C^{12}C^{14}N$

Transition			ν [MHz]	Ref.
rotational $N' - N''$	parity	fine structure $J' - J''$		
State: electronic $\tilde{X}\,^3\Sigma^-$; vibrational (0,0,0, 1^1,0)				
7← 6	+ ← −	8← 7	153 987.679(23) [a])	95McC
		7← 6	154 258.677(38)	
	− ← +	8← 7	154 381.333(21)	
		7← 6	154 646.191(23)	
		6← 5	154 443.933(39)	
8← 7	− ← +	9← 8	176 024.105(21)	
		8← 7	176 217.530(22)	
		7← 6	176 103.199(23)	
	+ ← −	9← 8	176 472.906(20)	
		8← 7	176 661.564(22)	
		7← 6	176 542.047(23)	
9← 8	+ ← −	10← 9	198 051.538(21)	
		9← 8	198 196.639(21)	
		8← 7	198 127.826(30)	
	− ← +	10← 9	198 555.581(21)	
		9← 8	198 697.066(21)	
		8← 7	198 624.372(21)	
11← 10	+ ← −	12← 11	242 090.345(38)	
		11← 10	242 181.954(20)	
		10← 9	242 158.042(21)	
	− ← +	12← 11	242 705.252(21)	
		11← 10	242 794.680(27)	
		10← 9	242 768.202(22)	
12← 11	− ← +	13← 12	264 104.638(22)	
		12← 11	264 180.911(21)	
		11← 10	264 168.161(22)	
	+ ← −	13← 12	264 774.807(23)	
		12← 11	264 849.181(28)	
		11← 10	264 834.526(28)	
13← 12	+ ← −	14← 13	286 116.081(21)	
		13← 12	286 180.911(27)	
		12← 11	286 176.044(21)	
	− ← +	14← 13	286 841.706(21)	
		13← 12	286 905.071(24)	
		12← 11	286 898.590(22)	
15 ← 14	+ ← −	16← 15	330 132.066(23)	
		15← 14	330 181.974(43)	
		14← 13	330 186.448(28)	
	− ← +	14← 13	331 020.662(34)	
16 ← 15	− ← +	17← 16	352 136.918(21)	
		15← 14	352 189.060(21)	

	+ ← −	17← 16	353 028.859(26)	
		15← 14	353 079.034(24)	
17 ← 16	+ ← −	18 ← 17	374 139.697(21)	
		17← 16	374 180.451(34)	
		16← 15	374 189.977(22)	
	− ← +	18 ← 17	375 086.981(26)	
		16← 15	375 135.539(30)	
18 ← 17	− ← +	19 ← 18	396 140.220(26)	
		17← 16	396 188.629 [b])	

[a]) The figures in parentheses are the authors' estimates of experimental uncertainty (1σ). [b]) Blended line.

Microwave data for $^{1}H^{12}C^{12}C^{14}N$

Transition			ν [MHz]	Ref.
rotational $N' - N''$	fine structure $J' - J''$	Parity		
State: electronic $\tilde{X}\,^3\Sigma^-$; vibrational (0,0,0,0,2^0) [a])				
7← 6	8← 7	− ← +	153 978.239(28) [b])	95McC
	6← 5		154 127.166(36)	
8← 7	9← 8	+ ← −	175 990.225(21)	
	8← 7		176 039.424(22)	
	7← 6		176 110.349(23)	
9← 8	10← 9	− ← +	197 998.885(21)	
	9← 8		198 041.798(22)	
	8← 7		198 099.810(30)	
11← 10	12← 11	− ← +	242 008.950(22)	
	11← 10		242 043.664(22)	
	10← 9		242 086.636(95)	
12← 11	13← 12	+ ← −	264 011.074(22)	
	12← 11		264 042.956(28)	
	11← 10		264 081.219(22)	
13← 12	14← 13	− ← +	286 011.347(21)	
	13← 12		286 041.095(23)	
	12← 11		286 075.800(23)	
15 ← 14	15 ← 14	− ← +	330 033.255(40)	
	14← 13		330 062.999(44)	
16 ← 15	17 ← 16	+ ← −	352 001.646(22)	
	15 ← 14		352 055.076(21)	
17 ← 16	18 ← 17	− ← +	373 994.988(21)	
	17 ← 16		374 019.274(34)	
	16 ← 15		374 045.900(21)	
18 ← 17	18 ← 17	+ ← −	396 009.860(28)	
	17 ← 16		396 035.190(38)	

[a]) Assignment due to Hung *et al.* (01Hu)
[b]) The figures in parentheses are the authors' estimates of experimental uncertainty (1σ).

Microwave data for $^{1}H^{12}C^{12}C^{14}N$

Transition			ν [MHz]	Ref.
rotational $N' - N''$	fine structure $J' - J''$	Parity		
State: electronic $\tilde{X}\,^3\Sigma^-$; vibrational *a*, not known (l = 0). Probably (0,0,0,1^1,1^1) [a])				
7← 6	8← 7	− ← +	154 105.587(30) [b])	95McC
	7← 6		154 162.744(48)	

	6← 5		154 254.450(55)	
8← 7	9← 8	+ ← –	176 136.250(22)	
	8← 7		176 184.575(30)	
	7← 6		176 256.430(24)	
9← 8	10← 9	– ← +	198 163.878(21)	
	9← 8		198 205.812(22)	
	8← 7		198 265.000(30)	
11← 10	12← 11	– ← +	242 212.795(28)	
	11← 10		242 246.762 [c])	
	10← 9		242 290.488(26)	
12← 11	13← 12	+ ← –	264 234.704(25)	
	12← 11		264 265.331(43)	
	11← 10		264 305.184(47)	
13← 12	14← 13	– ← +	286 255.263(23)	
	13← 12		286 283.661970)	
	12← 11		286 319.984(40)	
15 ← 14	16 ← 15	– ← +	330 292.388(120)	
	14← 13		330 348.851(44)	
16 ← 15	15 ← 14	+ ← –	352 362.426(23)	
17 ← 16	18 ← 17	– ← +	374 324.034(31)	
	17 ← 16		374 346.406(103)	
	16 ← 15		374 375.272(45)	

[a]) Assignment due to Hung *et al.* [01Hu].
[b]) The figures in parentheses are the authors' estimates of experimental uncertainty (1σ).
[c]) Blended line.

Microwave data for $^{1}H^{12}C^{12}C^{14}N$

Transition			ν [MHz]	Ref.
rotational $N' - N''$	fine structure $J' - J''$	Parity		
State: electronic $\tilde{X}\,^3\Sigma^-$; vibrational *b*, not known ($l = 0$) Probably $(0,0,0,2^0,0)$ [a])				
7← 6	6← 5	– ← +	154 397.547(31) [b])	95McC
8← 7	9← 8	+ ← –	176 299.310 [c])	
	7← 6		176 419.224(24)	
9← 8	10← 9	– ← +	198 346.262(20)	
	8← 7		198 447.305(22)	
10← 9	11← 10	+ ← –	220 391.041(25)	
	10← 9		220 428.883(28)	
	9← 8		220 478.690(21)	
11← 10	12← 11	– ← +	242 433.846(23)	
	11← 10		242 467.844(30)	
	10← 9		242 511.690(24)	
12← 11	13← 12	+ ← –	264 474.774(20)	
	12← 11		264 505.929(22)	
	11← 10		264 545.255(21)	
13← 12	14← 13	– ← +	286 514.103(23)	
	13← 12		286 542.855(34)	
	12← 11		286 578.831(25)	
15 ← 14	16 ← 15	– ← +	330 587.739(26)	
	15 ← 14		330 613.109(20)	
	14← 13		330 644.509(20)	
16 ← 15	17 ← 16	+ ← –	352 622.073(22)	
	16 ← 15		352 646.205(22)	
	15 ← 14		352 675.528(21)	

17 ← 16	18 ← 17	− ← +	374 654.681(20)
	17 ← 16		374 677.724(21)
	16 ← 15		374 705.832(20)

[a]) Assignment due to Hung *et al.* [01Hu].
[b]) The figures in parentheses are the authors' estimates of experimental uncertainty (1σ).
[c]) Blended line.

Molecular parameters for $^{1}H^{12}C^{12}C^{14}N$

Parameter		Value	Method	Ref.
State: electronic $\tilde{X}\,^3\Sigma^-$; vibrational (0,0,0,0,0)				
B	[MHz]	10 986.408 7(4) [a])	MW	95McC
D	[kHz]	4.168 7(9)		
λ	[MHz]	13 468(6)		
λ_D	[kHz]	5.5(3)		
γ	[MHz]	− 16.737(8)		
γ_D	[kHz]	−0.108(38)	MW	93En
$b_F(^{14}N)$	[MHz]	11.573(6)		
$c(^{14}N)$	[MHz]	− 28.291(43)		
$eQq_0\,(^{14}N)$	[MHz]	− 3.897(20)		
$b_F(^{1}H)$	[MHz]	− 41.723(9)		
$c(^{1}H)$	[MHz]	32.91(7)		
State: electronic $\tilde{X}\,^3\Sigma^-$; vibrational (0,0,0,0,1^1)				
B	[MHz]	10 988.525 1(3) [a])	MW	95McC
D	[kHz]	4.204 2(6)		
λ	[MHz]	13 062.6(3)		
λ_D	[kHz]	3.5(3)		
γ	[MHz]	− 16.119(3)		
o	[MHz]	853.0(3)		
p	[MHz]	0.579(8)		
q	[MHz]	40.560 7(6)		
q_D	[kHz]	− 0.113(1)		
State: electronic $\tilde{X}\,^3\Sigma^-$; vibrational (0,0,0,0,2^2)				
B	[MHz]	10 987.417 5(5) [a])	MW	95McC
D	[kHz]	4.313 7(10)		
λ	[MHz]	12 746.6(4)		
λ_D	[kHz]	9.0(5)		
γ	[MHz]	− 15.639(5)		
o_Δ	[kHz]	10.9(5)		
p_Δ	[kHz]	0.95(2)		
q_Δ	[kHz]	0.208 9(7)		
State: electronic $\tilde{X}\,^3\Sigma^-$; vibrational (0,0,0,0,3^3)				
B	[MHz]	10 988.940 1(7) [a])	MW	95McC
D	[kHz]	4.375 6(14)		
λ	[MHz]	12 448.1(3)		
λ_D	[kHz]	10.7(6)		
γ	[MHz]	− 14.844(10)		
State: electronic $\tilde{X}\,^3\Sigma^-$; vibrational (0,0,0, 1^1,0)				
A	[MHz]	− 75.7(9)(4) [a])	MW	95McC
B	[MHz]	11 021.408 6(4)		
D	[kHz]	4.340 0(10)		
λ	[MHz]	13 283.2(16)		
λ_D	[kHz]	5.9(5)		
γ	[MHz]	− 16.744(8)		
o	[MHz]	271.7(12)		

p	[MHz]	0.15(1)		
q	[MHz]	27.905 3(9)		
q_D	[kHz]	– 0.106(2)		
State: electronic $\tilde{X}\,^3\Sigma^-$; vibrational (0,0,0,0,2^0) ^{b})				
B	[MHz]	11 003.004 1(5) ^{a})	MW	95McC
D	[kHz]	4.21 9(12)		
λ	[MHz]	13 033(11)		
γ	[MHz]	– 16.161(11)		
State: electronic $\tilde{X}\,^3\Sigma^-$; vibrational a, not known (l = 0). Probably (0,0,0,1^1,1^1) ^{b})				
B	[MHz]	11 011.956 5(7) ^{a})	MW	95McC
D	[kHz]	2.985 6(20)		
λ	[MHz]	13 144(14)		
λ_D	[kHz]	– 59.1(9)		
γ	[MHz]	– 16.324(16)		
State: electronic $\tilde{X}\,^3\Sigma^-$; vibrational b, not known (l = 0). Probably (0,0,0,2^0,0) ^{b})				
B	[MHz]	11 022.249(6) ^{a})	MW	95McC
D	[kHz]	3.958 8(13)		
λ	[MHz]	13 052(11)		
λ_D	[kHz]	– 41.4(4)		
γ	[MHz]	– 16.256(10)		

^{a}) The numbers in parentheses are 1 standard deviation of the least-squares fit, in units of the last quoted decimal place.
^{b}) Parameter constrained to this value in the least-squares fit.

Microwave data for $^2H^{12}C^{12}C^{14}N$ (DCCN)

Transition: rotational $N'-N''$	fine structure $J'-J''$	Parity	ν [MHz]	Ref.
State: electronic $\tilde{X}\,^3\Sigma^-$; vibrational (0,0,0,0,0)				
8← 7	9← 8	+ ← –	158 452.780(20) ^{a})	95McC
	8← 7		158 494.595(20)	
	7← 6		158 553.392(20)	
9← 8	10← 9	– ← +	178 267.390(20)	
	9← 8		178 304.174(20)	
	8← 7		178 352.608(20)	
10← 9	11← 10	+ ← –	198 079.896(20)	
	10← 9		198 112.983(20)	
	9← 8		198 154.287(90)	
12← 11	13← 12	+ ← –	237 699.709(20)	
	12← 11		237 727.855(21)	
	11← 10		237 760.300(20)	
13← 12	14← 13	– ← +	257 507.296(20)	
	13← 12		257 533.736(21)	
	12← 11		257 563.353(20)	
14← 13	15 ← 14	+ ← –	277 313.446(20)	
	14← 13		277 338.481(21)	
	13← 12		277 365.879(20)	
15 ← 14	16 ← 15	– ← +	297 118.106(20)	
	15 ← 14		297 142.020(21)	
	14 ← 13		297 167.613(20)	
16 ← 15	17 ← 16	+ ← –	316 921.184(20)	
	16 ← 15		316 944.177(20)	
	15 ← 14		316 968.273(20)	

17 ← 16	18 ← 17	− ← +	336 722.803(20)	
	17 ← 16		336 745.026(21)	
	16 ← 15		336 767.898(20)	
18 ← 17	19 ← 18	+ ← −	356 522.738(20)	
	18 ← 17		356 544.314(21)	
	17 ← 16		356 566.214(20)	
19 ← 18	20 ← 19	− ← +	376 321.098(20)	
	19 ← 18		376 342.145(24)	
	18 ← 17		376 363.234(20)	

[a]) The figures in parentheses are the authors' estimates of experimental uncertainty (1σ).

Microwave data for $^{2}H^{12}C^{12}C^{14}N$ (DCCN)

Transition			ν [MHz]	Ref.
rotational $N' - N''$	parity	fine structure $J' - J''$		
State: electronic $\tilde{X}\,^3\Sigma^-$; vibrational (0,0,0,0,1[1])				
8← 7	− ← +	9← 8	158 274.330(20) [a])	95McC
		8← 7	158 464.488(20)	
		7← 6	158 345.069(20)	
	+ ← −	9← 8	159 090.573(20)	
		8← 7	159 267.073(20)	
		7← 6	159 133.398(20)	
9← 8	+ ← −	10← 9	178 082.286(20)	
		9← 8	178 224.251(20)	
		8← 7	178 151.088(20)	
	− ← +	10← 9	178 998.257(20)	
		9← 8	179 129.917(20)	
		8← 7	179 046.048(20)	
10← 9	− ← +	11← 10	197 884.774(20)	
		10← 9	197 995.158(20)	
		9← 8	197 949.866(22)	
	+ ← −	11← 10	198 900.692(20)	
		10← 9	199 003.061(20)	
		9← 8	198 949.440(20)	
12← 11	− ← +	13← 12	237 479.105(21)	
		12← 11	237 552.475(21)	
		11← 10	237 536.571(20)	
13← 12	+ ← −	14← 13	257 272.492(21)	
		13← 12	257 334.661(21)	
		12← 11	257 326.699(20)	
	− ← +	14← 13	258 588.825(20)	
		13← 12	258 646.794(21)	
		12← 11	258 634.295(21)	
14← 13	− ← +	15 ← 14	277 063.838(22)	
		14← 13	277 117.499(22)	
		13← 12	277 115.201(22)	
	+ ← −	15 ← 14	278 480.272(20)	
		14← 13	278 530.520(21)	
		13← 12	278 524.342(20)	
15 ← 14	+ ← −	16← 15	296 853.242(21)	
		15← 14	296 900.402(24)	
		14← 13	296 902.142(21)	
	− ← +	16← 15	298 369.835(21)	

		15← 14	298 414.307(21)	
		14← 13	298 412.626(20)	
16 ← 15	− ← +	17← 16	316 640.768(24)	
	+ ← −	17← 16	318 257.667(20)	
		16← 15	318 297.326(21)	
		15← 14	318 299.202(20)	
17 ← 16	+ ← −	18 ← 17	336 426.859(20)	
		17← 16	336 464.926(21)	
		16← 15	336 471.774(20)	
	− ← +	18 ← 17	338 143.676(21)	
		17← 16	338 179.796(21)	
		16← 15	338 184.082(20)	
18 ← 17	− ← +	19 ← 18	356 211.168(20)	
		18 ← 17	356 246.048(22)	
		17← 16	356 254.491(20)	
	+ ← −	19 ← 18	358 027.982(20)	
		17← 16	358 067.495(20)	
19 ← 18	+ ← −	20 ← 19	375 993.837(21)	
		19 ← 18	376 026.113(29)	
		18 ← 17	376 035.807(21)	
	− ← +	20 ← 19	377 910.350(22)	
		18 ← 17	377 949.018(22)	

[a]) The figures in parentheses are the authors' estimates of experimental uncertainty (1σ).

Microwave data for $^{2}H^{12}C^{12}C^{14}N$ (DCCN)

Transition			ν [MHz]	Ref.
rotational $N' - N''$	fine structure $J' - J''$	Parity [a])		
State: electronic $\tilde{X}\,^3\Sigma^-$; vibrational (0,0,0,0,2[2])				
8← 7	9← 8	− ← +	158 800.529 [b])	95McC
		+ ← −	158 800.529 [b])	
	7← 6	− ← +	158 736.318 [b])	
		+ ← −	158 736.318 [b])	
9← 8	10← 9	+ ← −	178 715.834 [b])	
		− ← +	178 715.834 [b])	
	9← 8	+ ← −	179 145.667 [b])	
		− ← +	179 145.667 [b])	
	8← 7	+ ← −	178 698.243(22) [c])	
		− ← +	178 698.933(24)	
10← 9	11← 10	− ← +	198 615.590(21)	
		+ ← −	198 616.450(21)	
	10← 9	− ← +	198 936.790(21)	
		+ ← −	198 937.515(22)	
	9← 8	− ← +	198 622.924(22)	
		+ ← −	198 623.763(22)	
12← 11	13← 12	− ← +	238 389.001(21)	
		+ ← −	238 884.826(21)	
	11← 10	− ← +	238 417.279(21)	
		+ ← −	238 418.759(21)	
16 ← 15	17 ← 16	− ← +	317 881.636(20)	
		+ ← −	317 884.826(20)	
	16 ← 15	− ← +	317 976.294(25)	
		+ ← −	317 979.200(29)	

	15 ← 14	− ← +	317 917.955(20)	
		+ ← −	317 921.318(20)	
17 ← 16	18 ← 17	− ← +	337 751.710(21)	
	17 ← 16	+ ← −	337 829.670(23)	
		− ← +	337 833.368(23)	
	16 ← 15	+ ← −	337 784.131(21)	
		− ← +	337 788.151(21)	
18 ← 17	19 ← 18	− ← +	357 611.190(22)	
		+ ← −	357 615.909(22)	
	18 ← 17	− ← +	357 683.543(25)	
		+ ← −	357 688.023(24)	
	17 ← 16	− ← +	357 647.640(21)	
		+ ← −	357 652.355(21)	
19 ← 18	20 ← 19	+ ← −	377 472.679(21)	
	18 ← 17	+ ← −	377 508.912(21)	
		− ← +	377 514.458(21)	

[a]) The relative parity was assumed to be as shown.
[b]) Blended line.
[c]) The figures in parentheses are the authors' estimates of experimental uncertainty (1σ).

Microwave data for $^{2}H^{12}C^{12}C^{14}N$ (DCCN)

Transition			ν [MHz]	Ref.
rotational $N' - N''$	fine structure $J' - J''$	Parity		
State: electronic $\tilde{X}\,^3\Sigma^-$; vibrational (0,0,0,0,3[3])				
9← 8	9← 8	[a])	179 717.375(21) [b])	95McC
10← 9	11← 10	[a])	198 766.881(22)	
	10 ← 9	[a])	199 438.070(21)	
13← 12	14← 13	[a])	258 541.705(24)	
14← 13	15 ← 14	[a])	278 448.982(21)	
	13 ← 12	[a])	278 462.784(22)	
15 ← 14	16 ← 15	[a])	298 350.847(21)	
16 ← 15	17 ← 16	[a])	318 248.521(21)	
	16 ← 15	[a])	318 430.412(22)	
	15 ← 14	[a])	318 272.650(21)	
17 ← 16	17 ← 16	[a])	338 297.353(22)	
	16 ← 15	[a])	338 169.135(21)	
18 ← 17	19 ← 18	[a])	358 033.128(21)	
	18 ← 17	[a])	358 061.448(21)	
	17 ← 16	[a])	358 166.762(23)	
19 ← 18	20 ← 19	[a])	377 920.722(33)	

[a]) Parity doubling not resolved.
[b]) The figures in parentheses are the authors' estimates of experimental uncertainty (1σ).

Microwave data for $^{2}H^{12}C^{12}C^{14}N$ (DCCN)

Transition			ν [MHz]	Ref.
rotational $N' - N''$	parity	fine structure $J' - J''$		
State: electronic $\tilde{X}\,^3\Sigma^-$; vibrational (0,0,0, 1[1],0)				
9← 8	+ ← −	10← 9	178 584.113(21) [a])	95McC
		9← 8	178 723.924(21)	
		8← 7	178 647.261(21)	

	− ← +	10← 9	179 212.605(21)
		9← 8	179 346.454(21)
		8← 7	179 263.243(21)
10← 9	− ← +	11← 10	198 442.301(21)
		9← 8	198 502.829(22)
	+ ← −	11← 10	199 139.341(21)
		10← 9	199 243.190(21)
		9← 8	199 190.206(21)
12← 11	− ← +	13← 12	238 147.875(23)
		12← 11	238 219.708(28)
		11← 10	238 202.432(22)
13← 12	+ ← −	14← 13	257 996.725(22)
		13← 12	258 057.825(23)
		12← 11	258 048.839(22)
14← 13	− ← +	15← 14	277 843.777(28)
		14← 13	277 896.627(41)
		13← 12	277 893.537(28)
15 ← 14	+ ← −	16← 15	297 532.947(54)
		14← 13	297 736.880(24)
16 ← 15	− ← +	17← 16	317 532.947(54)
		16← 15	317 574.242(28)
		15← 14	317 578.596(22)
	+ ← −	17← 16	318 641.234 [b])
		16← 15	318 681.479(27)
		15← 14	318 683.749(23)
17 ← 16	+ ← −	18 ← 17	337 374.876(22)
		17← 16	337 412.408(24)
		16← 15	337 418.994(21)
	− ← +	18 ← 17	338 551.338(28)
		17← 16	338 587.916(38)
		16← 15	338 592.667(22)
18 ← 17	− ← +	19 ← 18	357 215.392(22)
		18 ← 17	357 249.641(46)
		17← 16	357 258.065(25)
	+ ← −	19 ← 18	358 459.872(22)
		18 ← 17	358 493.608(26)
		17← 16	358 500.262(22)
19 ← 18	+ ← −	20← 19	377 054.221(23)
		18 ← 17	377 095.771(23)
	− ← +	20← 19	378 366.717(26)
		19 ← 18	378 397.863(59)
		18 ← 17	378 406.144(27)

[a]) The figures in parentheses are the authors' estimates of experimental uncertainty (1σ).
[b]) Blended line.

Microwave data for $^{2}H^{12}C^{12}C^{14}N$ (DCCN)

Transition			ν [MHz]	Ref.
rotational $N' - N''$	fine structure $J' - J''$	Parity		
State: electronic $\tilde{X}\,^3\Sigma^-$; vibrational (0,0,0,0,2^0) [a])				
8← 7	9← 8	+ ← −	158 747.565(22) [b])	95McC
9← 8	10← 9	− ← +	178 599.318(21)	
	9← 8		178 636.064(21)	

	8← 7		178 685.218(21)
10← 9	11← 10	+ ← –	198 449.063(21)
	10← 9		198 481.982(21)
	9← 8		198 523.965(21)
12← 11	13← 12	+ ← –	238 143.508(22)
	12← 11		238 171.413(23)
	11← 10		238 204.416(30)
13← 12	14← 13	– ← +	257 988.603(21)
	13← 12		258 014.676(22)
	12← 11		258 044.907(21)
14← 13	15 ← 14	+ ← –	277 832.272(24)
	14← 13		277 856.888(31)
	13← 12		277 884.895(24)
15 ← 14	16 ← 15	– ← +	297 674.610(22)
	15 ← 14		297 698.041(33)
	14← 13		297 724.296(22)
16 ← 15	17 ← 16	+ ← –	317 515.637(27)
	16 ← 15		317 537.963(50)
	15 ← 14		317 562.736(20)
17 ← 16	18 ← 17	– ← +	337 335.050(21)
	17 ← 16		337 376.801(22)
	16 ← 15		337 400.266(21)
18 ← 17	19 ← 18	+ ← –	357 193.032(21)
	17 ← 16		357 236.530(21)
19 ← 18	18 ← 17	– ← +	377 071.680(22)

[a]) Assignment due to Hung *et al.* [01Hu].
[b]) The figures in parentheses are the authors' estimates of experimental uncertainty (1σ).

Molecular parameters for $^{2}H^{12}C^{12}C^{14}N$ (DCCN)

Parameter		Value	Method	Ref.
State: electronic $\tilde{X}\,^3\Sigma^-$; vibrational (0,0,0,0,0)				
B	[MHz]	9 906.370 8(4) [a])	MW	95McC
D	[kHz]	3.660 1(7)		
λ	[MHz]	13 602(5)		
λ_D	[kHz]	15.3(3)		
γ	[MHz]	– 15.093(8)		
State: electronic $\tilde{X}\,^3\Sigma^-$; vibrational (0,0,0,0,1^1)				
B	[MHz]	9 922.983 5(2) [a])	MW	95McC
D	[kHz]	3.564 4(4)		
λ	[MHz]	13 259.3(9)		
γ	[MHz]	– 14.705(3)		
λ_D	[kHz]	7.7(2)		
o	[MHz]	740.2(8)		
p	[MHz]	0.568(9)		
q	[MHz]	50.627 6(4)		
q_D	[kHz]	– 0.306 7(7)		
State: electronic $\tilde{X}\,^3\Sigma^-$; vibrational (0,0,0,0,2^2)				
B	[MHz]	9 937.084 6(4) [a])	MW	95McC
D	[kHz]	3.667 7(7)		
λ	[MHz]	12 996.1(4)		
λ_D	[kHz]	14.6(4)		
γ	[MHz]	– 14.467(4)		

o_Δ	[kHz]	6.9(4)		
p_Δ	[kHz]	0.797(12)		
q_Δ	[kHz]	0.0.199 1(5)		
State: electronic $\tilde{X}\,^3\Sigma^-$; vibrational (0,0,0,0,3[3])				
B	[MHz]	9 949.495 4(5) [a])	MW	95McC
D	[kHz]	4.060 2(9)		
λ	[MHz]	12 767.5(3)		
λ_D	[kHz]	21.6(4)		
γ	[MHz]	– 14.080(5)		
State: electronic $\tilde{X}\,^3\Sigma^-$; vibrational (0,0,0, 1[1],0)				
A	[MHz]	– 85.3(9)(17) [a])	MW	95McC
B	[MHz]	9 942.837 7(4)		
D	[kHz]	3.419 7(8)		
λ	[MHz]	13 259(3)		
λ_D	[kHz]	1.6(4)		
γ	[MHz]	– 14.978(9)		
o	[MHz]	437.5(17)		
p	[MHz]	0.290(15)		
q	[MHz]	34 795(10)		
o_D	[kHz]	– 11.0(4)		
q_D	[kHz]	– 0.373(2)		
State: electronic $\tilde{X}\,^3\Sigma^-$; vibrational (0,0,0,0,2[0]) [b])				
B	[MHz]	9 924.766 2(5) [a])	MW	95McC
D	[kHz]	3.323 2(10)		
λ	[MHz]	13 472(8)		
λ_D	[kHz]	– 1.4(4)		
γ	[MHz]	– 15.021(10)		

[a]) The numbers in parentheses are 1 standard deviation of the least-squares fit, in units of the last quoted decimal place.
[b]) Assignment due to Hung *et al.* [01Hu].

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3.2.1.2.24 HC_4N

Microwave data for $^1H^{12}C_4{}^{14}N$

Transition: rotational $N' - N''$	fine structure $J' - J''$	Hyperfine [a]) $F_1' - F_1''$	$F' - F''$	ν [MHz]	Ref.
State: electronic $\tilde{X}\,^3\Sigma^-$; vibrational zero-point level					
1 ← 0	2 ← 1	1 ← 0	$1\frac{1}{2} \leftarrow \frac{1}{2}$	5 953.805(5) [b])	99Tan
		1 ← 1	$\frac{1}{2} \leftarrow \frac{1}{2}$	5 960.424(5)	
			$1\frac{1}{2} \leftarrow \frac{1}{2}$	5 950.367(5)	
		2 ← 1	$1\frac{1}{2} \leftarrow \frac{1}{2}$	5 966.556(5)	

			$1\frac{1}{2} \leftarrow 1\frac{1}{2}$	5 992.823(5)
			$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	5 957.199(5)
		$2 \leftarrow 2$	$1\frac{1}{2} \leftarrow 1\frac{1}{2}$	5 955.225(5)
			$2\frac{1}{2} \leftarrow 2\frac{1}{2}$	5 946.700(5)
		$3 \leftarrow 2$	$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	5 969.077(5)
			$2\frac{1}{2} \leftarrow 2\frac{1}{2}$	5 996.168(5)
			$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	5 959.995(5)
	$1 \leftarrow 1$	$0 \leftarrow 0$	$\frac{1}{2} \leftarrow \frac{1}{2}$	20 885.257(5)
		$1 \leftarrow 1$	$1\frac{1}{2} \leftarrow 1\frac{1}{2}$	20 880.044(5)
		$1 \leftarrow 2$	$1\frac{1}{2} \leftarrow 1\frac{1}{2}$	20 842.465(5)
			$1\frac{1}{2} \leftarrow 2\frac{1}{2}$	20 869.559(5)
		$2 \leftarrow 1$	$1\frac{1}{2} \leftarrow \frac{1}{2}$	20 865.455(5)
			$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	20 875.953(5)
		$2 \leftarrow 2$	$1\frac{1}{2} \leftarrow 1\frac{1}{2}$	20 854.110(5)
			$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	20 838.364(5)
			$1\frac{1}{2} \leftarrow 2\frac{1}{2}$	20 881.200(5)
			$2\frac{1}{2} \leftarrow 2\frac{1}{2}$	20 865.455(5)
$2 \leftarrow 1$	$1 \leftarrow 0$	$0 \leftarrow 1$	$\frac{1}{2} \leftarrow \frac{1}{2}$	25 491.573(5)
		$1 \leftarrow 1$	$\frac{1}{2} \leftarrow 1\frac{1}{2}$	25 474.062(5)
			$1\frac{1}{2} \leftarrow \frac{1}{2}$	25 485.222(5)
			$1\frac{1}{2} \leftarrow 1\frac{1}{2}$	25 485.140(5)
		$2 \leftarrow 1$	$1\frac{1}{2} \leftarrow \frac{1}{2}$	25 457.798(5)
			$1\frac{1}{2} \leftarrow 1\frac{1}{2}$	25 457.724(5)
			$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	25 470.414(5)
	$2 \leftarrow 1$	$1 \leftarrow 0$	$1\frac{1}{2} \leftarrow \frac{1}{2}$	9 210.307(5)
		$2 \leftarrow 1$	$1\frac{1}{2} \leftarrow \frac{1}{2}$	9 202.219(5)
			$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	9 209.724(5)
		$3 \leftarrow 2$	$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	9 204.721(5)
			$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	9 212.242(5)
	$3 \leftarrow 2$	$2 \leftarrow 1$	$1\frac{1}{2} \leftarrow \frac{1}{2}$	9 981.199(5)
			$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	9 977.129(5)
		$3 \leftarrow 2$	$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	9 983.238(5)
			$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	9 978.866(5)
		$4 \leftarrow 3$	$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	9 984.180(5)
			$4\frac{1}{2} \leftarrow 3\frac{1}{2}$	9 980.033(5)
	$2 \leftarrow 2$	$1 \leftarrow 1$	$1\frac{1}{2} \leftarrow 1\frac{1}{2}$	24 141.757(5)
		$2 \leftarrow 2$	$2\frac{1}{2} \leftarrow 2\frac{1}{2}$	24 132.568(5)
		$3 \leftarrow 3$	$2\frac{1}{2} \leftarrow 2\frac{1}{2}$	24 089.755(5)
			$3\frac{1}{2} \leftarrow 3\frac{1}{2}$	24 117.699(5)
$3 \leftarrow 2$	$2 \leftarrow 1$	$1 \leftarrow 0$	$1\frac{1}{2} \leftarrow \frac{1}{2}$	12 465.630(5)
		$2 \leftarrow 1$	$1\frac{1}{2} \leftarrow \frac{1}{2}$	12 444.686(5)
			$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	12 460.900(5)
		$3 \leftarrow 2$	$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	12 446.460(5)
			$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	12 461.895(5)
	$3 \leftarrow 2$	$2 \leftarrow 1$	$1\frac{1}{2} \leftarrow \frac{1}{2}$	13 812.073(5)

			$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	13 814.661(5)
		$3 \leftarrow 2$	$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	13 811.969(5)
			$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	13 814.661(5)
		$4 \leftarrow 3$	$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	13 813.147(5)
			$4\frac{1}{2} \leftarrow 3\frac{1}{2}$	13 815.689(5)
	$4 \leftarrow 3$	$3 \leftarrow 2$	$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	14 295.406(5)
			$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	14 293.376(5)
		$4 \leftarrow 3$	$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	14 296.542(5)
			$4\frac{1}{2} \leftarrow 3\frac{1}{2}$	14 294.368(5)
		$5 \leftarrow 4$	$4\frac{1}{2} \leftarrow 3\frac{1}{2}$	14 296.974(5)
			$5\frac{1}{2} \leftarrow 4\frac{1}{2}$	14 294.914(5)
$4 \leftarrow 3$	$3 \leftarrow 2$	$2 \leftarrow 1$	$1\frac{1}{2} \leftarrow \frac{1}{2}$	17 654.034(5)
			$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	17 651.676(5)
		$3 \leftarrow 2$	$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	17 643.100(5)
			$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	17 650.030(5)
		$4 \leftarrow 3$	$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	17 643.491(5)
			$4\frac{1}{2} \leftarrow 3\frac{1}{2}$	17 650.064(5)
	$4 \leftarrow 3$	$3 \leftarrow 2$	$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	18 417.959(5)
			$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	18 419.327(5)
		$4 \leftarrow 3$	$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	18 418.032(5)
			$4\frac{1}{2} \leftarrow 3\frac{1}{2}$	18 419.405(5)
		$5 \leftarrow 4$	$4\frac{1}{2} \leftarrow 3\frac{1}{2}$	18 418.620(5)
			$5\frac{1}{2} \leftarrow 4\frac{1}{2}$	18 419.935(5)
	$5 \leftarrow 4$	$4 \leftarrow 3$	$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	18 742.761(5)
			$4\frac{1}{2} \leftarrow 3\frac{1}{2}$	18 741.660(5)
		$5 \leftarrow 4$	$4\frac{1}{2} \leftarrow 3\frac{1}{2}$	18 743.464(5)
			$5\frac{1}{2} \leftarrow 4\frac{1}{2}$	18 742.283(5)
		$6 \leftarrow 5$	$5\frac{1}{2} \leftarrow 4\frac{1}{2}$	18 743.681(5)
			$6\frac{1}{2} \leftarrow 5\frac{1}{2}$	18 742.567(5)
$5 \leftarrow 4$	$4 \leftarrow 3$	$3 \leftarrow 2$	$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	22 541.605(5)
			$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	22 544.983(5)
		$4 \leftarrow 3$	$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	22 540.636(5)
			$4\frac{1}{2} \leftarrow 3\frac{1}{2}$	22 544.142(5)
		$5 \leftarrow 4$	$4\frac{1}{2} \leftarrow 3\frac{1}{2}$	22 540.840(5)
			$5\frac{1}{2} \leftarrow 4\frac{1}{2}$	22 544.192(5)
	$5 \leftarrow 4$	$4 \leftarrow 3$	$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	23 023.189(5)
			$4\frac{1}{2} \leftarrow 3\frac{1}{2}$	23 024.039(5)
		$5 \leftarrow 4$	$4\frac{1}{2} \leftarrow 3\frac{1}{2}$	23 023.284(5)
			$5\frac{1}{2} \leftarrow 4\frac{1}{2}$	23 024.127(5)
		$6 \leftarrow 5$	$5\frac{1}{2} \leftarrow 4\frac{1}{2}$	23 023.636(5)
			$6\frac{1}{2} \leftarrow 5\frac{1}{2}$	23 024.446(5)
	$6 \leftarrow 5$	$5 \leftarrow 4$	$4\frac{1}{2} \leftarrow 3\frac{1}{2}$	23 254.639(5)
			$5\frac{1}{2} \leftarrow 4\frac{1}{2}$	23 253.992(5)
		$6 \leftarrow 5$	$5\frac{1}{2} \leftarrow 4\frac{1}{2}$	23 255.104(5)
			$6\frac{1}{2} \leftarrow 5\frac{1}{2}$	23 254.412(5)

		7 ← 6	$6\frac{1}{2} \leftarrow 5\frac{1}{2}$	23 255.215(5)
			$7\frac{1}{2} \leftarrow 6\frac{1}{2}$	23 254.562(5)
6 ← 5	5 ← 4	4 ← 3	$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	27 304.287(5)
			$4\frac{1}{2} \leftarrow 3\frac{1}{2}$	27 306.221(5)
		5 ← 4	$4\frac{1}{2} \leftarrow 3\frac{1}{2}$	27 303.733(5)
			$5\frac{1}{2} \leftarrow 4\frac{1}{2}$	27 305.716(5)
		6 ← 5	$5\frac{1}{2} \leftarrow 4\frac{1}{2}$	27 303.875(5)
			$6\frac{1}{2} \leftarrow 5\frac{1}{2}$	27 305.803(5)
	6 ← 5	5 ← 4	$4\frac{1}{2} \leftarrow 3\frac{1}{2}$	27 628.188(5)
			$5\frac{1}{2} \leftarrow 4\frac{1}{2}$	27 628.746(5)
		6 ← 5	$5\frac{1}{2} \leftarrow 4\frac{1}{2}$	27 628.287(5)
			$6\frac{1}{2} \leftarrow 5\frac{1}{2}$	27 628.842(5)
		7 ← 6	$6\frac{1}{2} \leftarrow 5\frac{1}{2}$	27 628.493(5)
			$7\frac{1}{2} \leftarrow 6\frac{1}{2}$	27 629.052(5)
	7 ← 6	6 ← 5	$5\frac{1}{2} \leftarrow 4\frac{1}{2}$	27 800.584(5)
			$6\frac{1}{2} \leftarrow 5\frac{1}{2}$	27 800.186(5)
		7 ← 6	$6\frac{1}{2} \leftarrow 5\frac{1}{2}$	27 800.905(5)
			$7\frac{1}{2} \leftarrow 6\frac{1}{2}$	27 800.471(5)
		8 ← 7	$7\frac{1}{2} \leftarrow 6\frac{1}{2}$	27 801.000(5)
			$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	27 800.584(5)
7 ← 6	6 ← 5	5 ← 4	$4\frac{1}{2} \leftarrow 3\frac{1}{2}$	32 002.170(5)
			$5\frac{1}{2} \leftarrow 4\frac{1}{2}$	32 003.379(5)
		6 ← 5	$5\frac{1}{2} \leftarrow 4\frac{1}{2}$	32 001.842(5)
			$6\frac{1}{2} \leftarrow 5\frac{1}{2}$	32 003.051(5)
		7 ← 6	$6\frac{1}{2} \leftarrow 5\frac{1}{2}$	32 001.928(5)
			$7\frac{1}{2} \leftarrow 6\frac{1}{2}$	32 003.145(5)
	7 ← 6	6 ← 5	$5\frac{1}{2} \leftarrow 4\frac{1}{2}$	32 233.047(5)
			$6\frac{1}{2} \leftarrow 5\frac{1}{2}$	32 233.472(5)
		7 ← 6	$6\frac{1}{2} \leftarrow 5\frac{1}{2}$	32 233.149(5)
			$7\frac{1}{2} \leftarrow 6\frac{1}{2}$	32 233.575(5)
		8 ← 7	$7\frac{1}{2} \leftarrow 6\frac{1}{2}$	32 233.250(5)
			$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	32 233.664(5)
	8 ← 7	7 ← 6	$6\frac{1}{2} \leftarrow 5\frac{1}{2}$	32 366.002(5)
			$7\frac{1}{2} \leftarrow 6\frac{1}{2}$	32 365.728(5)
		8 ← 7	$7\frac{1}{2} \leftarrow 6\frac{1}{2}$	32 366.230(5)
		9 ← 8	$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	32 366.230(5)
			$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	32 366.002(5)

[a]) Coupling scheme: $\boldsymbol{J} = \boldsymbol{N} + \boldsymbol{S}$; $\boldsymbol{F}_1 = \boldsymbol{J} + \boldsymbol{I}_1$; $\boldsymbol{F} = \boldsymbol{F}_1 + \boldsymbol{I}_2$ where $\boldsymbol{I}_1$ is the ^{14}N nuclear spin and $\boldsymbol{I}_2$ is the ^{1}H nuclear spin.
[b]) The figures in parentheses are the authors' estimates of experimental uncertainty (1σ).

Molecular parameters for $^1H^{12}C_4{}^{14}N$

Parameter		Value	Method	Ref.
State: electronic $\tilde{X}\,^3\Sigma^-$; vibrational zero-point level				
B	[MHz]	2 302.398 02(47) [a])	FTMW	99Tan
D	[kHz]	0.119 3(68)		
λ	[MHz]	11 720.898 9(24)		
λ_D	[kHz]	0.85(38)		
γ	[MHz]	– 2.994 3(19)		
γ_D	[kHz]	0.0 [b])		
$b_F(^{14}N)$	[MHz]	7.805 1(72)		
$c(^{14}N)$	[MHz]	– 18.752 4(88)		
$eQq_0(^{14}N)$	[MHz]	– 3.999(18)		
$b_F(^1H)$	[MHz]	– 36.602 4(94)		
$c(^1H)$	[MHz]	25.870(14)		

[a]) The numbers in parentheses represent 2.5 standard deviations of the least-squares fit, in units of the last quoted decimal place.
[b]) Parameter constrained to this value.

References for HC_4N

99Tan Tang, J., Sumiyoshi, Y., Endo, Y. : Chem. Phys. Letters **315** (1999) 69.

3.2.1.2.25 HC_6N

Microwave data for $^1H^{12}C_6{}^{14}N$

Transition: rotational $N' - N''$	fine structure $J' - J''$	Hyperfine [a]) $F_1' - F_1''$	Hyperfine [a]) $F' - F''$	ν [MHz]	Ref.
State: electronic $\tilde{X}\,^3\Sigma^-$; vibrational zero-point level					
5 ← 4	5 ← 4	4 ← 3	$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	8 412.555(5) [b])	00Go
		5 ← 4	$4\frac{1}{2} \leftarrow 3\frac{1}{2}$	8 412.600(5)	
		6 ← 5	$5\frac{1}{2} \leftarrow 4\frac{1}{2}$	8 412.863(5)	
		4 ← 3	$4\frac{1}{2} \leftarrow 3\frac{1}{2}$	8 413.145(5)	
		5 ← 4	$5\frac{1}{2} \leftarrow 4\frac{1}{2}$	8 413.195(5)	
		6 ← 5	$6\frac{1}{2} \leftarrow 5\frac{1}{2}$	8 413.448(5)	
6 ← 5	5 ← 4	6 ← 5	$5\frac{1}{2} \leftarrow 4\frac{1}{2}$	9 503.209(5)	
		5 ← 4	$4\frac{1}{2} \leftarrow 3\frac{1}{2}$	9 503.623(5)	
		4 ← 3	$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	9 504.379(5)	
		6 ← 5	$6\frac{1}{2} \leftarrow 5\frac{1}{2}$	9 506.289(5)	
		5 ← 4	$5\frac{1}{2} \leftarrow 4\frac{1}{2}$	9 506.737(5)	
		4 ← 3	$4\frac{1}{2} \leftarrow 3\frac{1}{2}$	9 507.470(5)	
	6 ← 5	5 ← 4	$4\frac{1}{2} \leftarrow 3\frac{1}{2}$	10 095.330(5)	
		6 ← 5	$5\frac{1}{2} \leftarrow 4\frac{1}{2}$	10 095.403(5)	
		7 ← 6	$6\frac{1}{2} \leftarrow 5\frac{1}{2}$	10 095.548(5)	
		5 ← 4	$5\frac{1}{2} \leftarrow 4\frac{1}{2}$	10 095.715(5)	
		6 ← 5	$6\frac{1}{2} \leftarrow 5\frac{1}{2}$	10 095.788(5)	
		7 ← 6	$7\frac{1}{2} \leftarrow 6\frac{1}{2}$	10 095.950(5)	
	7 ← 6	6 ← 5	$6\frac{1}{2} \leftarrow 5\frac{1}{2}$	10 486.196(5)	

		7 ← 6	$7\frac{1}{2} \leftarrow 6\frac{1}{2}$	10 486.694(5)
		8 ← 7	$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	10 487.118(5)
		6 ← 5	$6\frac{1}{2} \leftarrow 5\frac{1}{2}$	10 487.667(5)
		7 ← 6	$7\frac{1}{2} \leftarrow 6\frac{1}{2}$	10 488.185(5)
		8 ← 7	$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	10 488.603(5)
7 ← 6	6 ← 5	7 ← 6	$6\frac{1}{2} \leftarrow 5\frac{1}{2}$	11 298.231(5)
		6 ← 5	$5\frac{1}{2} \leftarrow 4\frac{1}{2}$	11 298.580(5)
		5 ← 4	$4\frac{1}{2} \leftarrow 3\frac{1}{2}$	11 299.165(5)
		7 ← 6	$7\frac{1}{2} \leftarrow 6\frac{1}{2}$	11 300.552(5)
		6 ← 5	$6\frac{1}{2} \leftarrow 5\frac{1}{2}$	11 300.925(5)
		5 ← 4	$5\frac{1}{2} \leftarrow 4\frac{1}{2}$	11 301.486(5)
	7 ← 6	7 ← 6	$6\frac{1}{2} \leftarrow 5\frac{1}{2}$	11 777.785(5)
		6 ← 5	$5\frac{1}{2} \leftarrow 4\frac{1}{2}$	11 778.035(5)
		6 ← 6	$6\frac{1}{2} \leftarrow 5\frac{1}{2}$	11 778.146(5)
		8 ← 7	$7\frac{1}{2} \leftarrow 6\frac{1}{2}$	11 778.200(5)
		7 ← 5	$6\frac{1}{2} \leftarrow 5\frac{1}{2}$	11 778.268(5)
		7 ← 6	$7\frac{1}{2} \leftarrow 6\frac{1}{2}$	11 778.375(5)
		8 ← 7	$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	11 778.490(5)
	8 ← 7	7 ← 6	$7\frac{1}{2} \leftarrow 6\frac{1}{2}$	12 101.714(5)
		8 ← 7	$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	12 102.109(5)
		9 ← 8	$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	12 102.437(5)
		7 ← 6	$6\frac{1}{2} \leftarrow 5\frac{1}{2}$	12 102.860(5)
		8 ← 7	$7\frac{1}{2} \leftarrow 6\frac{1}{2}$	12 103.266(5)
		9 ← 8	$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	12 103.588(5)
8 ← 7	7 ← 6	8 ← 7	$7\frac{1}{2} \leftarrow 6\frac{1}{2}$	13 067.894(5)
		7 ← 6	$6\frac{1}{2} \leftarrow 5\frac{1}{2}$	13 068.175(5)
		6 ← 5	$5\frac{1}{2} \leftarrow 4\frac{1}{2}$	13 068.625(5)
		8 ← 7	$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	13 069.668(5)
		7 ← 6	$7\frac{1}{2} \leftarrow 6\frac{1}{2}$	13 069.961(5)
		6 ← 5	$6\frac{1}{2} \leftarrow 5\frac{1}{2}$	13 070.403(5)
	8 ← 7	7 ← 6	$6\frac{1}{2} \leftarrow 5\frac{1}{2}$	13 460.708(5)
		8 ← 7	$7\frac{1}{2} \leftarrow 6\frac{1}{2}$	13 460.823(5)
		9 ← 8	$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	13 460.833(5)
		7 ← 6	$7\frac{1}{2} \leftarrow 6\frac{1}{2}$	13 460.853(5)
		8 ← 7	$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	13 460.967(5)
		9 ← 8	$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	13 461.054(5)
	9 ← 8	8 ← 7	$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	13 731.769(5)
		9 ← 8	$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	13 732.087(5)
		10 ← 9	$10\frac{1}{2} \leftarrow 9\frac{1}{2}$	13 732.339(5)
		8 ← 9	$7\frac{1}{2} \leftarrow 6\frac{1}{2}$	13 732.668(5)
		9 ← 8	$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	13 732.992(5)
		10 ← 9	$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	13 733.241(5)
9 ← 8	8 ← 7	9 ← 8	$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	14 818.147(5)
		8 ← 7	$7\frac{1}{2} \leftarrow 6\frac{1}{2}$	14 818.368(5)
		7 ← 6	$6\frac{1}{2} \leftarrow 5\frac{1}{2}$	14 818.723(5)

		9 ← 8	$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	14 819.519(5)
		8 ← 7	$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	14 819.749(5)
		7 ← 6	$7\frac{1}{2} \leftarrow 6\frac{1}{2}$	14 820.095(5)
	10 ← 9	9 ← 8	$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	15 372.806(5)
		10 ← 9	$10\frac{1}{2} \leftarrow 9\frac{1}{2}$	15 373.061(5)
		11 ← 10	$11\frac{1}{2} \leftarrow 10\frac{1}{2}$	15 373.262(5)
		9 ← 8	$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	15 373.516(5)
		10 ← 9	$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	15 373.778(5)
		11 ← 10	$10\frac{1}{2} \leftarrow 9\frac{1}{2}$	15 373.974(5)
10 ← 9	9 ← 8	10 ← 9	$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	16 553.714(5)
		9 ← 8	$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	16 553.891(5)
		8 ← 7	$7\frac{1}{2} \leftarrow 6\frac{1}{2}$	16 554.170(5)
		10 ← 9	$10\frac{1}{2} \leftarrow 9\frac{1}{2}$	16 554.793(5)
		9 ← 8	$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	16 554.973(5)
		8 ← 7	$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	16 555.247(5)
	11 ← 10	10 ← 9	$10\frac{1}{2} \leftarrow 9\frac{1}{2}$	17 022.172(5)
		11 ← 10	$11\frac{1}{2} \leftarrow 10\frac{1}{2}$	17 022.379(5)
		12 ← 11	$12\frac{1}{2} \leftarrow 11\frac{1}{2}$	17 022.538(5)
		10 ← 9	$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	17 022.739(5)
		11 ← 10	$10\frac{1}{2} \leftarrow 9\frac{1}{2}$	17 022.951(5)
		12 ← 11	$12\frac{1}{2} \leftarrow 11\frac{1}{2}$	17 023.109(5)

[a]) Coupling scheme: $\boldsymbol{J} = \boldsymbol{N} + \boldsymbol{S}$; $\boldsymbol{F}_1 = \boldsymbol{J} + \boldsymbol{I}_1$; $\boldsymbol{F} = \boldsymbol{F}_1 + \boldsymbol{I}_2$ where $\boldsymbol{I}_1$ is the ^{14}N nuclear spin and $\boldsymbol{I}_2$ is the ^{1}H nuclear spin.
[b]) The figures in parentheses are the authors' estimates of experimental uncertainty (1σ).

Molecular parameters for $^{1}H^{12}C_6{}^{14}N$

Parameter		Value	Method	Ref.
State: electronic $\tilde{X}\,^3\Sigma^-$; vibrational zero-point level				
B	[MHz]	841.307 28(7) [a])	FTMW	00Go
D	[Hz]	10.3(5)		
λ	[MHz]	10 729.75(6)		
λ_D	[Hz]	– 130(50)		
γ	[MHz]	– 0.946(3)		
$b_F(^1H)$	[MHz]	– 26.27(2)		
$c(^1H)$	[MHz]	18.42(4)		
$b_F(^{14}N)$	[MHz]	5.448(9)		
$c(^{14}N)$	[MHz]	– 12.97(3)		
$eQq_0(^{14}N)$	[MHz]	–4.09(2)		

[a]) The numbers in parentheses represent 1 standard deviation of the least-squares fit, in units of the last quoted decimal place.

Microwave data for $^{1}H^{12}C_6{}^{15}N$

Transition				ν [MHz]	Ref.
rotational $N' - N''$	fine structure $J' - J''$	Hyperfine [a]) $F_1' - F_1''$	$F' - F''$		
State: electronic $\tilde{X}\,^3\Sigma^-$; vibrational zero-point level					
5 ← 4	5 ← 4	$5\frac{1}{2} \leftarrow 4\frac{1}{2}$	5 ← 4	8 222.443(5) [b])	00Go
			6 ← 5	8 223.028(5)	
		$4\frac{1}{2} \leftarrow 3\frac{1}{2}$	5 ← 4	8 223.211(5)	

6 ← 5	6 ← 5	$6\frac{1}{2} \leftarrow 5\frac{1}{2}$	6 ← 5	9 867.155(5)
		$5\frac{1}{2} \leftarrow 4\frac{1}{2}$	5 ← 4	9 867.275(5)
		$6\frac{1}{2} \leftarrow 5\frac{1}{2}$	7 ← 6	9 867.555(5)
		$5\frac{1}{2} \leftarrow 4\frac{1}{2}$	6 ← 5	9 867.678(5)
7 ← 6	6 ← 5	$5\frac{1}{2} \leftarrow 4\frac{1}{2}$	5 ← 4	11 028.558(5)
		$6\frac{1}{2} \leftarrow 5\frac{1}{2}$	6 ← 5	11 029.286(5)
		$5\frac{1}{2} \leftarrow 4\frac{1}{2}$	6 ← 5	11 030.849(5)
		$6\frac{1}{2} \leftarrow 5\frac{1}{2}$	7 ← 6	11 031.567(5)
	7 ← 6	$7\frac{1}{2} \leftarrow 6\frac{1}{2}$	7 ← 6	11 511.800(5)
		$6\frac{1}{2} \leftarrow 5\frac{1}{2}$	6 ← 5	11 511.893(5)
		$7\frac{1}{2} \leftarrow 6\frac{1}{2}$	8 ← 7	11 512.088(5)
		$6\frac{1}{2} \leftarrow 5\frac{1}{2}$	7 ← 6	11 512.183(5)
	8 ← 7	$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	9 ← 8	11 839.834(5)
			8 ← 7	11 840.985(5)
8 ← 7	7 ← 6	$6\frac{1}{2} \leftarrow 5\frac{1}{2}$	6 ← 5	12 759.513(5)
		$7\frac{1}{2} \leftarrow 6\frac{1}{2}$	7 ← 6	12 760.077(5)
		$6\frac{1}{2} \leftarrow 5\frac{1}{2}$	7 ← 6	12 761.276(5)
		$7\frac{1}{2} \leftarrow 6\frac{1}{2}$	8 ← 7	12 761.836(5)
	8 ← 7	$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	8 ← 7	13 156.415(5)
		$7\frac{1}{2} \leftarrow 6\frac{1}{2}$	7 ← 6	13 156.487(5)
		$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	9 ← 8	13 156.6415)
		$7\frac{1}{2} \leftarrow 6\frac{1}{2}$	8 ← 7	13 156.708(5)
	9 ← 8	$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	10 ← 9	13 431.708(5)
		$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	9 ← 8	13 432.111(5)
		$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	9 ← 8	13 432.616(5)
		$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	8 ← 7	13 433.018(5)
9 ← 8	8 ← 7	$7\frac{1}{2} \leftarrow 6\frac{1}{2}$	7 ← 6	14 471.555(5)
		$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	8 ← 7	14 471.999(5)
		$7\frac{1}{2} \leftarrow 6\frac{1}{2}$	8 ← 7	14 472.929(5)
		$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	9 ← 8	14 473.370(5)
	9 ← 8	$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	9 ← 8	14 801.015(5)
		$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	8 ← 7	14 801.070(5)
		$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	10 ← 9	14 801.193(5)
		$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	11 ← 10	14 801.248(5)
	10 ← 9	$10\frac{1}{2} \leftarrow 9\frac{1}{2}$	11 ← 10	15 034.444(5)
		$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	10 ← 9	15 034.766(5)
		$10\frac{1}{2} \leftarrow 9\frac{1}{2}$	10 ← 9	15 035.165(5)
		$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	9 ← 8	15 035.490(5)
10 ← 9	9 ← 8	$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	8 ← 7	16 169.187(5)
		$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	9 ← 8	16 169.533(5)
		$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	9 ← 8	16 170.266(5)
		$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	10 ← 9	16 170.612(5)
	10 ← 9	$10\frac{1}{2} \leftarrow 9\frac{1}{2}$	10 ← 9	16 445.604(5)
		$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	9 ← 8	16 445.604(5)
		$10\frac{1}{2} \leftarrow 9\frac{1}{2}$	11 ← 10	16 445.645(5)

		$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	$10 \leftarrow 9$	16 445.745(5)
	$11 \leftarrow 10$	$11\frac{1}{2} \leftarrow 10\frac{1}{2}$	$12 \leftarrow 11$	16 645.466(5)
		$10\frac{1}{2} \leftarrow 9\frac{1}{2}$	$11 \leftarrow 10$	16 645.725(5)
		$11\frac{1}{2} \leftarrow 10\frac{1}{2}$	$11 \leftarrow 10$	16 646.043(5)
		$10\frac{1}{2} \leftarrow 9\frac{1}{2}$	$10 \leftarrow 9$	16 646.306(5)

[a]) Coupling scheme: $\boldsymbol{J} = \boldsymbol{N} + \boldsymbol{S}$; $\boldsymbol{F}_1 = \boldsymbol{J} + \boldsymbol{I}_1$; $\boldsymbol{F} = \boldsymbol{F}_1 + \boldsymbol{I}_2$ where $\boldsymbol{I}_1$ is the ^{14}N nuclear spin and $\boldsymbol{I}_2$ is the ^{1}H nuclear spin.
[b]) The figures in parentheses are the authors' estimates of experimental uncertainty (1σ).

Molecular parameters for $^1H^{12}C_6{}^{15}N$

Parameter		Value	Method	Ref.
State: electronic $\tilde{X}\,^3\Sigma^-$; vibrational zero-point level				
B	[MHz]	822.287 00(8) [a])	FTMW	00Go
D	[Hz]	10.1(5)		
λ	[MHz]	10 729.83(8)		
λ_D	[Hz]	– 170(50)		
γ	[MHz]	– 0.928(4)		
$b_F(^1H)$	[MHz]	– 26.29(1)		
$c(^1H)$	[MHz]	18.41(6)		
$b_F(^{15}N)$	[MHz]	– 7.65(1)		
$c(^{15}N)$	[MHz]	18.14(6)		

[a]) The numbers in parentheses represent 1 standard deviation of the least-squares fit, in units of the last quoted decimal place.

Reference for HC_6N

00Go Gordon, V.D., McCarthy, M.C., Apponi, A.J., Thaddeus, P. : Astrophys. J. **540** (2000) 286.

3.2.1.2.26 HCCP

Microwave data for $^1H^{12}C^{12}C^{31}P$

Transition				ν [MHz]	Ref.
rotational $N' - N''$	fine structure $J' - J''$	Hyperfine [a]) $F_1' - F_1''$	$F' - F''$		
State: electronic $\tilde{X}\,^3\Sigma^-$; vibrational (0,0,0,0,0)					
$8 \leftarrow 7$	$9 \leftarrow 8$	$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	$10 \leftarrow 9$	91 408.479	97Ah
		$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	$9 \leftarrow 8$	91 401.704	
			$8 \leftarrow 7$	91 402.483	
	$8 \leftarrow 7$	$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	[b])	89 967.908	
		$7\frac{1}{2} \leftarrow 6\frac{1}{2}$	[b])	89 965.738	
$9 \leftarrow 8$	$9 \leftarrow 8$	$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	[b])	101 212.648	
		$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	[b])	101 210.939	
	$8 \leftarrow 7$	$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	$9 \leftarrow 8$	99 466.262	
			$8 \leftarrow 7$	99 465.152	
		$7\frac{1}{2} \leftarrow 6\frac{1}{2}$	$7 \leftarrow 6$	99 471.859	
$10 \leftarrow 9$	$11 \leftarrow 10$	$11\frac{1}{2} \leftarrow 10\frac{1}{2}$	[b])	113 476.007	
	$10 \leftarrow 9$	$10\frac{1}{2} \leftarrow 9\frac{1}{2}$	[b])	112 457.107	
		$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	[b])	112 455.726	
	$9 \leftarrow 8$	$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	$10 \leftarrow 9$	111 014.878	
			$9 \leftarrow 8$	111 013.905	

		$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	$9 \leftarrow 8$	111 020.058
			$8 \leftarrow 7$	111 019.108
$11 \leftarrow 10$	$12 \leftarrow 11$	$12\frac{1}{2} \leftarrow 11\frac{1}{2}$	[b])	124 571.631
		$11\frac{1}{2} \leftarrow 10\frac{1}{2}$	[b])	124 568.188
	$11 \leftarrow 10$	$11\frac{1}{2} \leftarrow 10\frac{1}{2}$	[b])	123 701.223
		$10\frac{1}{2} \leftarrow 9\frac{1}{2}$	[b])	123 700.089
	$10 \leftarrow 9$	$10\frac{1}{2} \leftarrow 9\frac{1}{2}$	[b])	122 499.137
		$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	[b])	122 498.399
$12 \leftarrow 11$	$13 \leftarrow 12$	$13\frac{1}{2} \leftarrow 12\frac{1}{2}$	[b])	135 695.323
		$12\frac{1}{2} \leftarrow 11\frac{1}{2}$	[b])	135 692.458
	$12 \leftarrow 11$	$12\frac{1}{2} \leftarrow 11\frac{1}{2}$	[b])	134 945.008
		$11\frac{1}{2} \leftarrow 10\frac{1}{2}$	[b])	134 944.025
	$11 \leftarrow 10$	$11\frac{1}{2} \leftarrow 10\frac{1}{2}$	[b])	133 924.376
		$10\frac{1}{2} \leftarrow 9\frac{1}{2}$	[b])	133 927.448
$13 \leftarrow 12$	$14 \leftarrow 13$	$14\frac{1}{2} \leftarrow 13\frac{1}{2}$	[b])	146 840.318
		$13\frac{1}{2} \leftarrow 12\frac{1}{2}$	[b])	146 837.968
	$13 \leftarrow 12$	$13\frac{1}{2} \leftarrow 12\frac{1}{2}$	[b])	146 188.275
		$12\frac{1}{2} \leftarrow 11\frac{1}{2}$	[b])	146 187.475
	$12 \leftarrow 11$	$12\frac{1}{2} \leftarrow 11\frac{1}{2}$	[b])	145 316.215
$14 \leftarrow 13$	$15 \leftarrow 14$	$15\frac{1}{2} \leftarrow 14\frac{1}{2}$	[b])	158 001.914
		$14\frac{1}{2} \leftarrow 13\frac{1}{2}$	[b])	157 999.914
	$14 \leftarrow 13$	$14\frac{1}{2} \leftarrow 13\frac{1}{2}$	[b])	157 431.167
		$13\frac{1}{2} \leftarrow 12\frac{1}{2}$	[b])	157 430.449
	$13 \leftarrow 12$	$13\frac{1}{2} \leftarrow 12\frac{1}{2}$	[b])	156 679.158
		$12\frac{1}{2} \leftarrow 11\frac{1}{2}$	[b])	156 681.251
$15 \leftarrow 14$	$16 \leftarrow 15$	$16\frac{1}{2} \leftarrow 15\frac{1}{2}$	[b])	169 176.320
		$15\frac{1}{2} \leftarrow 14\frac{1}{2}$	[b])	169 174.624
	$15 \leftarrow 14$	[c])	[c])	168 673.168
	$14 \leftarrow 13$	$14\frac{1}{2} \leftarrow 13\frac{1}{2}$	[b])	168 019.715
		$13\frac{1}{2} \leftarrow 12\frac{1}{2}$	[b])	168 021.434
$16 \leftarrow 15$	$17 \leftarrow 16$	$17\frac{1}{2} \leftarrow 16\frac{1}{2}$	[b])	180 360.847
		$16\frac{1}{2} \leftarrow 15\frac{1}{2}$	[b])	180 359.369
	$16 \leftarrow 15$	[c])	[c])	179 915.033
	$15 \leftarrow 14$	$15\frac{1}{2} \leftarrow 14\frac{1}{2}$	[b])	179 342.769
		$14\frac{1}{2} \leftarrow 13\frac{1}{2}$	[b])	179 344.218
$18 \leftarrow 17$	$19 \leftarrow 18$	$19\frac{1}{2} \leftarrow 18\frac{1}{2}$	[b])	202 752.149
		$18\frac{1}{2} \leftarrow 17\frac{1}{2}$	[b])	202 751.072
	$18 \leftarrow 17$	[c])	[c])	202 396.866
	$17 \leftarrow 16$	$17\frac{1}{2} \leftarrow 16\frac{1}{2}$	[b])	201 949.594
		$16\frac{1}{2} \leftarrow 15\frac{1}{2}$	[b])	201 950.678
$19 \leftarrow 18$	$20 \leftarrow 19$	$20\frac{1}{2} \leftarrow 19\frac{1}{2}$	[b])	213 956.149
		$19\frac{1}{2} \leftarrow 18\frac{1}{2}$	[b])	213 955.146
	$19 \leftarrow 18$	[c])	[c])	213 636.841
$20 \leftarrow 19$	$21 \leftarrow 20$	$21\frac{1}{2} \leftarrow 20\frac{1}{2}$	[b])	225 164.108
		$20\frac{1}{2} \leftarrow 19\frac{1}{2}$	[b])	225 163.204
	$20 \leftarrow 19$	[c])	[c])	224 876.120

	19 ← 18	[c])	[c])	224 519.461
21 ← 20	22 ← 21	$22\frac{1}{2} \leftarrow 21\frac{1}{2}$	[b])	236 375.242
		$21\frac{1}{2} \leftarrow 20\frac{1}{2}$	[b])	236 374.467
	21 ← 20	[c])	[c])	236 114.585
	20 ← 19	[c])	[c])	235 793.841
22 ← 21	23 ← 22	[c])	[c])	247 588.562
	22 ← 21	[c])	[c])	247 352.309
	21 ← 20	[c])	[c])	247 062.722
23 ← 22	24 ← 23	[c])	[c])	258 804.346
	23 ← 22	[c])	[c])	258 589.269
	22 ← 21	[c])	[c])	258 326.821
24 ← 23	25 ← 24	[c])	[c])	270 021.625
	24 ← 23	[c])	[c])	269 825.315
	23 ← 22	[c])	[c])	269 586.792
25 ← 24	25 ← 24	[c])	[c])	281 060.528
	24 ← 23	[c])	[c])	280 843.071
26 ← 25	27 ← 26	[c])	[c])	292 459.342
	26 ← 25	[c])	[c])	292 294.797
	25 ← 24	[c])	[c])	292 096.034
27 ← 26	28 ← 27	[c])	[c])	303 679.202
	27 ← 26	[c])	[c])	303 528.080
	26 ← 25	[c])	[c])	303 346.001
28 ← 27	29 ← 28	[c])	[c])	314 899.309
	28 ← 27	[c])	[c])	314 760.379
	27 ← 26	[c])	[c])	314 593.155
29 ← 28	30 ← 29	[c])	[c])	326 119.594
	29 ← 28	[c])	[c])	325 991.672
	28 ← 27	[c])	[c])	325 837.845
30 ← 29	31 ← 30	[c])	[c])	337 339.817
	30 ← 29	[c])	[c])	337 221.871
	29 ← 28	[c])	[c])	337 080.137
31 ← 30	32 ← 31	[c])	[c])	348 559.870
	31 ← 30	[c])	[c])	348 450.985
	30 ← 29	[c])	[c])	348 320.095

[a]) Coupling scheme: $\boldsymbol{J} = \boldsymbol{N} + \boldsymbol{S}$; $\boldsymbol{F}_1 = \boldsymbol{J} + \boldsymbol{I}_1$; $\boldsymbol{F} = \boldsymbol{F}_1 + \boldsymbol{I}_2$ where $\boldsymbol{I}_1$ is the ^{31}P nuclear spin and $\boldsymbol{I}_2$ is the ^{1}H nuclear spin.
[b]) ^{1}H hyperfine structure not resolved.
[c]) Neither ^{31}P nor ^{1}H hyperfine structure resolved.

Molecular parameters for ^{1}H^{12}C^{12}C^{31}P

Parameter		Value	Method	Ref.
State: electronic $\tilde{X}\,^{3}\Sigma^{-}$; vibrational (0,0,0,0,0)				
B	[MHz]	5 623.115 58(58) [a])	MW	97Ah
D	[kHz]	1.537 31(43)		
λ	[MHz]	63 429.42(111)		
λ_D	[kHz]	24.47(52)		
γ	[MHz]	– 30.092(22)		
$b_F(^{31}P)$	[MHz]	145.71(147)		
$c(^{31}P)$	[MHz]	– 418.9(59)		
$b_F(^{1}H)$	[MHz]	– 26.34(180)		
$c(^{1}H)$	[MHz]	21.8(144)		

[a]) The numbers in parentheses are 3 standard deviations of the least-squares fit, in units of the last quoted decimal place.

Microwave data for $^{2}H^{12}C^{12}C^{31}P$ (DCCP)

Transition rotational $N' - N''$	Transition fine structure $J' - J''$	ν [MHz]	Ref.
State: electronic $\tilde{X}\,^3\Sigma^-$; vibrational (0,0,0,0,0)			
26 ← 25	27 ← 26	267 397.363	97Ah
	26 ← 25	267 207.859	
	25 ← 24	266 981.238	
27 ← 26	28 ← 27	277 652.765	
	27 ← 26	277 478.191	
	26 ← 25	277 270.026	
29 ← 28	30 ← 29	298 165.211	
	29 ← 28	298 016.368	
	28 ← 27	297 839.492	
30 ← 29	31 ← 30	308 422.042	
	30 ← 29	308 284.224	
	29 ← 28	308 120.710	
31 ← 30	32 ← 31	318 678.922	
	31 ← 30	318 551.224	
32 ← 31	33 ← 32	328 935.875	
	32 ← 31	328 817.308	
	31 ← 30	328 676.845	
33 ← 32	34 ← 33	339 192.593	
	33 ← 32	339 082.443	
	32 ← 31	338 951.986	
34 ← 33	35 ← 34	349 449.057	
	34 ← 33	349 346.632	
	33 ← 32	349 225.297	
35 ← 34	36 ← 35	359 705.171	
	35 ← 34	359 609.822	
	34 ← 33	359 496.786	

Molecular parameters for $^{2}H^{12}C^{12}C^{31}P$ (DCCP)

Parameter		Value	Method	Ref.
State: electronic $\tilde{X}\,^3\Sigma^-$; vibrational (0,0,0,0,0)				
B	[MHz]	5 140.236 64(159) [a])	MW	97Ah
D	[kHz]	1.211 14(78)		
λ	[MHz]	63 565.9(186)		
λ_D	[kHz]	20.92(57)		
γ	[MHz]	– 27.455(108)		

a) The numbers in parentheses are 3 standard deviations of the least-squares fit, in units of the last quoted decimal place.

Microwave data for $^{1}H^{13}C^{13}C^{31}P$

Transition rotational $N' - N''$	Transition fine structure $J' - J''$	Transition Hyperfine [a]) $F_1' - F_1''$	ν [MHz]	Ref.
State: electronic $\tilde{X}\,^3\Sigma^-$; vibrational (0,0,0,0,0)				
12 ← 11	13 ← 12	$13\frac{1}{2} \leftarrow 12\frac{1}{2}$	130 288.248	97Ah
		$12\frac{1}{2} \leftarrow 11\frac{1}{2}$	130 285.121	
	12 ← 11	$12\frac{1}{2} \leftarrow 11\frac{1}{2}$	129 502.352	
13 ← 12	14 ← 13	$14\frac{1}{2} \leftarrow 13\frac{1}{2}$	140 976.579	

		$13\frac{1}{2} \leftarrow 12\frac{1}{2}$	140 974.135
	$13 \leftarrow 12$	$13\frac{1}{2} \leftarrow 12\frac{1}{2}$	140 293.426
		$12\frac{1}{2} \leftarrow 11\frac{1}{2}$	140 292.515
$14 \leftarrow 13$	$15 \leftarrow 14$	$15\frac{1}{2} \leftarrow 14\frac{1}{2}$	151 681.962
		$14\frac{1}{2} \leftarrow 13\frac{1}{2}$	151 679.879
	$14 \leftarrow 13$	$14\frac{1}{2} \leftarrow 13\frac{1}{2}$	151 982.635
$15 \leftarrow 14$	$16 \leftarrow 15$	$16\frac{1}{2} \leftarrow 15\frac{1}{2}$	162 400.606
		$15\frac{1}{2} \leftarrow 14\frac{1}{2}$	162 398.866
	$15 \leftarrow 14$	b)	161 871.891
	$14 \leftarrow 13$	$14\frac{1}{2} \leftarrow 13\frac{1}{2}$	161 187.338
$16 \leftarrow 15$	$17 \leftarrow 16$	$17\frac{1}{2} \leftarrow 16\frac{1}{2}$	173 129.667
		$16\frac{1}{2} \leftarrow 15\frac{1}{2}$	173 128.100
	$16 \leftarrow 15$	b)	172 660.542
	$15 \leftarrow 14$	$15\frac{1}{2} \leftarrow 14\frac{1}{2}$	172 061.722
$17 \leftarrow 16$	$17 \leftarrow 16$	b)	183 448.592
	$16 \leftarrow 15$	$16\frac{1}{2} \leftarrow 15\frac{1}{2}$	182 918.605
$18 \leftarrow 17$	$19 \leftarrow 18$	$19\frac{1}{2} \leftarrow 18\frac{1}{2}$	194 611.906
		$18\frac{1}{2} \leftarrow 17\frac{1}{2}$	194 609.906
	$18 \leftarrow 17$	b)	194 236.144
$19 \leftarrow 18$	$20 \leftarrow 19$	$20\frac{1}{2} \leftarrow 19\frac{1}{2}$	205 360.482
		$19\frac{1}{2} \leftarrow 18\frac{1}{2}$	205 359.409
	$19 \leftarrow 18$	b)	205 023.063
$20 \leftarrow 19$	$21 \leftarrow 20$	$21\frac{1}{2} \leftarrow 20\frac{1}{2}$	216 114.123
		$20\frac{1}{2} \leftarrow 19\frac{1}{2}$	216 113.143
	$20 \leftarrow 19$	b)	215 809.373
	$19 \leftarrow 18$	$19\frac{1}{2} \leftarrow 18\frac{1}{2}$	215 432.824
		$18\frac{1}{2} \leftarrow 17\frac{1}{2}$	215 433.646
$21 \leftarrow 20$	$22 \leftarrow 21$	$22\frac{1}{2} \leftarrow 21\frac{1}{2}$	226 871.130
		$21\frac{1}{2} \leftarrow 20\frac{1}{2}$	226 870.282
	$21 \leftarrow 20$	b)	226 594.903
	$20 \leftarrow 19$	b)	226 256.202
$22 \leftarrow 21$	$23 \leftarrow 22$	$23\frac{1}{2} \leftarrow 22\frac{1}{2}$	237 630.911
		$22\frac{1}{2} \leftarrow 21\frac{1}{2}$	237 630.162
	$22 \leftarrow 21$	b)	237 379.856
	$21 \leftarrow 20$	b)	237 073.649
$23 \leftarrow 22$	$24 \leftarrow 23$	b)	248 164.056
	$23 \leftarrow 22$	b)	247 886.139
$24 \leftarrow 23$	$25 \leftarrow 24$	b)	259 156.209
	$24 \leftarrow 23$	b)	258 947.321
	$23 \leftarrow 22$	b)	258 694.506
$25 \leftarrow 24$	$26 \leftarrow 25$	b)	269 921.111
	$25 \leftarrow 24$	b)	269 729.907
	$24 \leftarrow 23$	b)	269 499.048
$26 \leftarrow 25$	$27 \leftarrow 26$	b)	280 687.216
	$26 \leftarrow 25$	b)	280 511.594
	$25 \leftarrow 24$	b)	280 300.407
$27 \leftarrow 26$	$28 \leftarrow 27$	b)	291 453.962
	$27 \leftarrow 26$	b)	291 292.440
	$26 \leftarrow 25$	b)	291 098.618

28 ← 27	29 ← 28	[b])	302 221.124
	28 ← 27	[b])	301 894.148
29 ← 28	30 ← 29	[b])	312 988.596
	29 ← 28	[b])	312 851.223
	28 ← 27	[b])	312 687.170
30 ← 29	31 ← 30	[b])	323 756.057
	30 ← 29	[b])	323 629.261
	29 ← 28	[b])	323 477.741
31 ← 30	32 ← 31	[b])	334 523.494
	31 ← 30	[b])	334 406.195
	30 ← 29	[b])	334 266.094
32 ← 31	33 ← 32	[b])	345 290.663
	32 ← 31	[b])	345 182.101
	31 ← 30	[b])	345 052.306
33 ← 32	34 ← 33	[b])	356 057.578
	33 ← 32	[b])	355 956.910
	32 ← 31	[b])	355 836.600
34 ← 33	35 ← 34	[b])	366 823.951
	34 ← 33	[b])	366 730.598
	33 ← 32	[b])	366 618.976
35 ← 34	36 ← 35	[b])	377 589.761
	35 ← 34	[b])	377 503.110
	34 ← 33	[b])	377 399.303

[a]) Coupling scheme: $\boldsymbol{J} = \boldsymbol{N} + \boldsymbol{S}$; $\boldsymbol{F}_1 = \boldsymbol{J} + \boldsymbol{I}_1$; $\boldsymbol{F} = \boldsymbol{F}_1 + \boldsymbol{I}_2$ where $\boldsymbol{I}_1$ is the ^{31}P nuclear spin. Neither ^{13}C nor ^{1}H hyperfine structure is resolved.
[b]) ^{31}P hyperfine structure not resolved.

Molecular parameters for $^{1}H^{13}C^{13}C^{31}P$

Parameter		Value	Method	Ref.
State: electronic $\tilde{X}\,^3\Sigma^-$; vibrational (0,0,0,0,0)				
B	[MHz]	5 396.348 60(69) [a])	MW	97Ah
D	[kHz]	1.413 03(40)		
λ	[MHz]	63 469.9(29)		
λ_D	[kHz]	23.21(52)		
γ	[MHz]	– 28.832(31)		
$b_F(^{31}P)$	[MHz]	140.6(78)		
$c(^{31}P)$	[MHz]	– 443.9(167)		

[a]) The numbers in parentheses are 3 standard deviations of the least-squares fit, in units of the last quoted decimal place.

References for HCCP

97Ah Ahmad, I.K., Ozeki, H., Saito, S. : J. Chem. Phys. **107** (1997) 1301.

3.2.1.2.27 HC_2S

Microwave data for $^{1}H^{12}C^{12}C^{32}S$

Transition				ν	Ref.
spin Ω	rotational $J' - J''$	parity e/f [a])	hyperfine $F' - F''$	[MHz]	
State: electronic $\tilde{X}\,^2\Pi$; vibrational zero point level					
$\frac{3}{2}$	$5\frac{1}{2} \leftarrow 4\frac{1}{2}$	e, f	6 ← 5	64 550.697 [c])	91Sa
		e, f	5 ← 4	64 551.147	
$\frac{1}{2}$	$5\frac{1}{2} \leftarrow 4\frac{1}{2}$	f	6 ← 5	64 772.804	

		f	5 ← 4	64 773.256	
		e	6 ← 5	64 646.442	
		e	5 ← 4	64 646.846	
$\frac{3}{2}$	$6\frac{1}{2} \leftarrow 5\frac{1}{2}$	*e*	b)	76 286.989(11)	92Vr
		f	b)	76 286.989(11)	
$\frac{1}{2}$	$6\frac{1}{2} \leftarrow 5\frac{1}{2}$	*e*	b)	76 411.602(10)	
		f	b)	76 537.975(10)	
$\frac{3}{2}$	$7\frac{1}{2} \leftarrow 6\frac{1}{2}$	*e*	b)	88 022.863(10)	
		f	b)	88 022.863(10)	
$\frac{3}{2}$	$7\frac{1}{2} \leftarrow 6\frac{1}{2}$	*e*	b)	88176.359(10)	
		f	b)	88 302.737(10)	
$\frac{3}{2}$	$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	*e*	b)	99 758.487(10)	
		f	b)	99 758.487(10)	
$\frac{1}{2}$	$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	*e*	b)	99 940.852(10)	
		f	b)	100 067.252(10)	
$\frac{3}{2}$	$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	*e,f*	b)	111 493.835	91Sa
$\frac{1}{2}$	$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	*f*	b)	111 831.490	
		e	b)	111 705.072	
$\frac{3}{2}$	$10\frac{1}{2} \leftarrow 9\frac{1}{2}$	*e,f*	b)	123 228.880	
$\frac{1}{2}$	$10\frac{1}{2} \leftarrow 9\frac{1}{2}$	*f*	b)	123 595.426	
		e	b)	123 468.962	
$\frac{3}{2}$	$11\frac{1}{2} \leftarrow 10\frac{1}{2}$	*e,f*	b)	134 963.586	
$\frac{1}{2}$	$11\frac{1}{2} \leftarrow 10\frac{1}{2}$	*f*	b)	135 358.988	
		e	b)	135 232.502	
$\frac{3}{2}$	$12\frac{1}{2} \leftarrow 11\frac{1}{2}$	*e,f*	b)	146 697.875	
$\frac{1}{2}$	$12\frac{1}{2} \leftarrow 11\frac{1}{2}$	*f*	b)	147 122.174	
		e	b)	146 995.640	
$\frac{3}{2}$	$13\frac{1}{2} \leftarrow 12\frac{1}{2}$	*e*	b)	158 431.758(10)	92Vr
		f	b)	158 431.758(10)	
$\frac{1}{2}$	$13\frac{1}{2} \leftarrow 12\frac{1}{2}$	*e*	b)	158 758.370(11)	
		f	b)	158 884.909(11)	
$\frac{3}{2}$	$14\frac{1}{2} \leftarrow 13\frac{1}{2}$	*e*	b)	170 165.192(10)	
		f	b)	170 165.192(10)	
$\frac{1}{2}$	$14\frac{1}{2} \leftarrow 13\frac{1}{2}$	*e*	b)	170 520.647(12)	
		f	b)	170 647.239(10)	
$\frac{3}{2}$	$15\frac{1}{2} \leftarrow 14\frac{1}{2}$	*e*	b)	181 897.817(30)	
		f	b)	181 898.404(10)	
$\frac{1}{2}$	$15\frac{1}{2} \leftarrow 14\frac{1}{2}$	*e*	b)	182 282.414(12)	
		f	b)	182 409.084(10)	
$\frac{3}{2}$	$16\frac{1}{2} \leftarrow 15\frac{1}{2}$	*e*	b)	193 630.265(20)	
		f	b)	193 630.915(20)	
$\frac{1}{2}$	$16\frac{1}{2} \leftarrow 15\frac{1}{2}$	*e*	b)	194 043.659(10)	
$\frac{1}{2}$	$18\frac{1}{2} \leftarrow 17\frac{1}{2}$	*e*	b)	217 564.528(12)	
		f	b)	217 691.343(11)	
$\frac{3}{2}$	$19\frac{1}{2} \leftarrow 18\frac{1}{2}$	*e*	b)	228 824.107	91Sa
		f	b)	228 825.085	
$\frac{1}{2}$	$19\frac{1}{2} \leftarrow 18\frac{1}{2}$	*e*	b)	229 323.986	
		f	b)	229 450.891	
$\frac{3}{2}$	$20\frac{1}{2} \leftarrow 19\frac{1}{2}$	*e*	b)	240 554.064(70)	92Vr

		f	[b])	240 555.232(90)	
$\frac{1}{2}$	$20\frac{1}{2} \leftarrow 19\frac{1}{2}$	*e*	[b])	241 082.817(10)	
		f	[b])	241 209.809(10)	
$\frac{3}{2}$	$21\frac{1}{2} \leftarrow 20\frac{1}{2}$	*e*	[b])	252 283.445	91Sa
		f	[b])	252 284.591	
$\frac{1}{2}$	$21\frac{1}{2} \leftarrow 20\frac{1}{2}$	*e*	[b])	252 840.931	
		f	[b])	252 968.017	
$\frac{3}{2}$	$22\frac{1}{2} \leftarrow 21\frac{1}{2}$	*e*	[b])	264 012.091	
		f	[b])	264 013.347	
$\frac{1}{2}$	$22\frac{1}{2} \leftarrow 21\frac{1}{2}$	*e*	[b])	264 598.337(10)	92Vr
		f	[b])	264 725.484(18)	
$\frac{3}{2}$	$23\frac{1}{2} \leftarrow 22\frac{1}{2}$	*e*	[b])	275 739.935(20)	
		f	[b])	275 741.316(20)	
$\frac{1}{2}$	$23\frac{1}{2} \leftarrow 22\frac{1}{2}$	*e*	[b])	276 354.988(11)	
		f	[b])	276 482.189(10)	
$\frac{3}{2}$	$24\frac{1}{2} \leftarrow 23\frac{1}{2}$	*e*	[b])	287 467.060(11)	
		f	[b])	287 468.545(11)	
$\frac{1}{2}$	$24\frac{1}{2} \leftarrow 23\frac{1}{2}$	*e*	[b])	288 110.856(11)	
		f	[b])	288 238.167(12)	
$\frac{3}{2}$	$25\frac{1}{2} \leftarrow 24\frac{1}{2}$	*e*	[b])	299 193.314(12)	
		f	[b])	299 194.958(20)	
$\frac{1}{2}$	$25\frac{1}{2} \leftarrow 24\frac{1}{2}$	*f*	[b])	299 993.262(10)	
$\frac{3}{2}$	$29\frac{1}{2} \leftarrow 28\frac{1}{2}$	*e*	[b])	346 089.716(10)	
		f	[b])	346 091.816(10)	
$\frac{1}{2}$	$29\frac{1}{2} \leftarrow 28\frac{1}{2}$	*e*	[b])	346 877.151(10)	
$\frac{3}{2}$	$31\frac{1}{2} \leftarrow 30\frac{1}{2}$	*e*	[b])	369 532.167(10)	
		f	[b])	369 534.532(10)	
$\frac{3}{2}$	$32\frac{1}{2} \leftarrow 31\frac{1}{2}$	*e*	[b])	381 251.813(10)	
		f	[b])	381 254.340(10)	
$\frac{1}{2}$	$32\frac{1}{2} \leftarrow 31\frac{1}{2}$	*e*	[b])	382 125.249(10)	
		f	[b])	382 253.372(10)	
$\frac{3}{2}$	$33\frac{1}{2} \leftarrow 32\frac{1}{2}$	*e*	[b])	392 970.358(30)	
		f	[b])	392 973.063(20)	
$\frac{1}{2}$	$33\frac{1}{2} \leftarrow 32\frac{1}{2}$	*e*	[b])	393 872.473(15)	
		f	[b])	394 000.705(10)	

[a]) States with parity equal to $\pm(-1)^{J-0.5}$ are labeled *e* and *f* respectively.
[b]) Proton hyperfine structure not resolved.
[c]) The figures in parentheses are the authors' estimate of experimental uncertainty, in units of the last quoted decimal place.

Microwave data for $^{1}H^{12}C^{12}C^{32}S$

Transition		ν	Ref.
rotational $N' - N''$	fine structure $J' - J''$ [a])	[MHz]	
State: electronic $\tilde{X}\,^2\Pi$; vibrational $v_4 = 1$, lower vibronic component ($\mu^2\Sigma$)			
$20 \leftarrow 19$	$19\frac{1}{2} \leftarrow 18\frac{1}{2}$	233 193.478	96Ta
$21 \leftarrow 20$	$21\frac{1}{2} \leftarrow 20\frac{1}{2}$	250 041.719	
$22 \leftarrow 21$	$21\frac{1}{2} \leftarrow 20\frac{1}{2}$	256 756.046	

23 ← 22	$22\frac{1}{2} \leftarrow 21\frac{1}{2}$	268 536.266	
	$23\frac{1}{2} \leftarrow 22\frac{1}{2}$	273 601.605	
24 ← 23	$23\frac{1}{2} \leftarrow 22\frac{1}{2}$	280 315.645	
25 ← 24	$24\frac{1}{2} \leftarrow 23\frac{1}{2}$	292 094.236	
26 ← 25	$25\frac{1}{2} \leftarrow 24\frac{1}{2}$	303 871.978	
27 ← 26	$26\frac{1}{2} \leftarrow 25\frac{1}{2}$	315 648.841	
	$27\frac{1}{2} \leftarrow 26\frac{1}{2}$	320 711.311	
28 ← 27	$28\frac{1}{2} \leftarrow 27\frac{1}{2}$	332 486.501	
29 ← 28	$28\frac{1}{2} \leftarrow 27\frac{1}{2}$	339 199.726	
	$29\frac{1}{2} \leftarrow 28\frac{1}{2}$	344 260.647	
30 ← 29	$30\frac{1}{2} \leftarrow 29\frac{1}{2}$	356 033.787	
31 ← 30	$30\frac{1}{2} \leftarrow 29\frac{1}{2}$	362 746.686	
32 ← 31	$31\frac{1}{2} \leftarrow 30\frac{1}{2}$	374 518.591	
	$32\frac{1}{2} \leftarrow 31\frac{1}{2}$	379 576.828	
State: electronic $\tilde{X}\,^2\Pi$; vibrational $v_5 = 1$, lower vibronic component ($\mu^2\Sigma$)			
19 ← 18	$19\frac{1}{2} \leftarrow 18\frac{1}{2}$	228 884.972	96Ta
20 ← 19	$19\frac{1}{2} \leftarrow 18\frac{1}{2}$	229 758.099	
21 ← 20	$20\frac{1}{2} \leftarrow 19\frac{1}{2}$	241 512.842	
	$21\frac{1}{2} \leftarrow 20\frac{1}{2}$	252 396.364	
22 ← 21	$21\frac{1}{2} \leftarrow 20\frac{1}{2}$	253 266.912	
	$22\frac{1}{2} \leftarrow 21\frac{1}{2}$	264 151.057	
23 ← 22	$22\frac{1}{2} \leftarrow 21\frac{1}{2}$	265 020.167	
	$23\frac{1}{2} \leftarrow 22\frac{1}{2}$	275 905.014	
24 ← 23	$23\frac{1}{2} \leftarrow 22\frac{1}{2}$	276 772.624	
	$24\frac{1}{2} \leftarrow 23\frac{1}{2}$	287 658.217	
25 ← 24	$24\frac{1}{2} \leftarrow 23\frac{1}{2}$	288 524.299	
	$25\frac{1}{2} \leftarrow 24\frac{1}{2}$	299 410.518	
26 ← 25	$25\frac{1}{2} \leftarrow 24\frac{1}{2}$	300 275.005	
27 ← 26	$27\frac{1}{2} \leftarrow 26\frac{1}{2}$	322 912.602	
28 ← 27	$27\frac{1}{2} \leftarrow 26\frac{1}{2}$	323 773.821	
29 ← 28	$28\frac{1}{2} \leftarrow 27\frac{1}{2}$	335 521.736	
	$29\frac{1}{2} \leftarrow 28\frac{1}{2}$	346 411.161	
30 ← 29	$29\frac{1}{2} \leftarrow 28\frac{1}{2}$	347 268.720	
	$30\frac{1}{2} \leftarrow 29\frac{1}{2}$	358 158.945	
31 ← 30	$30\frac{1}{2} \leftarrow 29\frac{1}{2}$	359 014.595	
32 ← 31	$31\frac{1}{2} \leftarrow 30\frac{1}{2}$	370 759.459	
	$32\frac{1}{2} \leftarrow 31\frac{1}{2}$	381 651.464	
33 ← 32	$32\frac{1}{2} \leftarrow 31\frac{1}{2}$	382 503.440	
State: electronic $\tilde{X}\,^2\Pi$; vibrational $v_5 = 1$, upper vibronic component ($\kappa^2\Sigma$)			
19 ← 18	$19\frac{1}{2} \leftarrow 18\frac{1}{2}$	277 653.724	96Ta
20 ← 19	$19\frac{1}{2} \leftarrow 18\frac{1}{2}$	231 944.231	
	$20\frac{1}{2} \leftarrow 19\frac{1}{2}$	239 434.918	
21 ← 20	$20\frac{1}{2} \leftarrow 19\frac{1}{2}$	243 723.096	
	$21\frac{1}{2} \leftarrow 20\frac{1}{2}$	251 215.358	

22 ← 21	$21\frac{1}{2} \leftarrow 20\frac{1}{2}$	255 501.175
	$22\frac{1}{2} \leftarrow 21\frac{1}{2}$	262 995.220
23 ← 22	$22\frac{1}{2} \leftarrow 21\frac{1}{2}$	267 278.474
	$23\frac{1}{2} \leftarrow 22\frac{1}{2}$	274 774.356
24 ← 23	$23\frac{1}{2} \leftarrow 22\frac{1}{2}$	279 054.985
	$24\frac{1}{2} \leftarrow 23\frac{1}{2}$	286 552.785
25 ← 24	$24\frac{1}{2} \leftarrow 23\frac{1}{2}$	290 830.662
	$25\frac{1}{2} \leftarrow 24\frac{1}{2}$	298 330.493
26 ← 25	$26\frac{1}{2} \leftarrow 25\frac{1}{2}$	310 107.276
27 ← 26	$27\frac{1}{2} \leftarrow 26\frac{1}{2}$	321 883.330
28 ← 27	$28\frac{1}{2} \leftarrow 27\frac{1}{2}$	333 658.508
29 ← 28	$28\frac{1}{2} \leftarrow 27\frac{1}{2}$	337 924.230
	$29\frac{1}{2} \leftarrow 28\frac{1}{2}$	345 432.784
30 ← 29	$29\frac{1}{2} \leftarrow 28\frac{1}{2}$	349 206.128
	$30\frac{1}{2} \leftarrow 29\frac{1}{2}$	357 206.128
31 ← 30	$30\frac{1}{2} \leftarrow 29\frac{1}{2}$	361 465.051
	$31\frac{1}{2} \leftarrow 30\frac{1}{2}$	368 978.557
32 ← 31	$31\frac{1}{2} \leftarrow 30\frac{1}{2}$	373 233.872
	$32\frac{1}{2} \leftarrow 31\frac{1}{2}$	380 749. 917

[a]) ^{1}H hyperfine structure not resolved.

Microwave data for $^1H^{12}C^{12}C^{32}S$

Transition			ν [MHz]	Ref.
spin Ω	rotational $J' - J''$	parity e/f [a])		
State: electronic $\tilde{X}\,^2\Pi$; vibrational $v_4 = 1$, $^2\Delta$ vibronic component				
$\frac{5}{2}$	$19\frac{1}{2} \leftarrow 18\frac{1}{2}$	e, f	229 279.725	96Ta
$\frac{5}{2}$	$20\frac{1}{2} \leftarrow 19\frac{1}{2}$	e, f	241 033.156	
$\frac{5}{2}$	$21\frac{1}{2} \leftarrow 20\frac{1}{2}$	e, f	252 785.815	
$\frac{5}{2}$	$22\frac{1}{2} \leftarrow 21\frac{1}{2}$	e, f	264 537.853	
$\frac{5}{2}$	$23\frac{1}{2} \leftarrow 22\frac{1}{2}$	e, f	276 289.135	
$\frac{5}{2}$	$24\frac{1}{2} \leftarrow 23\frac{1}{2}$	e, f	288 039.663	
$\frac{5}{2}$	$25\frac{1}{2} \leftarrow 24\frac{1}{2}$	e, f	299 789.314	
$\frac{5}{2}$	$27\frac{1}{2} \leftarrow 26\frac{1}{2}$	e, f	323 286.097	
$\frac{5}{2}$	$28\frac{1}{2} \leftarrow 27\frac{1}{2}$	e, f	335 033.152	
$\frac{5}{2}$	$29\frac{1}{2} \leftarrow 28\frac{1}{2}$	e, f	346 779.260	
$\frac{5}{2}$	$30\frac{1}{2} \leftarrow 29\frac{1}{2}$	e, f	358 524.343	
$\frac{5}{2}$	$31\frac{1}{2} \leftarrow 30\frac{1}{2}$	e, f	370 268.399	
$\frac{5}{2}$	$32\frac{1}{2} \leftarrow 31\frac{1}{2}$	e, f	382 011.539	
State: electronic $\tilde{X}\,^2\Pi$; vibrational $v_5 = 1$, $^2\Delta$ vibronic component				
$\frac{3}{2}$	$16\frac{1}{2} \leftarrow 15\frac{1}{2}$	e	194 629.004	96Ta
		f	194 630.246	
$\frac{3}{2}$	$17\frac{1}{2} \leftarrow 16\frac{1}{2}$	e	206 421.216	
		f	206 422.612	
$\frac{3}{2}$	$18\frac{1}{2} \leftarrow 17\frac{1}{2}$	e	218 212.041	
		f	218 215.127	

$\frac{5}{2}$	$19\frac{1}{2} \leftarrow 18\frac{1}{2}$	*e*, *f*	229 279.725	
$\frac{3}{2}$	$19\frac{1}{2} \leftarrow 18\frac{1}{2}$	*e*	230 003.629	
		f	230 005.348	
$\frac{5}{2}$	$20\frac{1}{2} \leftarrow 19\frac{1}{2}$	*e*, *f*	241 033.156	
$\frac{3}{2}$	$20\frac{1}{2} \leftarrow 19\frac{1}{2}$	*e*	241 793.948	
		f	241 795.754	
$\frac{5}{2}$	$21\frac{1}{2} \leftarrow 20\frac{1}{2}$	*e*, *f*	252 785.815	
$\frac{3}{2}$	$21\frac{1}{2} \leftarrow 20\frac{1}{2}$	*e*	253 583.400	
		f	253 585.484	
$\frac{5}{2}$	$22\frac{1}{2} \leftarrow 21\frac{1}{2}$	*e*, *f*	264 537.853	
$\frac{3}{2}$	$22\frac{1}{2} \leftarrow 21\frac{1}{2}$	*e*	265 372.131	
		f	265 374.383	
$\frac{5}{2}$	$23\frac{1}{2} \leftarrow 22\frac{1}{2}$	*e*, *f*	276 289.135	
$\frac{3}{2}$	$23\frac{1}{2} \leftarrow 22\frac{1}{2}$	*e*	277 160.062	
		f	277 162.376	
$\frac{5}{2}$	$24\frac{1}{2} \leftarrow 23\frac{1}{2}$	*e*, *f*	288 039.663	
$\frac{3}{2}$	$24\frac{1}{2} \leftarrow 23\frac{1}{2}$	*e*	288 947.194	
		f	288 949.858	
$\frac{5}{2}$	$25\frac{1}{2} \leftarrow 24\frac{1}{2}$	*e*, *f*	299 789.314	
$\frac{3}{2}$	$25\frac{1}{2} \leftarrow 24\frac{1}{2}$	*e*	300 733.668	
		f	300 736.294	
$\frac{5}{2}$	$27\frac{1}{2} \leftarrow 26\frac{1}{2}$	*e*, *f*	323 286.097	
$\frac{3}{2}$	$27\frac{1}{2} \leftarrow 26\frac{1}{2}$	*f*	324 306.479	
$\frac{5}{2}$	$28\frac{1}{2} \leftarrow 27\frac{1}{2}$	*e*, *f*	335 033.152	
$\frac{3}{2}$	$28\frac{1}{2} \leftarrow 27\frac{1}{2}$	*e*	336 086.644	
		f	336 090.150	
$\frac{5}{2}$	$29\frac{1}{2} \leftarrow 28\frac{1}{2}$	*e*, *f*	346 779.260	
$\frac{3}{2}$	$29\frac{1}{2} \leftarrow 28\frac{1}{2}$	*e*	347 869.197	
		f	347 872.859	
$\frac{5}{2}$	$30\frac{1}{2} \leftarrow 29\frac{1}{2}$	*e*, *f*	358 524.343	
$\frac{3}{2}$	$30\frac{1}{2} \leftarrow 29\frac{1}{2}$	*e*	359 650.643	
		f	359 654.445	
$\frac{5}{2}$	$31\frac{1}{2} \leftarrow 30\frac{1}{2}$	*e*, *f*	370 268.399	
$\frac{3}{2}$	$31\frac{1}{2} \leftarrow 30\frac{1}{2}$	*e*	371 430.966	
		f	371 434.995	
$\frac{5}{2}$	$32\frac{1}{2} \leftarrow 31\frac{1}{2}$	*e*, *f*	382 011.539	
$\frac{3}{2}$	$32\frac{1}{2} \leftarrow 31\frac{1}{2}$	*e*	383 210.208	
		f	383 214.373	
$\frac{3}{2}$	$33\frac{1}{2} \leftarrow 32\frac{1}{2}$	*e*	394 988.310	
		f	394 992.734	
State: electronic $\tilde{X}\,^2\Pi$; vibrational $v_5 = 2$, $^2\Phi$ vibronic component				
$\frac{7}{2}$	$16\frac{1}{2} \leftarrow 15\frac{1}{2}$	*e*, *f*	194 607.438	96Ta
$\frac{7}{2}$	$17\frac{1}{2} \leftarrow 16\frac{1}{2}$	*e*, *f*	206 398.435	
$\frac{7}{2}$	$18\frac{1}{2} \leftarrow 17\frac{1}{2}$	*e*, *f*	218 188.941	
$\frac{7}{2}$	$19\frac{1}{2} \leftarrow 18\frac{1}{2}$	*e*, *f*	229 978.748	
$\frac{7}{2}$	$20\frac{1}{2} \leftarrow 19\frac{1}{2}$	*e*, *f*	241 767.815	
$\frac{7}{2}$	$21\frac{1}{2} \leftarrow 20\frac{1}{2}$	*e*, *f*	253 556.283	

$\frac{7}{2}$	$22\frac{1}{2} \leftarrow 21\frac{1}{2}$	e, f	265 344.014
$\frac{7}{2}$	$23\frac{1}{2} \leftarrow 22\frac{1}{2}$	e, f	277 130.956
$\frac{7}{2}$	$24\frac{1}{2} \leftarrow 23\frac{1}{2}$	e, f	288 917.137
$\frac{7}{2}$	$25\frac{1}{2} \leftarrow 24\frac{1}{2}$	e, f	300 702.435
$\frac{7}{2}$	$27\frac{1}{2} \leftarrow 26\frac{1}{2}$	e, f	324 270.447
$\frac{7}{2}$	$29\frac{1}{2} \leftarrow 28\frac{1}{2}$	e, f	347 934.739
$\frac{7}{2}$	$30\frac{1}{2} \leftarrow 29\frac{1}{2}$	e, f	359 615.398
$\frac{7}{2}$	$31\frac{1}{2} \leftarrow 30\frac{1}{2}$	e, f	371 395.020
$\frac{7}{2}$	$32\frac{1}{2} \leftarrow 31\frac{1}{2}$	e, f	383 173.601
$\frac{7}{2}$	$33\frac{1}{2} \leftarrow 32\frac{1}{2}$	e, f	394 950.952

[a]) States with parity equal to $\pm(-1)^{J-0.5}$ are labeled *e* and *f* respectively.

Molecular parameters for $^1H^{12}C^{12}C^{32}S$

Parameter		Value	Method	Ref.
State: electronic $\tilde{X}\,^2\Pi$; vibrational zero point level				
B	[MHz]	5 875.567 25(27) [a])	MW	92Vr
D	[kHz]	1.389 74(18)		
$A+\gamma$	[GHz]	– 5 543.8(183)		
γ	[MHz]	– 920.8(207)		
γ_D	[kHz]	– 4.40(15)		
p	[MHz]	126.819(21)		
p_D	[kHz]	1.383 2(138)		
q	[MHz]	– 0.281 4(33)		
$h_{1/2}(^1H)$ [b])	[MHz]	26.5(80)	MW	91Sa
$h_{3/2}(^1H)$ [c])	[MHz]	8.0(38)		
$d(^1H)$	[MHz]	13(26)		
State: electronic $\tilde{X}\,^2\Pi$; vibrational $v_4 = 1$, lower vibronic component ($\mu^2\Sigma$)				
B	[MHz]	5 894.337(1)	MW	96Ta
D	[kHz]	1.446 8(7)		
γ_{eff}	[MHz]	5 072.9(1)		
γ_D	[kHz]	1 19(1)		
State: electronic $\tilde{X}\,^2\Pi$; vibrational $v_5 = 1$, lower vibronic component ($\mu^2\Sigma$)				
B	[MHz]	5 881.125(10)	MW	96Ta
D	[kHz]	1.425 1(7)		
γ_{eff}	[MHz]	10 877.1(1)		
γ_D	[kHz]	– 1.22(1)		
State: electronic $\tilde{X}\,^2\Pi$; vibrational $v_5 = 1$, upper vibronic component ($\kappa^2\Sigma$)				
B	[MHz]	5 893.344(1)	MW	96Ta
D	[kHz]	1.394 2(6)		
γ_{eff}	[MHz]	7 474.3(1)		
γ_D	[kHz]	– 3.40(1)		
State: electronic $\tilde{X}\,^2\Pi$; vibrational $v_4 = 1$, $^2\Delta_{5/2}$ vibronic component				
B	[MHz]	5 880.018(2)	MW	96Ta
D	[kHz]	1.381 0(11)		
State: electronic $\tilde{X}\,^2\Pi$; vibrational $v_5 = 1$, $^2\Delta_{5/2}$ vibronic component				
B	[MHz]	5 883.142(1)	MW	96Ta
D	[kHz]	1.375 2(7)		

State: electronic $\tilde{X}\,^2\Pi$; vibrational $v_5 = 1$, $^2\Delta_{3/2}$ vibronic component				
B	[MHz]	5 898.665(1)	MW	96Ta
D	[kHz]	1.463 0(7)		
State: electronic $X\,^2\Pi$; vibrational $v_5 = 2$, $^2\Phi_{7/2}$ vibronic component				
B	[MHz]	5 897.966(1)	MW	96Ta
D	[kHz]	1.414 3(8)		

[a]) The numbers in parentheses are 3 standard deviation of the least-squares fit, in units of the last quoted decimal place.
[b]) $h_{1/2}(^1H) = a - (b+c)/2$.
[c]) $h_{3/2}(^1H) = a + (b+c)/2$.

Microwave data for $^2H^{12}C^{12}C^{32}S$ (DCCS)

Transition				
spin Ω	rotational $J' - J''$	parity e/f [a])	ν [MHz]	Ref.
State: electronic $X\,^2\Pi$; vibrational zero point level				
3/2	$15\frac{1}{2} \leftarrow 14\frac{1}{2}$	*e*	165 931.990	91Sa
		f	165 932.618	
1/2	$15\frac{1}{2} \leftarrow 14\frac{1}{2}$	*e*	166 257.291	
		f	166 429.598	
3/2	$16\frac{1}{2} \leftarrow 15\frac{1}{2}$	*e*	176 634.964	
		f	176 635.662	
1/2	$16\frac{1}{2} \leftarrow 15\frac{1}{2}$	*e*	176 986.877	
		f	177 159.078	
3/2	$17\frac{1}{2} \leftarrow 16\frac{1}{2}$	*e*	187 337.496	
		f	187 338.274	
1/2	$17\frac{1}{2} \leftarrow 16\frac{1}{2}$	*e*	187 715.906	
		f	187 888.144	
3/2	$21\frac{1}{2} \leftarrow 20\frac{1}{2}$	*e*	230 142.755	
		f	230 143.932	
1/2	$21\frac{1}{2} \leftarrow 20\frac{1}{2}$	*e*	230 627.008	
		f	230 799.459	
3/2	$22\frac{1}{2} \leftarrow 21\frac{1}{2}$	*e*	240 842.715	
		f	240 844.021	
1/2	$22\frac{1}{2} \leftarrow 21\frac{1}{2}$	*e*	241 353.556	
		f	241 525.927	
3/2	$23\frac{1}{2} \leftarrow 22\frac{1}{2}$	*e*	251 542.096	
		f	251 543.506	
1/2	$23\frac{1}{2} \leftarrow 22\frac{1}{2}$	*e*	252 079.379	
		f	252 251.748	
3/2	$24\frac{1}{2} \leftarrow 23\frac{1}{2}$	*e*	262 240.878	
		f	262 242.399	
1/2	$24\frac{1}{2} \leftarrow 23\frac{1}{2}$	*f*	262 976.958	
3/2	$25\frac{1}{2} \leftarrow 24\frac{1}{2}$	*e*	272 938.958	
		f	272 940.642	
1/2	$25\frac{1}{2} \leftarrow 24\frac{1}{2}$	*e*	273 529.052	
		f	273 701.564	
3/2	$26\frac{1}{2} \leftarrow 25\frac{1}{2}$	*e*	283 636.408	
		f	283 638.225	
3/2	$27\frac{1}{2} \leftarrow 26\frac{1}{2}$	*e*	294 333.140	

		f	294 335.090
$\frac{1}{2}$	$27\frac{1}{2} \leftarrow 26\frac{1}{2}$	*e*	294 976.132
$\frac{3}{2}$	$28\frac{1}{2} \leftarrow 27\frac{1}{2}$	*e*	305 029.181
		f	305 031.274
$\frac{1}{2}$	$28\frac{1}{2} \leftarrow 27\frac{1}{2}$	*e*	305 698.558
		f	305 871.107
$\frac{3}{2}$	$29\frac{1}{2} \leftarrow 28\frac{1}{2}$	*e*	315 724.478
		f	315 726.698
$\frac{1}{2}$	$29\frac{1}{2} \leftarrow 28\frac{1}{2}$	*e*	316 420.200
		f	316 592.788
$\frac{3}{2}$	$30\frac{1}{2} \leftarrow 29\frac{1}{2}$	*e*	326 418.956
		f	326 421.339
$\frac{1}{2}$	$30\frac{1}{2} \leftarrow 29\frac{1}{2}$	*e*	327 141.054
		f	327 313.738
$\frac{3}{2}$	$31\frac{1}{2} \leftarrow 30\frac{1}{2}$	*e*	337 112.631
		f	337 115.194
$\frac{1}{2}$	$31\frac{1}{2} \leftarrow 30\frac{1}{2}$	*e*	337 861.108
		f	338 033.783
$\frac{3}{2}$	$32\frac{1}{2} \leftarrow 31\frac{1}{2}$	*e*	347 805.513
		f	347 808.223
$\frac{1}{2}$	$32\frac{1}{2} \leftarrow 31\frac{1}{2}$	*e*	348 580.299
		f	348 753.037
$\frac{3}{2}$	$33\frac{1}{2} \leftarrow 32\frac{1}{2}$	*e*	358 497.539
		f	358 500.402
$\frac{1}{2}$	$33\frac{1}{2} \leftarrow 32\frac{1}{2}$	*e*	359 298.640
		f	359 471.424
$\frac{3}{2}$	$34\frac{1}{2} \leftarrow 33\frac{1}{2}$	*e*	369 188.682
		f	369 191.716
$\frac{1}{2}$	$34\frac{1}{2} \leftarrow 33\frac{1}{2}$	*e*	370 016.073
		f	370 188.886

[a]) States with parity equal to $\pm(-1)^{J-0.5}$ are labeled *e* and *f* respectively.

Microwave data for $^{2}H^{12}C^{12}C^{32}S$ (DCCS)

Transition		ν	Ref.
rotational $N' - N''$	fine structure $J' - J''$ [a])	[MHz]	
State: electronic $X^2\Pi$; vibrational $v_4 = 1$, lower vibronic component ($\mu^2\Sigma$)			
$21 \leftarrow 20$	$20\frac{1}{2} \leftarrow 19\frac{1}{2}$	222 249.651	96Ta
$22 \leftarrow 21$	$21\frac{1}{2} \leftarrow 20\frac{1}{2}$	233 017.657	
$23 \leftarrow 22$	$22\frac{1}{2} \leftarrow 21\frac{1}{2}$	243 785.100	
	$23\frac{1}{2} \leftarrow 22\frac{1}{2}$	251 571.965	
$24 \leftarrow 23$	$23\frac{1}{2} \leftarrow 22\frac{1}{2}$	254 551.938	
	$24\frac{1}{2} \leftarrow 23\frac{1}{2}$	262 329.578	
$25 \leftarrow 24$	$24\frac{1}{2} \leftarrow 23\frac{1}{2}$	265 318.179	
	$25\frac{1}{2} \leftarrow 24\frac{1}{2}$	273 086.192	
$26 \leftarrow 25$	$25\frac{1}{2} \leftarrow 24\frac{1}{2}$	276 083.713	
$28 \leftarrow 27$	$28\frac{1}{2} \leftarrow 27\frac{1}{2}$	305 349.953	
$29 \leftarrow 28$	$28\frac{1}{2} \leftarrow 27\frac{1}{2}$	308 375.871	

	$29\frac{1}{2} \leftarrow 28\frac{1}{2}$	316 102.404	
$30 \leftarrow 29$	$30\frac{1}{2} \leftarrow 29\frac{1}{2}$	326 853.736	
$31 \leftarrow 30$	$31\frac{1}{2} \leftarrow 30\frac{1}{2}$	337 603.891	
$32 \leftarrow 31$	$31\frac{1}{2} \leftarrow 30\frac{1}{2}$	340 660.717	
	$32\frac{1}{2} \leftarrow 31\frac{1}{2}$	348 352.903	
$33 \leftarrow 32$	$32\frac{1}{2} \leftarrow 31\frac{1}{2}$	351 420.562	
	$33\frac{1}{2} \leftarrow 32\frac{1}{2}$	359 100.679	
$34 \leftarrow 33$	$33\frac{1}{2} \leftarrow 32\frac{1}{2}$	362 179.424	
	$34\frac{1}{2} \leftarrow 33\frac{1}{2}$	369 847.241	
State: electronic $X^2\Pi$; vibrational $v_5 = 1$, lower vibronic component ($\mu^2\Sigma$)			
$22 \leftarrow 21$	$21\frac{1}{2} \leftarrow 20\frac{1}{2}$	231 498.445	96Ta
$23 \leftarrow 22$	$22\frac{1}{2} \leftarrow 21\frac{1}{2}$	242 204.358	
	$23\frac{1}{2} \leftarrow 22\frac{1}{2}$	250 590.112	
$24 \leftarrow 23$	$23\frac{1}{2} \leftarrow 22\frac{1}{2}$	252 909.614	
$25 \leftarrow 24$	$24\frac{1}{2} \leftarrow 23\frac{1}{2}$	263 614.236	
$26 \leftarrow 25$	$25\frac{1}{2} \leftarrow 24\frac{1}{2}$	274 318.190	
$29 \leftarrow 28$	$28\frac{1}{2} \leftarrow 27\frac{1}{2}$	306 425.911	
$30 \leftarrow 29$	$29\frac{1}{2} \leftarrow 28\frac{1}{2}$	317 127.146	
$31 \leftarrow 30$	$30\frac{1}{2} \leftarrow 29\frac{1}{2}$	327 827.530	
	$31\frac{1}{2} \leftarrow 30\frac{1}{2}$	336 282.412	
$32 \leftarrow 31$	$32\frac{1}{2} \leftarrow 31\frac{1}{2}$	346 991.781	
$33 \leftarrow 32$	$32\frac{1}{2} \leftarrow 31\frac{1}{2}$	349 225.982	
	$33\frac{1}{2} \leftarrow 32\frac{1}{2}$	357 700.699	
$34 \leftarrow 33$	$33\frac{1}{2} \leftarrow 32\frac{1}{2}$	359 923.975	
	$34\frac{1}{2} \leftarrow 33\frac{1}{2}$	368 408.998	
$35 \leftarrow 34$	$34\frac{1}{2} \leftarrow 33\frac{1}{2}$	370 621.139	
	$29\frac{1}{2} \leftarrow 28\frac{1}{2}$	346 411.161	
$30 \leftarrow 29$	$29\frac{1}{2} \leftarrow 28\frac{1}{2}$	347 268.720	
	$30\frac{1}{2} \leftarrow 29\frac{1}{2}$	358 158.945	
$31 \leftarrow 30$	$30\frac{1}{2} \leftarrow 29\frac{1}{2}$	359 014.595	
$32 \leftarrow 31$	$31\frac{1}{2} \leftarrow 30\frac{1}{2}$	370 759.459	
	$32\frac{1}{2} \leftarrow 31\frac{1}{2}$	381 651.464	
$33 \leftarrow 32$	$32\frac{1}{2} \leftarrow 31\frac{1}{2}$	382 503.440	

[a]) ^1H hyperfine structure not resolved.

Microwave data for $^2H^{12}C^{12}C^{32}S$ (DCCS)

Transition			ν [MHz]	Ref.
spin Ω	rotational $J' - J''$	parity e/f [a])		
State: electronic $X^2\Pi$; vibrational $v_4 = 1$, $^2\Delta$ vibronic component				
$\frac{5}{2}$	$15\frac{1}{2} \leftarrow 14\frac{1}{2}$	e, f	166 395.691	96Ta
$\frac{5}{2}$	$16\frac{1}{2} \leftarrow 15\frac{1}{2}$	e, f	177 128.572	
$\frac{5}{2}$	$17\frac{1}{2} \leftarrow 16\frac{1}{2}$	e, f	187 861.047	
$\frac{5}{2}$	$21\frac{1}{2} \leftarrow 20\frac{1}{2}$	e, f	230 785.823	
$\frac{5}{2}$	$22\frac{1}{2} \leftarrow 21\frac{1}{2}$	e, f	241 515.699	
$\frac{5}{2}$	$23\frac{1}{2} \leftarrow 22\frac{1}{2}$	e, f	252 244.919	

$\frac{5}{2}$	$24\frac{1}{2} \leftarrow 23\frac{1}{2}$	*e*, *f*	262 973.747	
$\frac{5}{2}$	$25\frac{1}{2} \leftarrow 24\frac{1}{2}$	*e*, *f*	273 701.564	
$\frac{5}{2}$	$27\frac{1}{2} \leftarrow 26\frac{1}{2}$	*e*, *f*	295 155.424	
$\frac{5}{2}$	$28\frac{1}{2} \leftarrow 27\frac{1}{2}$	*e*, *f*	305 881.288	
$\frac{5}{2}$	$29\frac{1}{2} \leftarrow 28\frac{1}{2}$	*e*, *f*	316 606.413	
$\frac{5}{2}$	$30\frac{1}{2} \leftarrow 29\frac{1}{2}$	*e*, *f*	327 330.741	
$\frac{5}{2}$	$32\frac{1}{2} \leftarrow 31\frac{1}{2}$	*e*, *f*	348 776.752	
$\frac{5}{2}$	$33\frac{1}{2} \leftarrow 32\frac{1}{2}$	*e*, *f*	359 498.754	
$\frac{5}{2}$	$34\frac{1}{2} \leftarrow 33\frac{1}{2}$	*e*, *f*	370 219.651	
$\frac{5}{2}$	$36\frac{1}{2} \leftarrow 35\frac{1}{2}$	*e*, *f*	391 658.693	
State: electronic $X^2\Pi$; vibrational $v_5 = 1$, $^2\Delta$ vibronic component				
$\frac{5}{2}$	$15\frac{1}{2} \leftarrow 14\frac{1}{2}$	*e*, *f*	166 316.881	96Ta
$\frac{5}{2}$	$16\frac{1}{2} \leftarrow 15\frac{1}{2}$	*e*, *f*	177 044.668	
$\frac{5}{2}$	$17\frac{1}{2} \leftarrow 16\frac{1}{2}$	*e*, *f*	187 772.043	
$\frac{5}{2}$	$21\frac{1}{2} \leftarrow 20\frac{1}{2}$	*e*	230 676.187	
		f	230 676.871	
$\frac{5}{2}$	$22\frac{1}{2} \leftarrow 21\frac{1}{2}$	*e*	241 400.950	
		f	241 401.743	
$\frac{5}{2}$	$23\frac{1}{2} \leftarrow 22\frac{1}{2}$	*e*	252 125.013	
		f	252 125.954	
$\frac{5}{2}$	$24\frac{1}{2} \leftarrow 23\frac{1}{2}$	*e*	262 849.593	
		f	262 849.593	
$\frac{5}{2}$	$25\frac{1}{2} \leftarrow 24\frac{1}{2}$	*e*	273 571.313	
		f	273 572.610	
$\frac{5}{2}$	$27\frac{1}{2} \leftarrow 26\frac{1}{2}$	*e*	295 014.833	
		f	295 016.569	
$\frac{5}{2}$	$28\frac{1}{2} \leftarrow 27\frac{1}{2}$	*e*	305 735.492	
		f	305 737.603	
$\frac{5}{2}$	$29\frac{1}{2} \leftarrow 28\frac{1}{2}$	*e*	316 455.432	
		f	316 457.698	
$\frac{5}{2}$	$30\frac{1}{2} \leftarrow 29\frac{1}{2}$	*e*	327 174.530	
		f	327 177.105	
$\frac{5}{2}$	$31\frac{1}{2} \leftarrow 30\frac{1}{2}$	*e*	337 892.721	
		f	337 895.715	
$\frac{5}{2}$	$32\frac{1}{2} \leftarrow 31\frac{1}{2}$	*f*	348 613.535	
$\frac{5}{2}$	$33\frac{1}{2} \leftarrow 32\frac{1}{2}$	*e*	359 326.759	
		f	359 330.474	
$\frac{5}{2}$	$34\frac{1}{2} \leftarrow 33\frac{1}{2}$	*e*	370 042.407	
		f	370 046.585	
$\frac{5}{2}$	$36\frac{1}{2} \leftarrow 35\frac{1}{2}$	*e*	391 470.878	
		f	391 476.025	

[a]) States with parity equal to $\pm(-1)^{J-0.5}$ are labeled *e* and *f* respectively.

Molecular parameters for $^{2}H^{12}C^{12}C^{32}S$ (DCCS)

Parameter		Value	Method	Ref.
State: electronic $X^2\Pi$; vibrational zero point level				
B	[MHz]	5 359.820 050(127) [a])	MW	91Sa, 02Sa
D	[kHz]	1.101 761(97)		
$A+\gamma$	[GHz]	– 8 090 [b])		
γ	[MHz]	– 3 952.908(131)		
γ_D	[kHz]	2.026(107)		
p	[MHz]	172.821 1(101)		
p_D	[kHz]	1.076 0(135)		
q	[MHz]	– 0.396 9(50)		
$h_{1/2}$	[MHz]	3.845 6(30)		
b	[MHz]	– 4.79(73)		
$h_{3/2}$	[MHz]	1.292 7(156)		
d	[MHz]	2.205 5(57)		
eQq_0	[MHz]	0.199 9(57)		
State: electronic $X^2\Pi$; vibrational $v_4 = 1$, lower vibronic component ($\mu^2\Sigma$)				
B	[MHz]	5 385.879(3)	MW	96Ta
D	[kHz]	1.434(4)		
H	[Hz]	0.011(2)		
γ_{eff}	[MHz]	7 894.2(3)		
γ_D	[kHz]	17.4(1)		
γ_H	[Hz]	1.12(5)		
State: electronic $X^2\Pi$; vibrational $v_5 = 1$, lower vibronic component ($\mu^2\Sigma$)				
B	[MHz]	5 357.306(5)	MW	96Ta
D	[kHz]	0.834(6)		
H	[Hz]	–0.009(2)		
γ_{eff}	[MHz]	8 296.9(5)		
γ_D	[kHz]	– 14.4(1)		
γ_H	[Hz]	– 0.84(8)		
State: electronic $X^2\Pi$; vibrational $v_4 = 1$, $^2\Delta_{5/2}$ vibronic component				
B	[MHz]	5 368.136(1)	MW	96Ta
D	[kHz]	1.106 1(5)		
State: electronic $X^2\Pi$; vibrational $v_5 = 1$, $^2\Delta_{5/2}$ vibronic component				
B	[MHz]	5 365.592(1)	MW	96Ta
D	[kHz]	1.103 7(5)		
d_Δ	[Hz]	0.594(7)		

[a]) The numbers in parentheses are 3 standard deviation of the least-squares fit, in units of the last quoted decimal place.
[b]) Parameter constrained to this value in the least-squares fit.

Microwave data for $^{1}H^{12}C^{12}C^{34}S$

Transition			ν	Ref.
spin Ω	rotational $J' - J''$	parity e/f [a])	[MHz]	
State: electronic $X^2\Pi$; vibrational zero point level				
$\frac{3}{2}$	$20\frac{1}{2} \leftarrow 19\frac{1}{2}$	e	235 196.393	96Ta
		f	235 197.342	
$\frac{3}{2}$	$21\frac{1}{2} \leftarrow 20\frac{1}{2}$	e	246 664.814	
		f	246 665.687	
$\frac{3}{2}$	$23\frac{1}{2} \leftarrow 22\frac{1}{2}$	e	269 598.815	
		f	269 600.109	
$\frac{3}{2}$	$24\frac{1}{2} \leftarrow 23\frac{1}{2}$	e	281 064.858	
		f	281 066.236	

$\frac{3}{2}$	$27\frac{1}{2} \leftarrow 26\frac{1}{2}$	*e*	315 458.149
		f	315 459.875
$\frac{3}{2}$	$28\frac{1}{2} \leftarrow 27\frac{1}{2}$	*e*	326 920.843
		f	326 922.669
$\frac{3}{2}$	$29\frac{1}{2} \leftarrow 28\frac{1}{2}$	*e*	338 382.656
$\frac{3}{2}$	$30\frac{1}{2} \leftarrow 29\frac{1}{2}$	*e*	349 843.544
		f	349 845.668
$\frac{3}{2}$	$31\frac{1}{2} \leftarrow 30\frac{1}{2}$	*e*	361 303.430
		f	361 305.719
$\frac{3}{2}$	$32\frac{1}{2} \leftarrow 31\frac{1}{2}$	*e*	372 762.346
		f	372 764.764

[a]) States with parity equal to ± $(-1)^{J-0.5}$ are labeled *e* and *f* respectively.

Molecular parameters for $^{1}H^{12}C^{12}C^{34}S$

Parameter		Value	Method	Ref.
State: electronic $X^2\Pi$, Ω=3/2; vibrational zero point level				
$B_{3/2}$	[MHz]	5 737.623(1) [a])	MW	96Ta
D	[kHz]	1.324 5(5)		
q	[kHz]	0.77(1)		

[a]) The numbers in parentheses are 3 standard deviation of the least-squares fit, in units of the last quoted decimal place.

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3.2.1.2.28 HC_3S

Microwave data for $^{1}H^{12}C_3^{32}S$

Transition				ν [MHz]	Ref.
spin Ω	rotational $J' - J''$	parity e/f [a])	hyperfine $F' - F''$		
State: electronic $\tilde{X}^2\Pi$; vibrational zero point level					
$\frac{1}{2}$	$1\frac{1}{2} \leftarrow \frac{1}{2}$	*e*	$2 \leftarrow 1$	8 027.549(3) [b])	94Hi
			$1 \leftarrow 1$	8 030.968(3)	
			$1 \leftarrow 0$	8 031.070(3)	
		f	$1 \leftarrow 1$	8 028.069(3)	
			$2 \leftarrow 1$	8 038.193(3)	
			$1 \leftarrow 0$	8 045.105(3)	
	$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	*e*	$3 \leftarrow 2$	13 384.043(3)	
			$2 \leftarrow 1$	13 385.070(3)	
			$2 \leftarrow 2$	13 388.482(3)	
		f	$2 \leftarrow 2$	13 385.719(3)	
			$3 \leftarrow 2$	13 394.332(3)	
			$2 \leftarrow 1$	13 395.840(3)	

	$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	*e*	$4 \leftarrow 3$	18 740.004(3)	
			$3 \leftarrow 2$	18 740.539(3)	
		f	$4 \leftarrow 3$	18 750.321(3)	
			$3 \leftarrow 2$	18 751.014(3)	
	$4\frac{1}{2} \leftarrow 3\frac{1}{2}$	*e*	$5 \leftarrow 4$	24 095.785(3)	
			$4 \leftarrow 3$	24 096.117(3)	
		f	$5 \leftarrow 4$	24 106.274(3)	
			$4 \leftarrow 3$	24 106.689(3)	
$\frac{1}{2}$	$13\frac{1}{2} \leftarrow 12\frac{1}{2}$	*e*	c)	72 293.806	94McC
		f	c)	72 309.198	
$\frac{3}{2}$	$13\frac{1}{2} \leftarrow 12\frac{1}{2}$	*e*	c)	72 867.722	
		f	c)	72 871.244	
$\frac{1}{2}$	$16\frac{1}{2} \leftarrow 15\frac{1}{2}$	*e*	c)	88 358.066	
		f	c)	88 376.156	
$\frac{3}{2}$	$16\frac{1}{2} \leftarrow 15\frac{1}{2}$	*e*	c)	89 057.684	
		f	c)	89 063.020	
$\frac{1}{2}$	$17\frac{1}{2} \leftarrow 16\frac{1}{2}$	*e*	c)	93 712.574	
		f	c)	93 731.738	
$\frac{3}{2}$	$17\frac{1}{2} \leftarrow 16\frac{1}{2}$	*e*	c)	94 454.037	
		f	c)	94 459.974	
$\frac{1}{2}$	$18\frac{1}{2} \leftarrow 17\frac{1}{2}$	*e*	c)	99 066.946	
		f	c)	99 087.239	
$\frac{3}{2}$	$18\frac{1}{2} \leftarrow 17\frac{1}{2}$	*e*	c)	99 850.145	
		f	c)	99 856.798	
$\frac{1}{2}$	$19\frac{1}{2} \leftarrow 18\frac{1}{2}$	*f*	c)	104 442.564	
$\frac{3}{2}$	$19\frac{1}{2} \leftarrow 18\frac{1}{2}$	*f*	c)	105 253.444	
$\frac{1}{2}$	$20\frac{1}{2} \leftarrow 19\frac{1}{2}$	*e*	c)	109 797.929	
		f	c)	109 797.929	
$\frac{3}{2}$	$20\frac{1}{2} \leftarrow 19\frac{1}{2}$	*e*	c)	110 641.801	
		f	c)	110 649.931	
$\frac{1}{2}$	$21\frac{1}{2} \leftarrow 20\frac{1}{2}$	*e*	c)	115 129.304	
		f	c)	115 153.164	
$\frac{3}{2}$	$21\frac{1}{2} \leftarrow 20\frac{1}{2}$	*e*	c)	116 037.317	
		f	c)	116 046.232	
$\frac{3}{2}$	$27\frac{1}{2} \leftarrow 26\frac{1}{2}$	*e*	c)	148 405.335	
		f	c)	148 419.807	
$\frac{3}{2}$	$28\frac{1}{2} \leftarrow 27\frac{1}{2}$	*e*	c)	153 799.044	
$\frac{3}{2}$	$29\frac{1}{2} \leftarrow 28\frac{1}{2}$	*e*	c)	159 192.572	
		f	c)	159 209.106	
$\frac{3}{2}$	$30\frac{1}{2} \leftarrow 29\frac{1}{2}$	*f*	c)	164 603.334	
$\frac{1}{2}$	$31\frac{1}{2} \leftarrow 30\frac{1}{2}$	*e*	c)	168 660.109	
		f	c)	168 699.487	
$\frac{3}{2}$	$31\frac{1}{2} \leftarrow 30\frac{1}{2}$	*e*	c)	169 978.578	
		f	c)	169 997.388	
$\frac{1}{2}$	$32\frac{1}{2} \leftarrow 31\frac{1}{2}$	*e*	c)	174 012.145	
		f	c)	174 053.382	
$\frac{3}{2}$	$32\frac{1}{2} \leftarrow 31\frac{1}{2}$	*e*	c)	175 371.104	
		f	c)	175 391.050	
$\frac{1}{2}$	$33\frac{1}{2} \leftarrow 32\frac{1}{2}$	*e*	c)	179 364.015	

		f	[c])	179 407.121
$\frac{3}{2}$	$33\frac{1}{2} \leftarrow 32\frac{1}{2}$	*f*	[c])	180 763.349
$\frac{1}{2}$	$34\frac{1}{2} \leftarrow 33\frac{1}{2}$	*e*	[c])	184 715.664
		f	[c])	184 760.712
$\frac{3}{2}$	$34\frac{1}{2} \leftarrow 33\frac{1}{2}$	*e*	[c])	186 155.213
		f	[c])	186 177.613
$\frac{3}{2}$	$35\frac{1}{2} \leftarrow 34\frac{1}{2}$	*e*	[c])	191 546.755
		f	[c])	191 570.444
$\frac{1}{2}$	$47\frac{1}{2} \leftarrow 46\frac{1}{2}$	*e*	[c])	254 265.726
		f	[c])	254 339.769
$\frac{1}{2}$	$48\frac{1}{2} \leftarrow 47\frac{1}{2}$	*e*	[c])	259 614.041
		f	[c])	259 690.442
$\frac{3}{2}$	$48\frac{1}{2} \leftarrow 47\frac{1}{2}$	*e*	[c])	261 602.286
		f	[c])	261 644.792
$\frac{1}{2}$	$49\frac{1}{2} \leftarrow 48\frac{1}{2}$	*e*	[c])	264 961.906
		f	[c])	265 041.053
$\frac{3}{2}$	$49\frac{1}{2} \leftarrow 48\frac{1}{2}$	*e*	[c])	266 988.190
		f	[c])	267 032.327
$\frac{1}{2}$	$50\frac{1}{2} \leftarrow 49\frac{1}{2}$	*e*	[c])	270 309.476
		f	[c])	270 391.137
$\frac{3}{2}$	$50\frac{1}{2} \leftarrow 49\frac{1}{2}$	*e*	[c])	272 373.618
		f	[c])	272 419.414
$\frac{1}{2}$	$51\frac{1}{2} \leftarrow 50\frac{1}{2}$	*e*	[c])	275 656.743
$\frac{3}{2}$	$51\frac{1}{2} \leftarrow 50\frac{1}{2}$	*e*	[c])	277 758.630
		f	[c])	277 806.087
$\frac{1}{2}$	$52\frac{1}{2} \leftarrow 51\frac{1}{2}$	*e*	[c])	281 003.909
		f	[c])	281 090.625

[a]) States with parity equal to $\pm(-1)^{J-0.5}$ are labeled *e* and *f* respectively.
[b]) The figures in parentheses are the authors' estimates of experimental uncertainty (1σ).
[c]) Proton hyperfine structure not resolved.

Molecular parameters for $^{1}H^{12}C_3{}^{32}S$

Parameter		Value	Method	Ref.
State: electronic $\tilde{X}\,^2\Pi$; vibrational zero point level				
B	[MHz]	2 688.469 9(1) [a])	MW	94McC
D	[kHz]	0.319 5(1)		
H	[Hz]	0.001 34(2)		
$A+\gamma$	[GHz]	1 326.7(3)		
γ	[MHz]	– 2 084.7(8)		
$p+2q$	[MHz]	9.733(2)		
P_D+2q_D	[kHz]	3.843(5)		
P_H+2q_H	[Hz]	– 0.106(1)		
q	[MHz]	– 1.167 2(3)		
$h_{1/2}(^1H)$ [b])	[MHz]	12.863(4)		94Hi
$b(^1H)$	[MHz]	– 14.5(3)		
$d(^1H)$	[MHz]	12.693(3)		

[a]) The numbers in parentheses are 1 standard deviation of the least-squares fit, in units of the last quoted decimal place.
[b]) $h_{1/2}(^1H) = a-(b+c)/2$.

Microwave data for $^{1}H^{12}C_3^{34}S$

Transition				ν [MHz]	Ref.
spin Ω	rotational $J' - J''$	parity e/f [a])	hyperfine $F' - F''$		
State: electronic $\tilde{X}^2\Pi$; vibrational zero point level					
$\frac{1}{2}$	$1\frac{1}{2} \leftarrow \frac{1}{2}$	e	$2 \leftarrow 1$	7 832.740(3) [b])	94Hi
			$1 \leftarrow 1$	7 836.154(3)	
			$1 \leftarrow 0$	7 836.250(3)	
		f	$1 \leftarrow 1$	7 833.142(3)	
			$2 \leftarrow 1$	7 843.283(3)	
			$1 \leftarrow 0$	7 850.198(3)	
	$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	e	$3 \leftarrow 2$	13 059.318(3)	
			$2 \leftarrow 1$	13 060.348(3)	
		f	$3 \leftarrow 2$	13 069.498(3)	
			$2 \leftarrow 1$	13 071.002(3)	

[a]) States with parity equal to $\pm(-1)^{J-0.5}$ are labeled e and f respectively.
[b]) The figures in parentheses are the authors' estimates of experimental uncertainty (1σ).

Molecular parameters for $^{1}H^{12}C_3^{34}S$

Parameter		Value	Method	Ref.
State: electronic $\tilde{X}^2\Pi$, $\Omega = \frac{1}{2}$; vibrational zero point level				
B	[MHz]	2 623.114 7(5) [a])	MW	94Hi
D	[kHz]	0.32 [b])		
A	[GHz]	1 328.8 [b])		
γ	[MHz]	– 2 084.7 [b])		
p	[MHz]	13.1(2)		
q	[MHz]	– 1.73(13)		
$h_{1/2}(^{1}H)$ [c])	[MHz]	12.87(10)		
$b(^{1}H)$	[MHz]	– 14.4(10)		
$d(^{1}H)$	[MHz]	12.712(9)		

[a]) The numbers in parentheses are 1 standard deviation of the least-squares fit, in units of the last quoted decimal place.
[b]) Parameter constrained to this value in the least-squares fit.
[c]) $h_{1/2}(^{1}H) = a - (b+c)/2$.

Microwave data for $^{2}H^{12}C_3^{32}S$ (DC_3S)

Transition				ν [MHz]	Ref.
spin Ω	rotational $J' - J''$	parity e/f [a])	hyperfine $F' - F''$		
State: electronic $\tilde{X}^2\Pi$; vibrational zero point level					
$\frac{1}{2}$	$1\frac{1}{2} \leftarrow \frac{1}{2}$	e	$\frac{1}{2} \leftarrow \frac{1}{2}$	7 526.695(3) [b])	94Hi
			$1\frac{1}{2} \leftarrow \frac{1}{2}$	7 526.415(3)	
			$1\frac{1}{2} \leftarrow 1\frac{1}{2}$	7 526.254(3)	
			$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	7 525.607(3)	
		f	$\frac{1}{2} \leftarrow \frac{1}{2}$	7 535.008(3)	
			$1\frac{1}{2} \leftarrow \frac{1}{2}$	7 536.269(3)	
			$1\frac{1}{2} \leftarrow 1\frac{1}{2}$	7 532.268(3)	
			$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	7 534.180(3)	
	$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	e	$1\frac{1}{2} \leftarrow \frac{1}{2}$	12 546.244(3)	

			$1\frac{1}{2} \leftarrow 1\frac{1}{2}$	12 546.521(3)	
			$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	12 546.057(3)	
			$2\frac{1}{2} \leftarrow 2\frac{1}{2}$	12 546.707(3)	
			$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	12 545.892(3)	
		f	$1\frac{1}{2} \leftarrow \frac{1}{2}$	12 554.964(3)	
			$1\frac{1}{2} \leftarrow 1\frac{1}{2}$	12 553.703(3)	
			$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	12 554.883(3)	
			$2\frac{1}{2} \leftarrow 2\frac{1}{2}$	12 552.97193)	
			$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	12 554.461(3)	
	$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	*e*	$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	17 566.153(3)	
			$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	17 566.053(3)	
			$4\frac{1}{2} \leftarrow 3\frac{1}{2}$	17 565.976(3)	
		f	$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	17 574.943(3)	
			$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	17 574.887(3)	
			$4\frac{1}{2} \leftarrow 3\frac{1}{2}$	17 574.706(3)	
$\frac{1}{2}$	$14\frac{1}{2} \leftarrow 13\frac{1}{2}$	*e*	c)	72 781.498	94McC
		f	c)	72 797.098	
$\frac{3}{2}$	$14\frac{1}{2} \leftarrow 13\frac{1}{2}$	*e*	c)	73 398.448	
		f	c)	73 403.399	
$\frac{1}{2}$	$16\frac{1}{2} \leftarrow 15\frac{1}{2}$	*e*	c)	82 819.471	
		f	c)	82 837.240	
$\frac{3}{2}$	$16\frac{1}{2} \leftarrow 15\frac{1}{2}$	*f*	c)	83 526.830	
$\frac{1}{2}$	$17\frac{1}{2} \leftarrow 16\frac{1}{2}$	*f*	c)	87 857.216	
$\frac{3}{2}$	$17\frac{1}{2} \leftarrow 16\frac{1}{2}$	*e*	c)	88 581.271	
		f	c)	88 588.390	
$\frac{1}{2}$	$20\frac{1}{2} \leftarrow 19\frac{1}{2}$	*e*	c)	102 894.012	
		f	c)	102 916.856	
$\frac{3}{2}$	$20\frac{1}{2} \leftarrow 19\frac{1}{2}$	*e*	c)	103 762.448	
		f	c)	103 772.151	
$\frac{1}{2}$	$21\frac{1}{2} \leftarrow 20\frac{1}{2}$	*e*	c)	107 912.301	
		f	c)	107 936.587	
$\frac{3}{2}$	$21\frac{1}{2} \leftarrow 20\frac{1}{2}$	*e*	c)	108 822.440	
		f	c)	108 833.095	
$\frac{1}{2}$	$22\frac{1}{2} \leftarrow 21\frac{1}{2}$	*e*	c)	112 930.455	
		f	c)	112 956.246	
$\frac{3}{2}$	$22\frac{1}{2} \leftarrow 21\frac{1}{2}$	*e*	c)	113 882.231	
		f	c)	113 893.880	
$\frac{3}{2}$	$31\frac{1}{2} \leftarrow 30\frac{1}{2}$	*e*	c)	159 409.400	
		f	c)	159 431.721	
$\frac{1}{2}$	$32\frac{1}{2} \leftarrow 31\frac{1}{2}$	*e*	c)	163 103.445	
		f	c)	163 147.501	
$\frac{3}{2}$	$32\frac{1}{2} \leftarrow 31\frac{1}{2}$	*e*	c)	164 466.616	
		f	c)	164 490.312	
$\frac{1}{2}$	$33\frac{1}{2} \leftarrow 32\frac{1}{2}$	*e*	c)	168 119.782	
		f	c)	168 165.968	
$\frac{1}{2}$	$34\frac{1}{2} \leftarrow 33\frac{1}{2}$	*e*	c)	173 135.903	
		f	c)	173 184.251	

$\frac{1}{2}$	$37\frac{1}{2} \leftarrow 36\frac{1}{2}$	*e*	[c])	188 183.091
		f	[c])	188 238.348
$\frac{1}{2}$	$38\frac{1}{2} \leftarrow 37\frac{1}{2}$	*e*	[c])	193 198.466
		f	[c])	193 256.063
$\frac{1}{2}$	$44\frac{1}{2} \leftarrow 43\frac{1}{2}$	*e*	[c])	223 285.736
		f	[c])	223 358.567
$\frac{3}{2}$	$44\frac{1}{2} \leftarrow 43\frac{1}{2}$	*e*	[c])	225 127.452
		f	[c])	225 170.012
$\frac{3}{2}$	$52\frac{1}{2} \leftarrow 51\frac{1}{2}$	*e*	[c])	265 537.314
		f	[c])	265 594.690

[a]) States with parity equal to $\pm (-1)^{J-0.5}$ are labeled *e* and *f* respectively.
[b]) The figures in parentheses are the authors' estimates of experimental uncertainty (1σ).
[c]) Deuteron hyperfine structure not resolved.

Molecular parameters for $^{2}H\,^{12}C_3\,^{32}S$ (DC_3S)

Parameter		Value	Method	Ref.
State: electronic $\tilde{X}\,^2\Pi$; vibrational zero point level				
B	[MHz]	2 520.644 5(1) [a])	MW	94McC
D	[kHz]	0.292 3(1)		
H	[Hz]	0.00104(3)		
$A+\gamma$	[GHz]	1 381.6(5)		
γ	[MHz]	– 2 584.3(14)		
$p+2q$	[MHz]	8.25(2)		
P_D+2q_D	[kHz]	3.93(1)		
P_H+2q_H	[Hz]	– 0.079(3)		
q	[MHz]	– 1.430(1)		
q_D	[kHz]	0.012 0(2)		
$h_{1/2}(^2H)$ [b])	[MHz]	2.082(3)	MW	94Hi
$b(^2H)$	[MHz]	– 2.67(17)		
$d(^2H)$	[MHz]	1.920(2)		
$eQq_0(^2H)$	[MHz]	0.184(3)		

[a]) The numbers in parentheses are 3 standard deviation of the least-squares fit, in units of the last quoted decimal place.
[b]) $h_{1/2}(^2H) = a - (b+c)/2$.

References for HC_3S

94Hi Hirahara, Y., Ohshima, Y., Endo, Y. : J. Chem. Phys. **101** (1994) 7342.

94McC McCarthy, M.C., Vrtilek, J.M., Gottlieb, E.W., Tao, F.-M., Gottlieb, C.A., Thaddeus, P. : Astrophys. J. **431** (1994) L127.

3.2.1.2.29 HC_4S

Microwave data for $^{1}H\,^{12}C_4\,^{32}S$

Transition			ν	Ref.
spin Ω	rotational $J' - J''$	hyperfine $F' - F''$	[MHz]	
State: electronic $\tilde{X}\,^2\Pi$; vibrational zero point level				
$\frac{3}{2}$	$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	$3 \leftarrow 2$	7 166.040(3) [a])	94Hi
		$2 \leftarrow 1$	7 167.079(3)	
	$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	$4 \leftarrow 3$	10 032.721(3)	
		$3 \leftarrow 2$	10 033.204(3)	
	$4\frac{1}{2} \leftarrow 3\frac{1}{2}$	$5 \leftarrow 4$	12 899.314(3)	

	$4 \leftarrow 3$	12 899.598(3)	
$5\frac{1}{2} \leftarrow 4\frac{1}{2}$	$6 \leftarrow 5$	15 765.877(3)	
	$5 \leftarrow 4$	15 766.069(3)	
$6\frac{1}{2} \leftarrow 5\frac{1}{2}$	$7 \leftarrow 6$	18 632.426(3)	
	$6 \leftarrow 5$	18 632.561(3)	
$7\frac{1}{2} \leftarrow 6\frac{1}{2}$	$8 \leftarrow 7$	21 498.956(3)	
	$7 \leftarrow 6$	21 499.048(3)	

[a]) The figures in parentheses are the authors' estimates of experimental uncertainty (1σ).

Molecular parameters for $^{1}H\,^{12}C_4\,^{32}S$

Parameter		Value	Method	Ref.
State: electronic $X^2\Pi$; vibrational zero point level				
B	[MHz]	1 435.325 5(2) [a])	MW	94Hi
D	[kHz]	0.047(3)		
A	[GHz]	– 1 000 [b])		
$h_{3/2}(^1H)$ [c])	[MHz]	3.632(13)		

[a]) The numbers in parentheses are 1 standard deviation of the least-squares fit, in units of the last quoted decimal place.
[b]) Parameter constrained to this value.
[c]) $h_{3/2}(^1H) = a + (b+c)/2$.

Microwave data for $^{2}H\,^{12}C_4\,^{32}S$ (DC_4S)

Transition				
spin Ω	rotational $J' - J''$	hyperfine $F' - F''$	ν [MHz]	Ref.
State: electronic $X^2\Pi$; vibrational zero point level				
$\frac{3}{2}$	$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	$4\frac{1}{2} \leftarrow 3\frac{1}{2}$	9 535.377(3) [a])	94Hi
		$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	9 535.499(3)	
		$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	9 535.535(3)	
	$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	$5\frac{1}{2} \leftarrow 4\frac{1}{2}$	12 259.806(3)	
		$4\frac{1}{2} \leftarrow 3\frac{1}{2}$	12 259.872(3)	
		$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	12 259.907(3)	
	$5\frac{1}{2} \leftarrow 4\frac{1}{2}$	$6\frac{1}{2} \leftarrow 5\frac{1}{2}$	14 984.212(3)	
		$5\frac{1}{2} \leftarrow 4\frac{1}{2}$	14 984.284(3)	
		$4\frac{1}{2} \leftarrow 3\frac{1}{2}$	14 984.284(3)	

[a]) The figures in parentheses are the authors' estimates of experimental uncertainty (1σ).

Molecular parameters for $^{1}H\,^{12}C_4\,^{32}S$

Parameter		Value	Method	Ref.
State: electronic $X^2\Pi$; vibrational zero point level				
B	[MHz]	1 364.062 0(9) [a])	MW	94Hi
D	[kHz]	0.04(2)		
A	[GHz]	– 1 000 [b])		
$h_{3/2}(^1H)$ [c])	[MHz]	0.63(4)		
eQq_0	[MHz]	0.20(9)		

[a]) The numbers in parentheses are 1 standard deviation of the least-squares fit, in units of the last quoted decimal place.
[b]) Parameter constrained to this value.
[c]) $h_{3/2}(^1H) = a + (b+c)/2$.

Reference for HC_4S
94Hi Hirahara, Y., Ohshima, Y., Endo, Y. : J. Chem. Phys. **101** (1994) 7342.

3.2.1.2.30 SiCN

Microwave data for $^{28}Si\,^{12}C^{14}N$

Transition spin Ω	rotational $J' - J''$	parity e/f [a])	ν [MHz]	Ref.
State: electronic $\tilde{X}^2\Pi$; vibrational zero point level				
$\frac{1}{2}$	$13\frac{1}{2} \leftarrow 12\frac{1}{2}$	*f*	149 402.070	00Ap
$\frac{3}{2}$	$13\frac{1}{2} \leftarrow 12\frac{1}{2}$	*e*	149 907.342	
		f	149 909.389	
$\frac{1}{2}$	$14\frac{1}{2} \leftarrow 13\frac{1}{2}$	*e*	160 441.068	
		f	160 464.171	
$\frac{3}{2}$	$14\frac{1}{2} \leftarrow 13\frac{1}{2}$	*e*	161 007.636	
		f	161 009.947	
$\frac{1}{2}$	$15\frac{1}{2} \leftarrow 14\frac{1}{2}$	*e*	171 502.789	
$\frac{3}{2}$	$15\frac{1}{2} \leftarrow 14\frac{1}{2}$	*f*	172 109.888	
$\frac{3}{2}$	$16\frac{1}{2} \leftarrow 15\frac{1}{2}$	*e*	183 205.676	
		f	183 208.799	
$\frac{3}{2}$	$23\frac{1}{2} \leftarrow 22\frac{1}{2}$	*e*	260 865.966	
		f	260 872.270	
$\frac{1}{2}$	$24\frac{1}{2} \leftarrow 23\frac{1}{2}$	*e*	271 014.611	
		f	271 032.841	
$\frac{3}{2}$	$24\frac{1}{2} \leftarrow 23\frac{1}{2}$	*e*	271955.382	
		f	271 962.114	
$\frac{1}{2}$	$25\frac{1}{2} \leftarrow 24\frac{1}{2}$	*e*	282 065.649	
		f	282 083.260	
$\frac{3}{2}$	$25\frac{1}{2} \leftarrow 24\frac{1}{2}$	*e*	283 043.355	
		f	283 050.721	
$\frac{1}{2}$	$26\frac{1}{2} \leftarrow 25\frac{1}{2}$	*e*	293 115.283	
		f	293 132.294	
$\frac{3}{2}$	$26\frac{1}{2} \leftarrow 25\frac{1}{2}$	*e*	294 129.860	
		f	294 137.818	
$\frac{1}{2}$	$27\frac{1}{2} \leftarrow 26\frac{1}{2}$	*e*	304 163.557	
		f	304 179.889	
$\frac{3}{2}$	$27\frac{1}{2} \leftarrow 26\frac{1}{2}$	*e*	305 214.863	
		f	305 223.409	
$\frac{1}{2}$	$28\frac{1}{2} \leftarrow 27\frac{1}{2}$	*e*	315 210.382	
		f	315 225.984	
$\frac{3}{2}$	$28\frac{1}{2} \leftarrow 27\frac{1}{2}$	*e*	316 298.316	
		f	316 307.480	
$\frac{1}{2}$	$29\frac{1}{2} \leftarrow 28\frac{1}{2}$	*e*	326 255.647	
		f	326 270.513	
$\frac{3}{2}$	$29\frac{1}{2} \leftarrow 28\frac{1}{2}$	*e*	327 380.113	
		f	327 389.911	
$\frac{1}{2}$	$30\frac{1}{2} \leftarrow 29\frac{1}{2}$	*e*	337 299.287	
		f	337 313.436	
$\frac{3}{2}$	$30\frac{1}{2} \leftarrow 29\frac{1}{2}$	*e*	338 460.231	
		f	338 470.784	

[a]) States with parity equal to $\pm(-1)^{J-0.5}$ are labeled *e* and *f* respectively.

Molecular parameters for $^{28}Si\,^{12}C^{14}N$.

Parameter		Value	Method	Ref.
State: electronic $\tilde{X}^2\Pi$; vibrational zero point level				
B	[MHz]	5 543.415 2(2) [a])	MW	00Ap
D	[kHz]	2.310 2(2)		
$A+\gamma$	[GHz]	2 124(6)		
γ	[MHz]	2 070(10)		
$p + 2q$	[MHz]	25.734(2)		
$p_D + 2\, q_D$	[kHz]	– 0.386(7)		
q	[MHz]	0.869(2)		
$h_{1/2}(^{14}N)$ [b])	[MHz]	15.676(20)		
$b(^{14}N)$	[MHz]	5.6(2)		
$d(^{14}N)$	[MHz]	20.033(2)		
eQq_0	[MHz]	– 5.031(3)		
eQq_2	[MHz]	2.3(5)		

[a]) The numbers in parentheses are 1 standard deviation of the least-squares fit, in units of the last quoted decimal place.
[b]) $h_{1/2}(^{14}N) = a - (b+c)/2$.

Reference for SiCN

00Ap Apponi, A.J., McCarthy, M.C., Gottlieb, C.A., Thaddeus, P. : Astrophys. J. **536** (2000) L55.

3.2.1.2.31 SiNC

Microwave data for $^{28}Si\,^{14}N^{12}C$

Transition			ν [MHz]	Ref.
spin Ω	rotational $J' - J''$	parity e/f [a])		
State: electronic $\tilde{X}^2\Pi$; vibrational zero point level				
$\frac{1}{2}$	$11\frac{1}{2} \leftarrow 10\frac{1}{2}$	e	146 750.465	00Ap
		f	146 764.377	
$\frac{1}{2}$	$12\frac{1}{2} \leftarrow 11\frac{1}{2}$	e	159 508.318	
		f	159 522.959	
$\frac{3}{2}$	$12\frac{1}{2} \leftarrow 11\frac{1}{2}$	e	160 271.231	
		f	160 275.161	
$\frac{1}{2}$	$13\frac{1}{2} \leftarrow 12\frac{1}{2}$	e	172 265.317	
		f	172 280.796	
$\frac{3}{2}$	$13\frac{1}{2} \leftarrow 12\frac{1}{2}$	e	173 088.477	
		f	173 093.070	
$\frac{1}{2}$	$14\frac{1}{2} \leftarrow 13\frac{1}{2}$	e	185 021.468	
		f	185 037.780	
$\frac{3}{2}$	$14\frac{1}{2} \leftarrow 13\frac{1}{2}$	e	185 904.690	
		f	185 909.985	
$\frac{1}{2}$	$15\frac{1}{2} \leftarrow 14\frac{1}{2}$	e	197 776.606	
		f	197 793.782	
$\frac{3}{2}$	$15\frac{1}{2} \leftarrow 14\frac{1}{2}$	e	198 719.806	
		f	198 725.863	
$\frac{1}{2}$	$18\frac{1}{2} \leftarrow 17\frac{1}{2}$	e	236 035.490	
		f	236 055.743	
$\frac{3}{2}$	$18\frac{1}{2} \leftarrow 17\frac{1}{2}$	e	237 157.963	
		f	237 166.557	

$\frac{1}{2}$	$19\frac{1}{2} \leftarrow 18\frac{1}{2}$	*e*	248 786.095
		f	248 807.492
$\frac{3}{2}$	$19\frac{1}{2} \leftarrow 18\frac{1}{2}$	*e*	249 968.028
		f	249 977.657
$\frac{1}{2}$	$21\frac{1}{2} \leftarrow 20\frac{1}{2}$	*e*	274 283.235
		f	274 307.084
$\frac{3}{2}$	$21\frac{1}{2} \leftarrow 20\frac{1}{2}$	*e*	275 583.690
		f	275 595.340
$\frac{1}{2}$	$22\frac{1}{2} \leftarrow 21\frac{1}{2}$	*e*	287 029.701
		f	287 054.832
$\frac{3}{2}$	$22\frac{1}{2} \leftarrow 21\frac{1}{2}$	*e*	288 389.253
		f	288 401.913
$\frac{1}{2}$	$24\frac{1}{2} \leftarrow 23\frac{1}{2}$	*e*	312 518.133
		f	312 545.938
$\frac{3}{2}$	$24\frac{1}{2} \leftarrow 23\frac{1}{2}$	*e*	313 995.152
		f	314 010.149
$\frac{1}{2}$	$25\frac{1}{2} \leftarrow 24\frac{1}{2}$	*e*	325 259.866
$\frac{3}{2}$	$25\frac{1}{2} \leftarrow 24\frac{1}{2}$	*e*	326 795.431
		f	326 811.745
$\frac{1}{2}$	$26\frac{1}{2} \leftarrow 25\frac{1}{2}$	*f*	338 030.779
$\frac{3}{2}$	$26\frac{1}{2} \leftarrow 25\frac{1}{2}$	*e*	339 593.748

[a]) States with parity equal to $\pm(-1)^{J-0.5}$ are labeled *e* and *f* respectively.

Molecular parameters for $^{28}Si\,^{14}N^{12}C$

Parameter		Value	Method	Ref.
State: electronic $\tilde{X}^2\Pi$; vibrational zero point level				
B	[MHz]	6 396.683 9(3) [a])	MW	00Ap
D	[kHz]	2.889 0(4)		
$A+\gamma$	[GHz]	1 763(4)		
γ	[MHz]	2 470(10)		
$p + 2q$	[MHz]	9.800(3)		
$p_D + 2\,q_D$	[kHz]	18.42(3)		
q	[MHz]	1.385(7)		
q_D	[kHz]	0.011(7)		
$h_{1/2}(^{14}N)$ [b])	[MHz]	3.206(4)		
$b(^{14}N)$	[MHz]	− 5.2(3)		
$d(^{14}N)$	[MHz]	2.706(4)		
eQq_0	[MHz]	− 1.417(2)		

[a]) The numbers in parentheses are 1 standard deviation of the least-squares fit, in units of the last quoted decimal place.
[b]) $h_{1/2}(^{14}N) = a - (b+c)/2$.

Reference for SiNC

00Ap Apponi, A.J., McCarthy, M.C., Gottlieb, C.A., Thaddeus, P.: Astrophys. J. **536** (2000) L55.

3.2.1.2.32 SiCCH

Microwave data for $^{28}Si^{12}C^{12}C^{12}H$

Transition			ν [MHz]	Ref.
spin Ω	rotational $J' - J''$	parity e/f [a])		
State: electronic $\tilde{X}^2\Pi$; vibrational zero point level				
$\frac{1}{2}$	$13\frac{1}{2} \leftarrow 12\frac{1}{2}$	*e*	146 462.715	00Ap
		f	146 492.504	
$\frac{3}{2}$	$13\frac{1}{2} \leftarrow 12\frac{1}{2}$	*e*	147 065.062	
		f	147 067.120	
$\frac{1}{2}$	$14\frac{1}{2} \leftarrow 13\frac{1}{2}$	*e*	157 310.228	
		f	157 339.660	
$\frac{3}{2}$	$14\frac{1}{2} \leftarrow 13\frac{1}{2}$	*e*	157 955.660	
		f	157 957.989	
$\frac{1}{2}$	$15\frac{1}{2} \leftarrow 14\frac{1}{2}$	*e*	168 157.151	
		f	168 186.224	
$\frac{3}{2}$	$15\frac{1}{2} \leftarrow 14\frac{1}{2}$	*e*	168 845.531	
		f	168 848.184	
$\frac{1}{2}$	$16\frac{1}{2} \leftarrow 15\frac{1}{2}$	*e*	179 003.414	
		f	179 032.087	
$\frac{3}{2}$	$16\frac{1}{2} \leftarrow 15\frac{1}{2}$	*e*	179 734.687	
		f	179 737.704	
$\frac{1}{2}$	$17\frac{1}{2} \leftarrow 16\frac{1}{2}$	*e*	189 849.026	
		f	189 877.268	
$\frac{1}{2}$	$24\frac{1}{2} \leftarrow 23\frac{1}{2}$	*f*	265 770.200	
$\frac{1}{2}$	$25\frac{1}{2} \leftarrow 24\frac{1}{2}$	*e*	276 584.127	
$\frac{1}{2}$	$26\frac{1}{2} \leftarrow 25\frac{1}{2}$	*e*	287 421.751	
		f	287 445.144	
$\frac{1}{2}$	$27\frac{1}{2} \leftarrow 26\frac{1}{2}$	*e*	298 258.131	
		f	298 280.967	
$\frac{3}{2}$	$29\frac{1}{2} \leftarrow 28\frac{1}{2}$	*e*	321 208.140	
		f	321 217.594	
$\frac{3}{2}$	$30\frac{1}{2} \leftarrow 29\frac{1}{2}$	*e*	332 082.598	
		f	332 092.594	
$\frac{3}{2}$	$31\frac{1}{2} \leftarrow 30\frac{1}{2}$	*e*	342 955.572	
		f	342 966.287	
$\frac{3}{2}$	$32\frac{1}{2} \leftarrow 31\frac{1}{2}$	*e*	353 827.157	
		f	353 838.492	
$\frac{1}{2}$	$33\frac{1}{2} \leftarrow 32\frac{1}{2}$	*e*	363 251.216	
		f	363 269.792	
$\frac{3}{2}$	$33\frac{1}{2} \leftarrow 32\frac{1}{2}$	*e*	364 697.191	
		f	364 709.196	
$\frac{1}{2}$	$34\frac{1}{2} \leftarrow 33\frac{1}{2}$	*e*	374 078.752	
		f	374 096.539	
$\frac{3}{2}$	$34\frac{1}{2} \leftarrow 33\frac{1}{2}$	*e*	375 565.812	
		f	375 578.501	

[a]) States with parity equal to $\pm(-1)^{J-0.5}$ are labeled *e* and *f* respectively.

Molecular parameters for $^{28}Si^{12}C^{12}C^{12}H$

Parameter		Value	Method	Ref.
State: electronic $\tilde{X}^2\Pi$; vibrational zero point level				
B	[MHz]	5 436.662 9(2) [a])	MW	00Ap
D	[kHz]	1.824 4(5)		
$A+\gamma$	[GHz]	2 169(4)		
γ	[MHz]	1 161(9)		
$p + 2q$	[MHz]	32.071(2)		
$p_D + 2\,q_D$	[kHz]	– 0.420(7)		
q	[MHz]	0.807(4)		
q_D	[kHz]	– 0.016(2)		
$h_{1/2}(^1H)$ [b])	[MHz]	14.969(5)		
$b(^1H)$	[MHz]	– 14.1(3)		
$d(^1H)$	[MHz]	9.475(3)		

[a]) The numbers in parentheses are 1 standard deviation of the least-squares fit, in units of the last quoted decimal place.
[b]) $h_{1/2}(^1H) = a - (b+c)/2$.

Reference for SiCCH

00Ap Apponi, A.J., McCarthy, M.C., Gottlieb, C.A., Thaddeus, P. : Astrophys. J. **536** (2000) L55.

3.2.1.2.33 NaCH

Microwave data for $^{23}Na^{12}C^{1}H$

Transition		ν [MHz]	Ref.
rotational $N' - N''$	fine structure $J' - J''$		
State: electronic $\tilde{X}^3\Sigma^-$; zero point vibrational level			
15← 14	16← 15	339 264.598(100) [a])	98Xin
	15← 14	339 286.033(100)	
	14← 13	339 310.762(100)	
16← 15	17← 16	361 828.480(100)	
	16← 15	361 848.725(100)	
	15← 14	361 871.620(100)	
17← 16	18← 17	384 381.298(100)	
	17← 16	384 400.637(100)	
	16← 15	384 421.894(100)	
18← 17	19← 18	406 922.395(100)	
	18← 17	406 940.848(100)	
	17← 16	406 960.817(100)	
19← 18	20← 19	429 451.093(100)	
	19← 18	429 468.733(100)	
	18← 17	429 487.864(100)	
20← 19	21← 20	451 966.669(100)	
	20← 19	451 983.638(100)	
	19← 18	452 001.991(100)	
21← 20	22← 21	474 468.543(100)	
	21← 20	474 485.057(100)	
	20← 19	474 502.566(100)	
22← 21	23← 22	496 956.056(100)	
	22← 21	496 972.038(100)	
	21← 20	496 988.919(100)	

23← 22	24← 23	519 428.601(100)	
	23← 22	519 444.040(100)	
	22← 21	519 460.524(100)	

[a]) The figures in parentheses are the authors' estimates of experimental uncertainty (1σ).

Molecular parameters for $^{23}Na^{12}C^{1}H$

Parameter		Value	Method	Ref.
State: electronic $\tilde{X}^3\Sigma^-$; zero point vibrational level				
B	[MHz]	11 322.317 5(34) [a])	MW	98Xin
D	[kHz]	28.497 8(41)		
λ	[MHz]	9 120(460)		
λ_D	[kHz]	1.3(17)		
γ	[MHz]	– 10.76(13)		
r_0(C – H)	[Å]	1.073		
r_0(Na – C)	[Å]	2.207		

[a]) The numbers in parentheses are 3 standard deviations of the least-squares fit, in units of the last quoted decimal place.

Microwave data for $^{23}Na^{12}C^{2}H$ (NaCD)

Transition		ν [MHz]	Ref.
rotational $N' – N''$	fine structure $J' – J''$		
State: electronic $\tilde{X}^3\Sigma^-$; zero point vibrational level			
22← 21	23← 22	439 155.189(100) [a])	98Xin
	22← 21	439 169.776(100)	
	21← 20	439 185.007(100)	
23← 22	24← 23	459 033.609(100)	
	23← 22	459 047.800(100)	
	22← 21	459 062.537(100)	
24← 23	25← 24	478 900.848(100)	
	24← 23	478 914.669(100)	
	23← 22	478 928.970(100)	
25← 24	26← 25	498 769.834(100)	
	25← 24	498 783.759(100)	
	24← 23	498 783.759(100)	
26← 25	27← 26	518 599.418(100)	
	26← 25	518 612.768(100)	
	25← 24	518 626.265(100)	

[a]) The figures in parentheses are the authors' estimates of experimental uncertainty (1σ).

Molecular parameters for $^{23}Na^{12}C^{2}H$ (NaCD)

Parameter		Value	Method	Ref.
State: electronic $\tilde{X}^3\Sigma^-$; zero point vibrational level				
B	[MHz]	10 000.13 6(43) [a])	MW	98Xin
D	[kHz]	20.335 5(36)		
λ	[MHz]	9 000(2900)		
λ_D	[kHz]	3.2(11)		
γ	[MHz]	– 9.75(24)		

[a]) The numbers in parentheses are 3 standard deviations of the least-squares fit, in units of the last quoted decimal place.

Reference for NaCH

98Xin Xin, J., Ziurys, L.M.: Astrophys. J. Letts. **508** (1998) L109.

3.2.1.2.34 KCH

Microwave data for $^{39}K^{12}C^{1}H$

Transition		ν [MHz]	Ref.
rotational $N' - N''$	fine structure $J' - J''$		
State: electronic $\tilde{X}^3\Sigma^-$; zero point vibrational level			
22← 21	23← 22	328 736.419(100) [a])	99Xin
	22← 21	328 746.435(100)	
	21← 20	328 757.199(100)	
23← 22	24← 23	343 626.845(100)	
	23← 22	343 636.584(100)	
	22← 21	343 647.034(100)	
24← 23	25← 24	358 510.146(100)	
	24← 23	358 519.664(100)	
	23← 22	358 529.735(100)	
25← 24	26← 25	373 386.160(100)	
	25← 24	373 395.418(100)	
	24← 23	373 405.239(100)	
26← 25	27← 26	388 254.381(100)	
	26← 25	388 263.517(100)	
	25← 24	388 273.045(100)	
27← 26	28← 27	403 114.758(100)	
	27← 26	403 123.618(100)	
	26← 25	403 132.948(100)	
28← 27	29← 28	417 966.782(100)	
	28← 27	417 975.511(100)	
	27← 26	417 984.608(100)	
29← 28	30← 29	432 956.056(100)	
	29← 28	432 956.056(100)	
	28← 27	432 956.056(100)	
30← 29	31← 30	447 644.626(100)	
	30← 29	447 653.093(100)	
	29← 28	447 661.876(100)	
31← 30	32← 31	462 469.927(100)	
	31← 30	462 478.339(100)	
	30← 29	462 486.936(100)	
32← 31	33← 32	477 285.715(100)	
	32← 31	477 293.988(100)	
	31← 30	477 302.492(100)	
33← 32	34← 33	492 091.721(100)	
	33← 32	492 099.889(100)	
	32← 31	492 108.201(100)	
34← 33	35← 34	506 887.577(100)	
	34← 33	506 895.702(100)	
	33← 32	506 903.896(100)	
35← 34	36← 35	521 673.009(100)	
	35← 34	521 680.973(100)	
	34← 33	521 689.168(100)	

[a]) The figures in parentheses are the authors' estimates of experimental uncertainty (1σ).

Molecular parameters for $^{39}K^{12}C^{1}H$

Parameter		Value	Method	Ref.
State: electronic $\tilde{X}^3\Sigma^-$; zero point vibrational level				
B	[MHz]	7 483.870 69(94) [a])	MW	99Xin
D	[kHz]	12.769 49(51)		
λ	[MHz]	8 240(740)		
λ_D	[kHz]	0.0 [b])		
γ	[MHz]	– 6.550(55)		
r_0(C – H)	[Å]	1.082		
r_0(K – C)	[Å]	2.526		

[a]) The numbers in parentheses are 3 standard deviations of the least-squares fit, in units of the last quoted decimal place.
[b]) Parameter constrained to this value.

Microwave data for $^{39}K^{12}C^{2}H$ (KCD)

Transition		ν [MHz]	Ref.
rotational $N' - N''$	fine structure $J' - J''$		
State: electronic $\tilde{X}^3\Sigma^-$; zero point vibrational level			
32← 31	33← 32	423 437.023(100) [a])	99Xin
	32← 31	423 444.510(100)	
	31← 30	423 452.126(100)	
33← 32	34← 33	436 589.688(100)	
	33← 32	436 597.086(100)	
	32← 31	436 604.612(100)	
34← 33	35← 34	449 735.073(100)	
	34← 33	449 742.374(100)	
	33← 32	449 749.725(100)	
35← 34	36← 35	462 872.727(100)	
	35← 34	462 880.003(100)	
	34← 33	462 887.277(100)	
36← 35	37← 36	476 002.579(100)	
	36← 35	476 009.713(100)	
	35← 34	476 016.983(100)	
37← 36	38← 37	489 124.322(100)	
	37← 36	489 131.483(100)	
	36← 35	489 138.677(100)	
38← 37	39← 38	502 237.924(100)	
	38← 37	502 244.935(100)	
	37← 36	502 251.988(100)	
39← 38	40← 39	515 342.788(100)	
	39← 38	515 349.877(100)	
	38← 37	515 356.872(100)	
40← 39	41← 40	528 439.061(100)	
	40← 39	528 445.993(100)	
	39← 38	528 453.006(100)	

[a]) The figures in parentheses are the authors' estimates of experimental uncertainty (1σ).

Molecular parameters for $^{39}K^{12}C^{2}H$ (KCD)

Parameter		Value	Method	Ref.
State: electronic $\tilde{X}\,^3\Sigma^-$; zero point vibrational level				
B	[MHz]	6 635.422 3(23) [a])	MW	99Xin
D	[kHz]	9.327 23(86)		
λ	[MHz]	8 100(2000)		
λ_D	[kHz]	0.0 [b])		
γ	[MHz]	– 5.98(19)		

[a]) The numbers in parentheses are 3 standard deviations of the least-squares fit, in units of the last quoted decimal place.
[b]) Parameter constrained to this value.

Reference for KCH

99Xin Xin, J., Ziurys, L.M. : J. Chem. Phys. **110** (1999) 3360.

3.2.1.2.35 MgOH

Microwave data for $^{24}Mg^{16}O\,^{1}H$

Transition			ν [MHz]	Ref.
rotational $N' - N''$	fine structure $J' - J''$	Hyperfine [a]) $F' - F''$		
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (0,0,0)				
3 ← 2	$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	2 ← 1	88 913.315	92Ba
		3 ← 2	88 913.215	
	$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	3 ← 2	88 951.128	
		4 ← 3	88 951.028	
5 ← 4	$4\frac{1}{2} \leftarrow 3\frac{1}{2}$	[b])	148 193.213	
	$5\frac{1}{2} \leftarrow 4\frac{1}{2}$	[b])	148 230.880	
6 ← 5	$5\frac{1}{2} \leftarrow 4\frac{1}{2}$	[b])	177 828.755	
	$6\frac{1}{2} \leftarrow 5\frac{1}{2}$	[b])	177 866.334	
7 ← 6	$6\frac{1}{2} \leftarrow 5\frac{1}{2}$	[b])	207 460.423	
	$7\frac{1}{2} \leftarrow 6\frac{1}{2}$	[b])	207 498.046	
8 ← 7	$7\frac{1}{2} \leftarrow 6\frac{1}{2}$	[b])	237 087.750	
	$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	[b])	237 125.358	
9 ← 8	$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	[b])	266 710.039	
	$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	[b])	266 747.652	
10 ← 9	$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	[b])	296 326.642	
	$10\frac{1}{2} \leftarrow 9\frac{1}{2}$	[b])	296 364.264	
11 ← 10	$10\frac{1}{2} \leftarrow 9\frac{1}{2}$	[b])	325 936.944	
	$11\frac{1}{2} \leftarrow 10\frac{1}{2}$	[b])	325 974.531	
12 ← 11	$11\frac{1}{2} \leftarrow 10\frac{1}{2}$	[b])	355 540.349	
	$12\frac{1}{2} \leftarrow 11\frac{1}{2}$	[b])	355 577.911	
13 ← 12	$12\frac{1}{2} \leftarrow 11\frac{1}{2}$	[b])	385 136.187	
	$13\frac{1}{2} \leftarrow 12\frac{1}{2}$	[b])	385 173.745	

[a]) Coupling scheme: $\boldsymbol{J} = \boldsymbol{N} + \boldsymbol{S}$; $\boldsymbol{F} = \boldsymbol{J} + \boldsymbol{I}_1$ where $\boldsymbol{I}_1$ is the ^{1}H nuclear spin.
[b]) Hyperfine structure not resolved.

Microwave data for $^{24}Mg^{16}O^{1}H$

Transition rotational $N' - N''$	rotational $J' - J''$	parity e/f[a])	ν [MHz]	Ref.
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (0,1^1,0), $^2\Pi$ vibronic component				
$9 \leftarrow 8$	$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	*e*	264 766.989	95Fl, 99Ap
		f	266 297.314	
	$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	*e*	264 807.391	
		f	266 339.700	
$10 \leftarrow 9$	$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	*e*	294 168.119	
		f	295 867.966	
	$10\frac{1}{2} \leftarrow 9\frac{1}{2}$	*e*	294 207.888	
		f	295 909.970	
$11 \leftarrow 10$	$10\frac{1}{2} \leftarrow 9\frac{1}{2}$	*e*	323 562.702	
		f	325 432.307	
	$11\frac{1}{2} \leftarrow 10\frac{1}{2}$	*e*	323 602.248	
		f	325 474.047	
$12 \leftarrow 11$	$11\frac{1}{2} \leftarrow 10\frac{1}{2}$	*e*	352 950.313	
		f	354 989.542	
	$12\frac{1}{2} \leftarrow 11\frac{1}{2}$	*e*	352 989.645	
		f	355 031.099	
$13 \leftarrow 12$	$12\frac{1}{2} \leftarrow 11\frac{1}{2}$	*e*	382 330.288	
		f	384 539.123	
	$13\frac{1}{2} \leftarrow 12\frac{1}{2}$	*e*	382 369.457	
		f	384 580.441	
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (0,2^0,0), $^2\Sigma$ vibronic component				
$9 \leftarrow 8$	$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	*f*	265 836.278	95Fl, 99Ap
	$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	*e*	265 876.502	
$10 \leftarrow 9$	$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	*f*	295 369.605	
	$10\frac{1}{2} \leftarrow 9\frac{1}{2}$	*e*	295 410.134	
$11 \leftarrow 10$	$10\frac{1}{2} \leftarrow 9\frac{1}{2}$	*f*	324 900.721	
	$11\frac{1}{2} \leftarrow 10\frac{1}{2}$	*e*	324 941.245	
$12 \leftarrow 11$	$11\frac{1}{2} \leftarrow 10\frac{1}{2}$	*f*	354 429.212	
	$12\frac{1}{2} \leftarrow 11\frac{1}{2}$	*e*	354 469.700	
$13 \leftarrow 12$	$12\frac{1}{2} \leftarrow 11\frac{1}{2}$	*f*	383 954.571	
	$13\frac{1}{2} \leftarrow 12\frac{1}{2}$	*e*	383 995.123	
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (0,2^2,0), $^2\Delta$ vibronic component				
$9 \leftarrow 8$	$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	*e*	264 411.525	95Fl, 99Ap
		f	264 467.829	
	$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	*e*	264 458.883	
		f	264 515.443	
$10 \leftarrow 9$	$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	*e*	293 759.546	
		f	293 836.640	
	$10\frac{1}{2} \leftarrow 9\frac{1}{2}$	*e*	293 805.740	
		f	293 882.793	
$11 \leftarrow 10$	$10\frac{1}{2} \leftarrow 9\frac{1}{2}$	*e*	323 097.237	
		f	323 198.733	
	$11\frac{1}{2} \leftarrow 10\frac{1}{2}$	*e*	323 142.161	
		f	323 243.900	
$12 \leftarrow 11$	$11\frac{1}{2} \leftarrow 10\frac{1}{2}$	*e*	352 423.122	

		f	352 553.731	
	$12\frac{1}{2} \leftarrow 11\frac{1}{2}$	*e*	352 467.148	
		f	352 598.383	
$13 \leftarrow 12$	$12\frac{1}{2} \leftarrow 11\frac{1}{2}$	*e*	381 736.723	
		f	381 901.023	
	$13\frac{1}{2} \leftarrow 12\frac{1}{2}$	*e*	381 780.156	
		f	381 944.878	
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational $(0,3^1,0)$, $^2\Pi$ vibronic component				
$9 \leftarrow 8$	$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	*e*	264 198.441	95Fl, 99Ap
		f	266 551.921	
	$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	*e*	264 240.426	
		f	266 596.348	
$10 \leftarrow 9$	$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	*e*	293 556.116	
		f	296 165.762	
	$10\frac{1}{2} \leftarrow 9\frac{1}{2}$	*e*	293 597.784	
		f	296 209.585	
$11 \leftarrow 10$	$10\frac{1}{2} \leftarrow 9\frac{1}{2}$	*e*	322 913.130	
		f	325 776.032	
	$11\frac{1}{2} \leftarrow 10\frac{1}{2}$	*e*	322 954.287	
		f	325 819.800	
$12 \leftarrow 11$	$11\frac{1}{2} \leftarrow 10\frac{1}{2}$	*e*	352 268.994	
		f	355 382.249	
	$12\frac{1}{2} \leftarrow 11\frac{1}{2}$	*e*	352 310.136	
		f	355 426.002	
$13 \leftarrow 12$	$12\frac{1}{2} \leftarrow 11\frac{1}{2}$	*e*	381 623.576	
		f	384 983.634	
	$13\frac{1}{2} \leftarrow 12\frac{1}{2}$	*e*	381 664.443	
		f	385 027.189	
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational $(0,3^3,0)$, $^2\Phi$ vibronic component				
$9 \leftarrow 8$	$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	*e*	263 430.278	95Fl, 99Ap
		f	263 439.025	
	$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	*e*	263 486.132	
		f	263 494.969	
$10 \leftarrow 9$	$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	*e*	292 665.271	
		f	292 679.583	
	$10\frac{1}{2} \leftarrow 9\frac{1}{2}$	*e*	292 718.171	
		f	292 732.503	
$11 \leftarrow 10$	$10\frac{1}{2} \leftarrow 9\frac{1}{2}$	*e*	321 887.629	
		f	321 909.843	
	$11\frac{1}{2} \leftarrow 10\frac{1}{2}$	*e*	321 938.453	
		f	321 960.812	
$12 \leftarrow 11$	$11\frac{1}{2} \leftarrow 10\frac{1}{2}$	*e*	351 096.899	
		f	351 129.674	
	$12\frac{1}{2} \leftarrow 11\frac{1}{2}$	*e*	351 146.053	
		f	351 179.000	
$13 \leftarrow 12$	$12\frac{1}{2} \leftarrow 11\frac{1}{2}$	*e*	380 292.016	
		f	380 339.860	
	$13\frac{1}{2} \leftarrow 12\frac{1}{2}$	*e*	380 338.584	
		f	380 386.774	
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational $(0,4^2,0)$, $^2\Delta$ vibronic component				
$9 \leftarrow 8$	$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	*e*	263 726.700	95Fl, 99Ap

		f	264 542.148
	$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	e	263 766.813
		f	264 590.286
$10 \leftarrow 9$	$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	e	293 022.109
		f	293 904.108
	$10\frac{1}{2} \leftarrow 9\frac{1}{2}$	e	293 062.025
		f	293 951.156
$11 \leftarrow 10$	$10\frac{1}{2} \leftarrow 9\frac{1}{2}$	e	322 314.183
		f	323 254.699
	$11\frac{1}{2} \leftarrow 10\frac{1}{2}$	e	323 354.403
		f	323 300.751
$12 \leftarrow 11$	$11\frac{1}{2} \leftarrow 10\frac{1}{2}$	e	351 602.485
		f	352 592.643
	$12\frac{1}{2} \leftarrow 11\frac{1}{2}$	e	351 643.039
		f	352 637.711

[a]) States with parity equal to ± $(-1)^{J-0.5}$ are labeled *e* and *f* respectively.

Molecular parameters for $^{24}Mg^{16}O^{1}H$

Parameter		Value	Method	Ref.
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (0,0,0)				
B	[MHz]	14 822.516 1(22) [a])	MW	92Ba
D	[kHz]	26.222 5(92)		
γ	[MHz]	37.567(36)		
$b(^1H)$	[MHz]	9.3(39)		
$c(^1H)$	[MHz]	– 4.8(28)		
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational $(0,1^1,0)$, $^2\Pi$ vibronic component				
B	[MHz]	14 757.180 7(66) [a])	MW	95Fl, 99Ap
D	[kHz]	26.546(25)		
γ	[MHz]	42.23(27)		
γ_D	[kHz]	– 4.10(72)		
q	[MHz]	– 85.134(13)		
q_D	[kHz]	0.413(49)		
p_Π [d])	[MHz]	– 2.16(13)		
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational $(0,2^0,0)$, $^2\Sigma$ vibronic component				
B	[MHz]	14 771.018(15) [a]), [b])	MW	99Ap
D	[kHz]	26.860(57)		
γ	[MHz]	40.15(39)		
γ_D	[kHz]	0.8(10)		
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational $(0,2^2,0)$, $^2\Delta$ vibronic component				
B	[MHz]	14 698.038 3(66) [a])	MW	99Ap
D	[kHz]	26.346(33)		
γ	[MHz]	50.60(27)		
γ_D	[kHz]	–14.20(72)		
q	[MHz]	– 79.96(12)		
q_D	[kHz]	2.39(54)		

State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (0,3[1],0), $^2\Pi$ vibronic component				
B	[MHz]	14 744.710 3(68) [a])	MW	99Ap
D	[kHz]	20.136(25)		
γ	[MHz]	43.15(28)		
γ_D	[kHz]	– 3.81(72)		
q	[MHz]	– 65.859(30)		
q_D	[kHz]	2.22(24)		
q_H	[Hz]	16.28(63)		
p_Π [d])	[MHz]	6.14(36)		
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (0,3[3],0), $^2\Phi$ vibronic component				
B	[MHz]	14 644.371 1(61) [a])	MW	99Ap
D	[kHz]	33.143(24)		
γ	[MHz]	64.08(71)		
γ_D	[kHz]	– 32.71(59)		
ρ [c])	[kHz]	32.686(59)		
State: electronic $X\,^2\Sigma^+$; vibrational (0,4[2],0), $^2\Delta$ vibronic component				
B	[MHz]	14 679.936 5(88) [a])	MW	99Ap
D	[kHz]	29.672(38)		
γ	[MHz]	43.389(75)		
q	[MHz]	0.923 6(38)		
q_D	[kHz]	– 8.922(71)		
q_H	[Hz]	41.00(48)		
q_1	[Hz]	–0.074 2(11)		
p_Δ [d])	[MHz]	3.188(75)		

[a]) The numbers in parenthesis are 3 standard deviations of the least-squares fit, in units of the last quoted decimal place.
[b]) The separation between the $v = 2$, $l = 0$ and ±2 levels, $4g_{22}$, was constrained to 10.5 cm^{-1} [95Bu] in the least-squares fit.
[c]) ρ is a higher-order l-type resonance parameter used to account for the splittings in the 3^3 states.
[d]) This parameter takes care of the different spin-rotation splittings in the l-type doubling components.

Microwave data for $^{25}Mg^{16}O\,^1H$

Transition: rotational $N' - N''$	Transition: fine structure $J' - J''$	Transition: Hyperfine [a]) $F' - F''$	ν [MHz]	Ref.
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (0,0,0)				
13 ← 12	$12\frac{1}{2} \leftarrow 11\frac{1}{2}$	10 ← 9	378 896.155	92Ba
		11 ← 10	378 899.136	
		12 ← 11	378 902.481	
		13 ← 12	378 906.384	
		14 ← 13	378 911.456 [b])	
		15 ← 14	378 911.456 [b])	
	$13\frac{1}{2} \leftarrow 12\frac{1}{2}$	14 ← 13	378 918.132 [b])	
		15 ← 14	378 918.132 [b])	
		13 ← 12	378 922.990	
		12 ← 11	378 926.793	
		11 ← 10	378 930.135	
		16 ← 15	378 933.240	

[a]) Coupling scheme: $\boldsymbol{J} = \boldsymbol{N} + \boldsymbol{S}$; $\boldsymbol{F} = \boldsymbol{J} + \boldsymbol{I}_2$ where $\boldsymbol{I}_1$ is the ^{25}Mg nuclear spin (I = 5/2).
[b]) Blended hyperfine components.

Molecular parameters for $^{25}Mg^{16}O^{1}H$

Parameter		Value	Method	Ref.
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (0,0,0)				
B	[MHz]	14 581.798 7(27) [a])	MW	92Ba
D	[kHz]	24.130 [b])		
γ	[MHz]	37.01(22)		
$b(^{25}Mg)$	[MHz]	– 304.4(46)		
$c(^{25}Mg)$	[MHz]	0.0 [b])		
$eQq_0(^{25}Mg)$	[MHz]	– 41(17)		

[a]) The numbers in parenthesis is 3 standard deviations of the least-squares fit, in units of the last quoted decimal place.
[b]) Parameter constrained to this value in the least-squares fit which was based on the N = 13←12 transition frequencies only.

Microwave data for $^{26}Mg^{16}O^{1}H$

Transition			ν [MHz]	Ref.
rotational $N' - N''$	fine structure $J' - J''$	Hyperfine [a]) $F' - F''$		
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (0,0,0)				
8 ← 7	$7\frac{1}{2} \leftarrow 6\frac{1}{2}$	[b])	229 709.481	92Ba
	$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	[b])	229 745.993	
9 ← 8	$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	[b])	258 410.366	
	$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	[b])	258 446.815	
10 ← 9	$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	[b])	287 105.878	
	$10\frac{1}{2} \leftarrow 9\frac{1}{2}$	[b])	287 142.369	
11 ← 10	$10\frac{1}{2} \leftarrow 9\frac{1}{2}$	[b])	315 795.605	
	$11\frac{1}{2} \leftarrow 10\frac{1}{2}$	[b])	315 832.014	
12 ← 11	$11\frac{1}{2} \leftarrow 10\frac{1}{2}$	[b])	344 478.734	
	$12\frac{1}{2} \leftarrow 11\frac{1}{2}$	[b])	344 515.113	
13 ← 12	$12\frac{1}{2} \leftarrow 11\frac{1}{2}$	[b])	373 154.786	
	$13\frac{1}{2} \leftarrow 12\frac{1}{2}$	[b])	373 191.138	

[a]) Coupling scheme: $\boldsymbol{J} = \boldsymbol{N} + \boldsymbol{S}$; $\boldsymbol{F} = \boldsymbol{J} + \boldsymbol{I}_1$ where $\boldsymbol{I}_1$ is the ^1H nuclear spin.
[b]) Hyperfine structure not resolved.

Molecular parameters for $^{26}Mg^{16}O^{1}H$

Parameter		Value	Method	Ref.
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (0,0,0)				
B	[MHz]	14 361.137 3(37) [a])	MW	92Ba
D	[kHz]	24.648(14)		
γ	[MHz]	36.433(4)		

[a]) The numbers in parenthesis is 3 standard deviations of the least-squares fit, in units of the last quoted decimal place.

Microwave data for $^{24}Mg^{16}O^{2}H$ (MgOD)

Transition			ν [MHz]	Ref.
rotational $N' - N''$	rotational $J' - J''$	parity e/f [a])		
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (0,0,0)				
7 ← 6	$6\frac{1}{2} \leftarrow 5\frac{1}{2}$	f	188 094.847	95Nu
	$7\frac{1}{2} \leftarrow 6\frac{1}{2}$	e	188 128.587	
8 ← 7	$7\frac{1}{2} \leftarrow 6\frac{1}{2}$	f	214 958.413	
	$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	e	214 992.079	
9 ← 8	$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	f	241 818.156	

	$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	*e*	241 851.798	
$10 \leftarrow 9$	$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	*f*	268 673.605	
	$10\frac{1}{2} \leftarrow 9\frac{1}{2}$	*e*	268 707.207	
$11 \leftarrow 10$	$10\frac{1}{2} \leftarrow 9\frac{1}{2}$	*f*	295 524.252	
	$11\frac{1}{2} \leftarrow 10\frac{1}{2}$	*e*	295 557.872	
$13 \leftarrow 12$	$12\frac{1}{2} \leftarrow 11\frac{1}{2}$	*f*	349 209.358	
	$13\frac{1}{2} \leftarrow 12\frac{1}{2}$	*e*	349 242.969	
$14 \leftarrow 13$	$13\frac{1}{2} \leftarrow 12\frac{1}{2}$	*f*	376 042.759	
	$14\frac{1}{2} \leftarrow 13\frac{1}{2}$	*e*	376 076.442	
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational $(0,1^1,0)$, $^2\Pi$ vibronic component				
$9 \leftarrow 8$	$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	*e*	241 053.319	95Nu
		f	242 864.123	
	$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	*e*	241 088.836	
		f	242 901.323	
$10 \leftarrow 9$	$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	*e*	267 824.243	
		f	269 835.281	
	$10\frac{1}{2} \leftarrow 9\frac{1}{2}$	*e*	267 859.576	
		f	269 872.265	
$11 \leftarrow 10$	$10\frac{1}{2} \leftarrow 9\frac{1}{2}$	*e*	294 590.555	
		f	296 801.335	
	$11\frac{1}{2} \leftarrow 10\frac{1}{2}$	*e*	294 625.651	
		f	296 838.152	
$12 \leftarrow 11$	$11\frac{1}{2} \leftarrow 10\frac{1}{2}$	*e*	312 351.577	
		f	323 761.834	
	$12\frac{1}{2} \leftarrow 11\frac{1}{2}$	*e*	321 386.560	
		f	323 798.498	
$13 \leftarrow 12$	$12\frac{1}{2} \leftarrow 11\frac{1}{2}$	*e*	348 107.014	
		f	350 716.238	
	$13\frac{1}{2} \leftarrow 12\frac{1}{2}$	*e*	348 141.873	
		f	350 752.822	
$14 \leftarrow 13$	$13\frac{1}{2} \leftarrow 12\frac{1}{2}$	*e*	374 856.272	
		f	377 664.144	
	$14\frac{1}{2} \leftarrow 13\frac{1}{2}$	*e*	374 891.113	
		f	377 700.624	
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational $(0,2^0,0)$, $^2\Sigma$ vibronic component				
$10 \leftarrow 9$	$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	*f*	269 643.224	99Ap
	$10\frac{1}{2} \leftarrow 9\frac{1}{2}$	*e*	269 679.327	
$11 \leftarrow 10$	$10\frac{1}{2} \leftarrow 9\frac{1}{2}$	*f*	296 607.298	
	$11\frac{1}{2} \leftarrow 10\frac{1}{2}$	*e*	296 643.419	
$12 \leftarrow 11$	$11\frac{1}{2} \leftarrow 10\frac{1}{2}$	*f*	323 570.567	
	$12\frac{1}{2} \leftarrow 11\frac{1}{2}$	*e*	323 606.766	
$13 \leftarrow 12$	$12\frac{1}{2} \leftarrow 11\frac{1}{2}$	*f*	350 532.832	
	$13\frac{1}{2} \leftarrow 12\frac{1}{2}$	*e*	350 569.076	
$14 \leftarrow 13$	$13\frac{1}{2} \leftarrow 12\frac{1}{2}$	*f*	377 493.935	
	$14\frac{1}{2} \leftarrow 13\frac{1}{2}$	*e*	377 530.160	
$17 \leftarrow 16$	$16\frac{1}{2} \leftarrow 15\frac{1}{2}$	*f*	458 367.596	
	$17\frac{1}{2} \leftarrow 16\frac{1}{2}$	*e*	458 403.930	
$18 \leftarrow 17$	$17\frac{1}{2} \leftarrow 16\frac{1}{2}$	*f*	485 321.239	

	$18\frac{1}{2} \leftarrow 17\frac{1}{2}$	*e*	485 357.586	

State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational $(0,2^2,0)$, $^2\Delta$ vibronic component

$10 \leftarrow 9$	$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	*e*	268 718.094	99Ap
		f	268 796.513	
	$10\frac{1}{2} \leftarrow 9\frac{1}{2}$	*e*	268 757.821	
		f	268 836.399	
$11 \leftarrow 10$	$10\frac{1}{2} \leftarrow 9\frac{1}{2}$	*e*	295 555.863	
		f	295 659.907	
	$11\frac{1}{2} \leftarrow 10\frac{1}{2}$	*e*	295 594.897	
		f	295 699.210	
$12 \leftarrow 11$	$11\frac{1}{2} \leftarrow 10\frac{1}{2}$	*e*	322 383.291	
		f	322 517.907	
	$12\frac{1}{2} \leftarrow 11\frac{1}{2}$	*e*	322 421.837	
		f	322 556.761	
$13 \leftarrow 12$	$12\frac{1}{2} \leftarrow 11\frac{1}{2}$	*e*	349 199.695	
		f	349 370.022	
	$13\frac{1}{2} \leftarrow 12\frac{1}{2}$	*e*	349 237.763	
		f	349 408.456	
$14 \leftarrow 13$	$13\frac{1}{2} \leftarrow 12\frac{1}{2}$	*f*	376 215.814	
	$14\frac{1}{2} \leftarrow 13\frac{1}{2}$	*f*	376 253.941	
$16 \leftarrow 15$	$15\frac{1}{2} \leftarrow 14\frac{1}{2}$	*e*	429 574.692	
		f	429 886.492	
	$16\frac{1}{2} \leftarrow 15\frac{1}{2}$	*e*	429 611.933	
		f	429 924.133	
$17 \leftarrow 16$	$16\frac{1}{2} \leftarrow 15\frac{1}{2}$	*e*	456 339.306	
		f	456 710.415	
	$17\frac{1}{2} \leftarrow 16\frac{1}{2}$	*e*	456 376.295	
		f	456 747.894	
$18 \leftarrow 17$	$17\frac{1}{2} \leftarrow 16\frac{1}{2}$	*e*	483 089.237	
		f	483 526.076	
	$18\frac{1}{2} \leftarrow 17\frac{1}{2}$	*e*	483 126.052	
		f	483 563.415	

State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational $(0,3^1,0)$, $^2\Pi$ vibronic component

$10 \leftarrow 9$	$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	*e*	268 348.968	99Ap
		f	271 468.846	
	$10\frac{1}{2} \leftarrow 9\frac{1}{2}$	*e*	268 385.686	
		f	271 507.641	
$11 \leftarrow 10$	$10\frac{1}{2} \leftarrow 9\frac{1}{2}$	*e*	295 176.153	
		f	298 605.124	
	$11\frac{1}{2} \leftarrow 10\frac{1}{2}$	*e*	295 212.646	
		f	298 643.799	
$12 \leftarrow 11$	$11\frac{1}{2} \leftarrow 10\frac{1}{2}$	*e*	322 000.605	
		f	325 737.549	
	$12\frac{1}{2} \leftarrow 11\frac{1}{2}$	*e*	322 036.929	
		f	325 776.115	
$13 \leftarrow 12$	$12\frac{1}{2} \leftarrow 11\frac{1}{2}$	*e*	348 821.844	
		f	352 865.655	
	$13\frac{1}{2} \leftarrow 12\frac{1}{2}$	*e*	348 858.161	
		f	352 904.224	
$14 \leftarrow 13$	$13\frac{1}{2} \leftarrow 12\frac{1}{2}$	*e*	375 639.940	

		f	379 989.097	
	$14\frac{1}{2} \leftarrow 13\frac{1}{2}$	*e*	375 676.156	
		f	380 027.590	
16 ← 15	$15\frac{1}{2} \leftarrow 14\frac{1}{2}$	*e*	429 265.142	
	$16\frac{1}{2} \leftarrow 15\frac{1}{2}$	*e*	429 301.314	
17 ← 16	$16\frac{1}{2} \leftarrow 15\frac{1}{2}$	*e*	456 071.782	
		f	461 326.192	
	$17\frac{1}{2} \leftarrow 16\frac{1}{2}$	*e*	456 107.902	
		f	461 364.491	
18 ← 17	$17\frac{1}{2} \leftarrow 16\frac{1}{2}$	*e*	482 874.116	
		f	488 425.774	
	$18\frac{1}{2} \leftarrow 17\frac{1}{2}$	*e*	482 910.224	
		f	488 464.056	
19 ← 18	$18\frac{1}{2} \leftarrow 17\frac{1}{2}$	*e*	509 671.825	
		f	515 518.060	
	$19\frac{1}{2} \leftarrow 18\frac{1}{2}$	*e*	509 707.938	
		f	515 556.218	
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational $(0,3^3,0)$, $^2\Phi$ vibronic component				
10 ← 9	$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	*e*	268 645.777	99Ap
		f	268 647.587	
	$10\frac{1}{2} \leftarrow 9\frac{1}{2}$	*e*	268 690.562	
		f	268 692.422	
11 ← 10	$10\frac{1}{2} \leftarrow 9\frac{1}{2}$	*e*	295 485.551	
		f	295 488.380	
	$11\frac{1}{2} \leftarrow 10\frac{1}{2}$	*e*	295 528.973	
		f	295 531.790	
12 ← 11	$11\frac{1}{2} \leftarrow 10\frac{1}{2}$	*e*	322 316.985	
		f	322 321.509	
	$12\frac{1}{2} \leftarrow 11\frac{1}{2}$	*e*	322 359.452	
		f	322 363.891	
13 ← 12	$12\frac{1}{2} \leftarrow 11\frac{1}{2}$	*e*	349 139.668	
		f	349 146.450	
	$13\frac{1}{2} \leftarrow 12\frac{1}{2}$	*e*	349 181.205	
		f	349 962.569	
13 ← 12	$13\frac{1}{2} \leftarrow 12\frac{1}{2}$	*e*	375 952.805	
		f	375 962.569	
	$14\frac{1}{2} \leftarrow 13\frac{1}{2}$	*e*	375 993.740	
		f	376 004.015	
16 ← 15	$15\frac{1}{2} \leftarrow 14\frac{1}{2}$	*e*	429 547.816	
	$16\frac{1}{2} \leftarrow 15\frac{1}{2}$	*f*	429 606.416	
17 ← 16	$16\frac{1}{2} \leftarrow 15\frac{1}{2}$	*e*	456 328.166	
	$17\frac{1}{2} \leftarrow 16\frac{1}{2}$	*f*	456 392.774	
19 ← 18	$18\frac{1}{2} \leftarrow 17\frac{1}{2}$	*e*	509 851.243	
	$19\frac{1}{2} \leftarrow 18\frac{1}{2}$	*f*	509 932.792	
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational $(0,4^4,0)$, $^2\Gamma$ vibronic component				
10 ← 9	$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	*e*	268 469.533	99Ap
		f	268 469.533	
	$10\frac{1}{2} \leftarrow 9\frac{1}{2}$	*e*	268 520.382	
		f	268 520.382	
11 ← 10	$10\frac{1}{2} \leftarrow 9\frac{1}{2}$	*e*	295 290.553	

		f	295 290.553
	$11\frac{1}{2} \leftarrow 10\frac{1}{2}$	*e*	295 339.135
		f	295 339.135
$12 \leftarrow 11$	$11\frac{1}{2} \leftarrow 10\frac{1}{2}$	*e*	322 102.897
		f	322 102.897
	$12\frac{1}{2} \leftarrow 11\frac{1}{2}$	*e*	322 149.711
		f	322 149.711
$13 \leftarrow 12$	$12\frac{1}{2} \leftarrow 11\frac{1}{2}$	*e*	348 906.034
		f	348 906.034
	$13\frac{1}{2} \leftarrow 12\frac{1}{2}$	*e*	348 951.492
		f	348 951.492
$17 \leftarrow 16$	$16\frac{1}{2} \leftarrow 15\frac{1}{2}$	*e*	456 012.589
		f	456 014.956
	$17\frac{1}{2} \leftarrow 16\frac{1}{2}$	*e*	459 054.733
		f	456 056.970
$18 \leftarrow 17$	$17\frac{1}{2} \leftarrow 16\frac{1}{2}$	*e*	482 759.931
		f	482 762.956
	$18\frac{1}{2} \leftarrow 17\frac{1}{2}$	*e*	482 801.516
		f	482 804.654
$19 \leftarrow 18$	$18\frac{1}{2} \leftarrow 17\frac{1}{2}$	*e*	509 494.152
		f	509 498.628
	$19\frac{1}{2} \leftarrow 18\frac{1}{2}$	*e*	509 535.345
		f	509 539.759

[a]) States with parity equal to $\pm(-1)^{J-0.5}$ are labeled *e* and *f* respectively.

Molecular parameters for $^{24}Mg^{16}O^{2}H$ (MgOD)

Parameter		Value	Method	Ref.
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (0,0,0)				
B	[MHz]	13 438.500 1(54) [a])	MW	95Nu
D	[kHz]	19.897(19)		
γ	[MHz]	33.69(19)		
γ_D	[kHz]	− 0.1(5)		
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational $(0,1^1,0)$, $^2\Pi$ vibronic component				
B	[MHz]	13 446.403 6(662) [a])	MW	95Nu
D	[kHz]	20.263(19)		
γ	[MHz]	36.78(25)		
γ_D	[kHz]	− 2.0(6)		
q	[MHz]	− 100.883(12)		
q_D	[kHz]	1.463(39)		
p_Π [d])	[MHz]	1.69(15)		
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational $(0,2^0,0)$, $^2\Sigma$ vibronic component				
B	[MHz]	13 483.435(11) [a]), [b])	MW	99Ap
D	[kHz]	21.470(50)		
γ	[MHz]	36.68(59)		
γ_D	[kHz]	1.3(17)		

State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (0,2^2,0), $^2\Delta$ vibronic component				
B	[MHz]	13 444.686 4(89) [a])	MW	99Ap
D	[kHz]	20.106(44)		
H	[Hz]	– 0.065(65)		
γ	[MHz]	40.51(15)		
γ_D	[kHz]	– 3.77(23)		
q	[MHz]	– 84.601(39)		
q_D	[kHz]	1.015(94)		
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (0,3^1,0), $^2\Pi$ vibronic component				
B	[MHz]	13 498.765 5(81) [a])	MW	99Ap
D	[kHz]	21.271(37)		
H	[Hz]	– 0.131(52)		
γ	[MHz]	37.35(14)		
γ_D	[kHz]	– 0.81(19)		
q	[MHz]	– 78.271 6(82)		
q_D	[kHz]	1.073(38)		
p_Π [d])	[MHz]	3.94(30)		
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (0,3^3,0), $^2\Phi$ vibronic component				
B	[MHz]	13 439.008 4(83) [a])	MW	99Ap
D	[kHz]	20.380(40)		
H	[Hz]	– 0.069(59)		
γ	[MHz]	47.16(24)		
γ_D	[kHz]	– 9.02(51)		
ρ [c])	[kHz]	– 0.332(54)		
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (0,4^4,0), $^2\Gamma$ vibronic component				
B	[MHz]	13 430.195 7(77) [a])	MW	99Ap
D	[kHz]	32.673(41)		
H	[Hz]	– 1.920(61)		
γ	[MHz]	52.53(14)		
γ_D	[kHz]	– 11.30(19)		
q	[Hz]	– 50.1(93)		
q_D	[Hz]	0.245(19)		
p_Γ [d])	[kHz]	– 3.0(280)		

[a]) The numbers in parenthesis are 3 standard deviations of the least-squares fit, in units of the last quoted decimal place.
[b]) The separation between the $v = 2$, $l = 0$ and ±2 levels, $4g_{22}$, was constrained to 11.8 cm^{-1} [95Bu] in the least-squares fit.
[c]) ρ is a higher-order l-type resonance parameter used to account for the splittings in the 3^3 states.
[d]) This parameter takes care of the different spin-rotation splittings in the l-type doubling components.

References for MgOH

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3.2.1.2.36 CaOH

Microwave data for $^{40}Ca^{16}O^{1}H$

Transition rotational $N' - N''$	fine structure $J' - J''$	Hyperfine [a]) $F' - F''$	ν [MHz]	Ref.
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (0,0,0)				
1← 0	$1\frac{1}{2} \leftarrow \frac{1}{2}$	1 ← 0	20 064.518	93Sc
		2 ← 1	20 063.429	
		1 ← 1	20 061.918	
	$\frac{1}{2} \leftarrow \frac{1}{2}$	1 ← 1	20 010.674	
		0 ← 1	20 010.674	
		1 ← 0	20 013.288	
2← 1	$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	3 ← 2	40 109.319	
		2 ← 1	40 109.534	
		2 ← 2	40 108.016	
	$1\frac{1}{2} \leftarrow 1\frac{1}{2}$	1 ← 1	40 023.691	
		1 ← 2	40 022.184	
		2 ← 1	40 023.172	
		2 ← 2	40 021.658	
3 ← 2	$2\frac{1}{2} \leftarrow 2\frac{1}{2}$	3 ← 3	60 032.144	
		2 ← 2	60 034.101	
	$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	4 ← 3	60 154.618	
		3 ← 2	60 154.715	
		3 ← 3	60 153.414	
	$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	2 ← 2	60 120.467	
4 ← 3	$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	[b])	80 164.301	92Zi
	$4\frac{1}{2} \leftarrow 3\frac{1}{2}$	[b])	80 199.073	
5 ← 4	$4\frac{1}{2} \leftarrow 3\frac{1}{2}$	[b])	100 207.681	
	$5\frac{1}{2} \leftarrow 4\frac{1}{2}$	[b])	100 242.455	
7 ← 6	$6\frac{1}{2} \leftarrow 5\frac{1}{2}$	[b])	140 289.927	
	$7\frac{1}{2} \leftarrow 6\frac{1}{2}$	[b])	140 324.681	
8 ← 7	$7\frac{1}{2} \leftarrow 6\frac{1}{2}$	[b])	160 328.270	
	$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	[b])	160 363.033	
9 ← 8	$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	[b])	180 364.388	
	$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	[b])	180 399.159	
11 ← 10	$10\frac{1}{2} \leftarrow 9\frac{1}{2}$	[b])	220 428.859	
	$11\frac{1}{2} \leftarrow 10\frac{1}{2}$	[b])	220 463.642	
12 ← 11	$11\frac{1}{2} \leftarrow 10\frac{1}{2}$	[b])	240 456.666	
	$12\frac{1}{2} \leftarrow 11\frac{1}{2}$	[b])	240 491.427	
13 ← 12	$12\frac{1}{2} \leftarrow 11\frac{1}{2}$	[b])	260 481.120	
	$13\frac{1}{2} \leftarrow 12\frac{1}{2}$	[b])	260 515.886	
14 ← 13	$13\frac{1}{2} \leftarrow 12\frac{1}{2}$	[b])	280 501.959	
	$14\frac{1}{2} \leftarrow 13\frac{1}{2}$	[b])	280 538.734	
15 ← 14	$14\frac{1}{2} \leftarrow 13\frac{1}{2}$	[b])	300 518.942	
	$15\frac{1}{2} \leftarrow 14\frac{1}{2}$	[b])	300 553.690	
16 ← 15	$15\frac{1}{2} \leftarrow 14\frac{1}{2}$	[b])	320 531.736	

	$16\frac{1}{2} \leftarrow 15\frac{1}{2}$	[b])	320 566.491	
$17 \leftarrow 16$	$16\frac{1}{2} \leftarrow 15\frac{1}{2}$	[b])	340 540.102	96Zi
	$17\frac{1}{2} \leftarrow 16\frac{1}{2}$	[b])	340 574.859	
$18 \leftarrow 17$	$17\frac{1}{2} \leftarrow 16\frac{1}{2}$	[b])	360 543.716	
	$18\frac{1}{2} \leftarrow 17\frac{1}{2}$	[b])	360 578.481	
$19 \leftarrow 18$	$18\frac{1}{2} \leftarrow 17\frac{1}{2}$	[b])	380 542.363	
	$19\frac{1}{2} \leftarrow 18\frac{1}{2}$	[b])	380 577.124	

[a]) Coupling scheme: $\boldsymbol{J} = \boldsymbol{N} + \boldsymbol{S}$; $\boldsymbol{F} = \boldsymbol{J} + \boldsymbol{I}_1$ where $\boldsymbol{I}_1$ is the ^{1}H nuclear spin.
[b]) Hyperfine structure not resolved.

Microwave data for ^{40}Ca^{16}O^{1}H

Transition			ν	Ref.
Rotational $N' - N''$	rotational $J' - J''$	parity e/f [a])	[MHz]	
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (0,1^1,0), $^2\Pi$ vibronic component				
$14 \leftarrow 13$	$13\frac{1}{2} \leftarrow 12\frac{1}{2}$	f	280 065.719	95Fl, 96Zi
	$14\frac{1}{2} \leftarrow 13\frac{1}{2}$	e	279 495.367	
		f	280 100.792	
$15 \leftarrow 14$	$14\frac{1}{2} \leftarrow 13\frac{1}{2}$	e	299 402.512	
		f	300 051.164	
	$15\frac{1}{2} \leftarrow 14\frac{1}{2}$	e	299 437.633	
		f	300 086.199	
$16 \leftarrow 15$	$15\frac{1}{2} \leftarrow 14\frac{1}{2}$	e	319 340.561	
		f	320 032.317	
	$16\frac{1}{2} \leftarrow 15\frac{1}{2}$	e	319 375.611	
		f	320 067.368	
$17 \leftarrow 16$	$16\frac{1}{2} \leftarrow 15\frac{1}{2}$	e	339 274.132	
		f	340 008.960	
	$17\frac{1}{2} \leftarrow 16\frac{1}{2}$	e	339 309.193	
		f	340 043.978	
$18 \leftarrow 17$	$17\frac{1}{2} \leftarrow 16\frac{1}{2}$	e	359 202.902	
		f	359 980.800	
	$18\frac{1}{2} \leftarrow 17\frac{1}{2}$	e	359 237.955	
		f	360 015.787	
$19 \leftarrow 18$	$18\frac{1}{2} \leftarrow 17\frac{1}{2}$	e	379 126.575	
		f	379 947.507	
	$19\frac{1}{2} \leftarrow 18\frac{1}{2}$	e	379 161.634	
		f	379 982.497	
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (0,2^0,0), $^2\Sigma$ vibronic component				
$14 \leftarrow 13$	$13\frac{1}{2} \leftarrow 12\frac{1}{2}$	f	279 364.005	95Fl, 96Zi
	$14\frac{1}{2} \leftarrow 13\frac{1}{2}$	e	279 399.015	
$15 \leftarrow 14$	$14\frac{1}{2} \leftarrow 13\frac{1}{2}$	f	299 297.922	
	$15\frac{1}{2} \leftarrow 14\frac{1}{2}$	e	299 332.961	
$16 \leftarrow 15$	$15\frac{1}{2} \leftarrow 14\frac{1}{2}$	f	319 227.345	
	$16\frac{1}{2} \leftarrow 15\frac{1}{2}$	e	319 262.362	
$17 \leftarrow 16$	$16\frac{1}{2} \leftarrow 15\frac{1}{2}$	f	339 151.879	
	$17\frac{1}{2} \leftarrow 16\frac{1}{2}$	e	339 186.930	
$18 \leftarrow 17$	$17\frac{1}{2} \leftarrow 16\frac{1}{2}$	f	359 071.300	

	$18\frac{1}{2} \leftarrow 17\frac{1}{2}$	*e*	359 106.442	
19 ← 18	$18\frac{1}{2} \leftarrow 17\frac{1}{2}$	*f*	378 985.347	
	$19\frac{1}{2} \leftarrow 18\frac{1}{2}$	*e*	379 020.360	
State: electronic $\widetilde{X}\,^2\Sigma^+$; vibrational $(0,2^2,0)$, $^2\Delta$ vibronic component				
14 ← 13	$13\frac{1}{2} \leftarrow 12\frac{1}{2}$	*e*	278 996.912	95Fl, 96Zi
		f	279 004.035	
	$14\frac{1}{2} \leftarrow 13\frac{1}{2}$	*e*	279 032.651	
		f	279 039.766	
15 ← 14	$14\frac{1}{2} \leftarrow 13\frac{1}{2}$	*e*	298 905.831	
		f	298 914.579	
	$15\frac{1}{2} \leftarrow 14\frac{1}{2}$	*e*	298 941.486	
		f	298 950.239	
16 ← 15	$15\frac{1}{2} \leftarrow 14\frac{1}{2}$	*e*	318 810.426	
		f	318 821.068	
	$16\frac{1}{2} \leftarrow 15\frac{1}{2}$	*e*	318 846.017	
		f	318 856.644	
17 ← 16	$16\frac{1}{2} \leftarrow 15\frac{1}{2}$	*e*	338 710.386	
		f	338 723.190	
	$17\frac{1}{2} \leftarrow 16\frac{1}{2}$	*e*	338 745.989	
		f	338 758.765	
18 ← 17	$17\frac{1}{2} \leftarrow 16\frac{1}{2}$	*e*	358 605.597	
		f	358 620.789	
	$18\frac{1}{2} \leftarrow 17\frac{1}{2}$	*e*	358 641.079	
		f	358 656.232	
19 ← 18	$18\frac{1}{2} \leftarrow 17\frac{1}{2}$	*e*	378 495.614	
		f	378 513.425	
	$19\frac{1}{2} \leftarrow 18\frac{1}{2}$	*e*	378 530.970	
		f	378 548.844	
State: electronic $\widetilde{X}\,^2\Sigma^+$; vibrational $(1,0,0)$, $^2\Pi$ vibronic component				
14 ← 13	$13\frac{1}{2} \leftarrow 12\frac{1}{2}$	*f*	278 632.967	95Fl, 96Zi
	$14\frac{1}{2} \leftarrow 13\frac{1}{2}$	*e*	278 667.515	
15 ← 14	$14\frac{1}{2} \leftarrow 13\frac{1}{2}$	*f*	298 516.278	
	$15\frac{1}{2} \leftarrow 14\frac{1}{2}$	*e*	298 550.835	
16 ← 15	$15\frac{1}{2} \leftarrow 14\frac{1}{2}$	*f*	318 395.303	
	$16\frac{1}{2} \leftarrow 15\frac{1}{2}$	*e*	318 429.849	
17 ← 16	$16\frac{1}{2} \leftarrow 15\frac{1}{2}$	*f*	338 269.998	
	$17\frac{1}{2} \leftarrow 16\frac{1}{2}$	*e*	338 304.567	
18 ← 17	$17\frac{1}{2} \leftarrow 16\frac{1}{2}$	*f*	358 139.925	
	$18\frac{1}{2} \leftarrow 17\frac{1}{2}$	*e*	358 174.481	
19 ← 18	$18\frac{1}{2} \leftarrow 17\frac{1}{2}$	*f*	378 004.834	
	$19\frac{1}{2} \leftarrow 18\frac{1}{2}$	*e*	378 039.349	

[a]) States with parity equal to $\pm(-1)^{J-0.5}$ are labeled *e* and *f* respectively.

Molecular parameters for $^{40}Ca^{16}O\,^{1}H$

Parameter		Value	Method	Ref.
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (0,0,0)				
B	[MHz]	10 023.084 1(10) [a])	MW	92Zi, 95Fl
D	[kHz]	11.570 7 (20)		
γ	[MHz]	34.765(19)		
$b_F(^1H)$	[MHz]	2.602(3)	MODR	93Sc
$c(^1H)$	[MHz]	2.053(10)		
μ	[D]	1.465(61)	OS	92St
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational $(0,1^1,0)$, $^2\Pi$ vibronic component				
B	[MHz]	9 996.751 8(17) [a])	MW	95Fl
D	[kHz]	11.769 6(29)		
γ	[MHz]	35.051(21)		
q	[MHz]	– 21.649 2(34)		
q_D	[kHz]	0.064(6)		
p_Π [b])	[MHz]	– 0.050(42)		
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational $(0,2^0,0)$, $^2\Sigma$ vibronic component				
B	[MHz]	9 982.838 7(23) [a])	MW	95Fl
D	[kHz]	11.923 9(40)		
γ	[MHz]	35.045(29)		
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational $(0,2^2,0)$, $^2\Delta$ vibronic component				
B	[MHz]	9 969.396 7(16) [a])	MW	95Fl
D	[kHz]	11.933 9(28)		
γ	[MHz]	35.569(20)		
q	[MHz]	– 21.131(17)		
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (1,0,0), $^2\Sigma$ vibronic component				
B	[MHz]	9 956.359 3(23) [a])	MW	95Fl
D	[kHz]	11.648 4(39)		
γ	[MHz]	34.549(29)		

[a]) The numbers in parenthesis are 3 standard deviations of the least-squares fit, in units of the last quoted decimal place.
[b]) This parameter takes care of the different spin-rotation splittings in the l-type doubling components.

Microwave data for $^{40}Ca^{16}O^{2}H$ (CaOD)

Transition			ν	Ref.
rotational $N' - N''$	fine structure $J' - J''$	Parity [a])	[MHz]	
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (0,0,0)				
11 ← 10	$10\frac{1}{2} \leftarrow 9\frac{1}{2}$	f	199 766.521	95Nu
	$11\frac{1}{2} \leftarrow 10\frac{1}{2}$	e	199 798.046	
12 ← 11	$11\frac{1}{2} \leftarrow 10\frac{1}{2}$	f	217 918.780	
	$12\frac{1}{2} \leftarrow 11\frac{1}{2}$	e	217 950.289	
13 ← 12	$12\frac{1}{2} \leftarrow 11\frac{1}{2}$	f	236 068.507	
	$13\frac{1}{2} \leftarrow 12\frac{1}{2}$	e	236 099.976	
14 ← 13	$13\frac{1}{2} \leftarrow 12\frac{1}{2}$	f	254 215.464	
	$14\frac{1}{2} \leftarrow 13\frac{1}{2}$	e	254 246.996	
15 ← 14	$14\frac{1}{2} \leftarrow 13\frac{1}{2}$	f	272 359.435	
	$15\frac{1}{2} \leftarrow 14\frac{1}{2}$	e	272 391.012	
16 ← 15	$15\frac{1}{2} \leftarrow 14\frac{1}{2}$	f	290 500.287	

	$16\frac{1}{2} \leftarrow 15\frac{1}{2}$	*e*	290 531.785	
17 ← 16	$16\frac{1}{2} \leftarrow 15\frac{1}{2}$	*f*	308 637.702	
	$17\frac{1}{2} \leftarrow 16\frac{1}{2}$	*e*	308 669.199	
18 ← 17	$17\frac{1}{2} \leftarrow 16\frac{1}{2}$	*f*	326 771.527	
	$18\frac{1}{2} \leftarrow 17\frac{1}{2}$	*e*	326 803.016	
19 ← 18	$18\frac{1}{2} \leftarrow 17\frac{1}{2}$	*f*	344 901.51	
	$19\frac{1}{2} \leftarrow 18\frac{1}{2}$	*e*	344 933.016	
20 ← 19	$19\frac{1}{2} \leftarrow 18\frac{1}{2}$	*f*	363 027.477	
	$20\frac{1}{2} \leftarrow 19\frac{1}{2}$	*e*	363 059.004	
21 ← 20	$20\frac{1}{2} \leftarrow 19\frac{1}{2}$	*f*	381 149.166	
	$21\frac{1}{2} \leftarrow 20\frac{1}{2}$	*e*	381 180.697	
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (1,0,0) $^2\Sigma$ vibronic component				
18 ← 17	$17\frac{1}{2} \leftarrow 16\frac{1}{2}$	*f*	324 766.053	95Nu
	$18\frac{1}{2} \leftarrow 17\frac{1}{2}$	*e*	324 797.015	
19 ← 18	$18\frac{1}{2} \leftarrow 17\frac{1}{2}$	*f*	342 784.299	
	$19\frac{1}{2} \leftarrow 18\frac{1}{2}$	*e*	342 815.568	
20 ← 19	$19\frac{1}{2} \leftarrow 18\frac{1}{2}$	*f*	360 798.825	
	$20\frac{1}{2} \leftarrow 19\frac{1}{2}$	*e*	360 830.085	
21 ← 20	$20\frac{1}{2} \leftarrow 19\frac{1}{2}$	*f*	378 809.157	
	$21\frac{1}{2} \leftarrow 20\frac{1}{2}$	*e*	378 840.365	
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (0,1^1,0) $^2\Pi$ vibronic component				
18 ← 17	$17\frac{1}{2} \leftarrow 16\frac{1}{2}$	*e*	326 433.326	95Nu
		f	327 258.425	
	$18\frac{1}{2} \leftarrow 17\frac{1}{2}$	*e*	326 465.303	
		f	327 290.199	
19 ← 18	$18\frac{1}{2} \leftarrow 17\frac{1}{2}$	*e*	344 544.407	
		f	345 414.948	
	$19\frac{1}{2} \leftarrow 18\frac{1}{2}$	*e*	344 576.488	
		f	345 446.620	
20 ← 19	$19\frac{1}{2} \leftarrow 18\frac{1}{2}$	*e*	362 651.057	
		f	363 567.235	
	$20\frac{1}{2} \leftarrow 19\frac{1}{2}$	*e*	362 682.927	
		f	363 598.921	
21 ← 20	$20\frac{1}{2} \leftarrow 19\frac{1}{2}$	*e*	380 753.725	
		f	381 715.115	
	$21\frac{1}{2} \leftarrow 20\frac{1}{2}$	*e*	380 785.474	
		f	381 736.833	
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (0,2^0,0) $^2\Sigma$ vibronic component				
18 ← 17	$17\frac{1}{2} \leftarrow 16\frac{1}{2}$	*f*	327 108.595	95Nu
	$18\frac{1}{2} \leftarrow 17\frac{1}{2}$	*e*	327 140.451	
19 ← 18	$18\frac{1}{2} \leftarrow 17\frac{1}{2}$	*f*	345 252.891	
	$19\frac{1}{2} \leftarrow 18\frac{1}{2}$	*e*	345 284.822	
20 ← 19	$19\frac{1}{2} \leftarrow 18\frac{1}{2}$	*f*	363 392.519	
	$20\frac{1}{2} \leftarrow 19\frac{1}{2}$	*e*	363 424.393	
21 ← 20	$20\frac{1}{2} \leftarrow 19\frac{1}{2}$	*f*	381 526.877	
	$21\frac{1}{2} \leftarrow 20\frac{1}{2}$	*e*	381 558.874	

State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational $(0,2^2,0)$ $^2\Delta$ vibronic component				
18 ← 17	$17\frac{1}{2} \leftarrow 16\frac{1}{2}$	*e*	326 878.395	95Nu
		f	326 905.271	
	$18\frac{1}{2} \leftarrow 17\frac{1}{2}$	*e*	326 910.522	
		f	326 937.363	
19 ← 18	$18\frac{1}{2} \leftarrow 17\frac{1}{2}$	*e*	345 013.302	
		f	345 045.325	
	$19\frac{1}{2} \leftarrow 18\frac{1}{2}$	*e*		
		f	345 077.216	
20 ← 19	$19\frac{1}{2} \leftarrow 18\frac{1}{2}$	*e*	363 144.400	
		f	363 181.190	
	$20\frac{1}{2} \leftarrow 19\frac{1}{2}$	*e*	363 176.522	
		f	363 213.261	
21 ← 20	$20\frac{1}{2} \leftarrow 19\frac{1}{2}$	*e*	381 270.963	
		f	381 313.523	

[a]) States with parity equal to ± $(-1)^{J-0.5}$ are labeled *e* and *f* respectively

Molecular parameters for $^{40}Ca^{16}O^{2}H$ (CaOD)

Parameter		Value	Method	Ref.
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (0,0,0)				
B	[MHz]	9 083.151 2(32) [a])	MW	95Nu
D	[kHz]	8.838 3(51)		
γ	[MHz]	31.514(64)		
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (1,0,0) $^2\Sigma$ vibronic component				
B	[MHz]	9 027.444(12) [a])	MW	95Nu
D	[kHz]	8.852(16)		
γ	[MHz]	30.48(93)		
γ_D	[kHz]	0.61(81)		
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational $(0,1^1,0)$ $^2\Pi$ vibronic component				
B	[MHz]	9 085.316 8(86) [a])	MW	95Nu
D	[kHz]	9.010(11)		
γ	[MHz]	32.33(66)		
γ_D	[kHz]	– 0.45(57)		
q	[MHz]	– 22.983(17)		
q_D	[kHz]	0.104(22)		
p_Π [b])	[MHz]	– 0.21(15)		
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational $(0,2^0,0)$ $^2\Sigma$ vibronic component				
B	[MHz]	9 093.536(12) [a])	MW	95Nu
D	[kHz]	9.255(16)		
γ	[MHz]	32.03(11)		
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational $(0,2^2,0)$ $^2\Delta$ vibronic component				
B	[MHz]	9 086.264 3(87) [a])	MW	95Nu
D	[kHz]	9.159(11)		
γ	[MHz]	32.139(78)		
q	[MHz]	– 23.425(25)		

[a]) The numbers in parenthesis are 3 standard deviations of the least-squares fit, in units of the last quoted decimal place.
[b]) This parameter takes care of the different spin-rotation splittings in the l-type doubling components.

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92St Steimle, T.C., Fletcher, D.A., Jung, K.Y., Scurlock, C.T. : J. Chem. Phys. **96** (1992) 2556.
92Zi Ziurys, L.M., Barclay, W.L., Anderson, M.A. : Astrophys. J. **384** (1992) L63.
93Sc Scurlock, C.T., Fletcher, D.A., Steimle, T.C. : J. Mol. Spectrosc. **159** (1993) 350.
95Fl Fletcher, D.A., Anderson, M.A., Barclay, W.L., Ziurys, L.M.: J. Chem. Phys. **102** (1995) 4334.
95Nu Nuccio, B.P., Apponi, A.J., Ziurys, L.M.: J. Chem. Phys. **103** (1995) 9193.
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3.2.1.2.37 SrOH

Microwave data for $^{88}Sr^{16}O^{1}H$

Transition rotational $N' - N''$	fine structure $J' - J''$	Hyperfine [a]) $F' - F''$	ν [MHz]	Ref.
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (0,0,0)				
1← 0	$1\frac{1}{2} \leftarrow \frac{1}{2}$	1 ← 1	14 976.934	93Fl
		2 ← 1	14 977.917	
		1 ← 0	14 978.646	
	$\frac{1}{2} \leftarrow \frac{1}{2}$	1 ← 1	14 868.511	
		0 ← 1	14 868.346	
		1 ← 0	14 870.225	
2← 1	$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	2 ← 2	29 918.580	
		3 ← 2	29 919.411	
		2 ← 1	29 919.566	
	$1\frac{1}{2} \leftarrow 1\frac{1}{2}$	2 ← 2	29 737.186	
		1 ← 2	28 737.427	
		2 ← 1	29 738.165	
		1 ← 1	29 738.416	
	$1\frac{1}{2} \leftarrow 1\frac{1}{2}$	1 ← 0	29 846.992	
		2 ← 1	29 846.586	
		1 ← 1	29 846.831	
3 ← 2	$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	3 ← 2	44 787.825	
		2 ← 1	44 787.937	
		2 ← 2	44 788.178	
	$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	3 ← 2	44 860.654	
		4 ← 3	44 860.586	
		3 ← 3	44 859.825	
6 ← 5	$5\frac{1}{2} \leftarrow 4\frac{1}{2}$	[b])	89 607.872	92An
	$6\frac{1}{2} \leftarrow 5\frac{1}{2}$	[b])	89 680.597	
7 ← 6	$6\frac{1}{2} \leftarrow 5\frac{1}{2}$	[b])	104 546.194	
	$7\frac{1}{2} \leftarrow 6\frac{1}{2}$	[b])	104 618.922	
9 ← 8	$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	[b])	134 419.461	
	$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	[b])	134 492.186	
10 ← 9	$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	[b])	149 354.008	
	$10\frac{1}{2} \leftarrow 9\frac{1}{2}$	[b])	149 426.760	
11 ← 10	$10\frac{1}{2} \leftarrow 9\frac{1}{2}$	[b])	164 287.027	
	$11\frac{1}{2} \leftarrow 10\frac{1}{2}$	[b])	164 359.769	

$12 \leftarrow 11$	$11\frac{1}{2} \leftarrow 10\frac{1}{2}$	[b])	179 218.294
	$12\frac{1}{2} \leftarrow 11\frac{1}{2}$	[b])	179 291.031
$13 \leftarrow 12$	$12\frac{1}{2} \leftarrow 11\frac{1}{2}$	[b])	194 147.725
	$13\frac{1}{2} \leftarrow 12\frac{1}{2}$	[b])	194 220.467
$14 \leftarrow 13$	$13\frac{1}{2} \leftarrow 12\frac{1}{2}$	[b])	209 075.093
	$14\frac{1}{2} \leftarrow 13\frac{1}{2}$	[b])	209 147.865
$15 \leftarrow 14$	$14\frac{1}{2} \leftarrow 13\frac{1}{2}$	[b])	224 000.282
	$15\frac{1}{2} \leftarrow 14\frac{1}{2}$	[b])	224 073.091
$16 \leftarrow 15$	$15\frac{1}{2} \leftarrow 14\frac{1}{2}$	[b])	238 923.121
	$16\frac{1}{2} \leftarrow 15\frac{1}{2}$	[b])	238 995.898
$17 \leftarrow 16$	$16\frac{1}{2} \leftarrow 15\frac{1}{2}$	[b])	253 843.472
	$17\frac{1}{2} \leftarrow 16\frac{1}{2}$	[b])	253 916.241
$18 \leftarrow 17$	$17\frac{1}{2} \leftarrow 16\frac{1}{2}$	[b])	268 761.163
	$18\frac{1}{2} \leftarrow 17\frac{1}{2}$	[b])	268 833.924
$19 \leftarrow 18$	$18\frac{1}{2} \leftarrow 17\frac{1}{2}$	[b])	283 676.005
	$19\frac{1}{2} \leftarrow 18\frac{1}{2}$	[b])	283 748.806
$20 \leftarrow 19$	$19\frac{1}{2} \leftarrow 18\frac{1}{2}$	[b])	298 587.908
	$20\frac{1}{2} \leftarrow 19\frac{1}{2}$	[b])	298 660.700
$21 \leftarrow 20$	$20\frac{1}{2} \leftarrow 19\frac{1}{2}$	[b])	313 496.668
	$21\frac{1}{2} \leftarrow 20\frac{1}{2}$	[b])	313 569.467
$22 \leftarrow 21$	$21\frac{1}{2} \leftarrow 20\frac{1}{2}$	[b])	328 402.151
	$22\frac{1}{2} \leftarrow 21\frac{1}{2}$	[b])	328 474.959
$23 \leftarrow 22$	$22\frac{1}{2} \leftarrow 21\frac{1}{2}$	[b])	343 304.173
	$23\frac{1}{2} \leftarrow 22\frac{1}{2}$	[b])	343 376.996
$24 \leftarrow 23$	$23\frac{1}{2} \leftarrow 22\frac{1}{2}$	[b])	358 202.620
	$24\frac{1}{2} \leftarrow 23\frac{1}{2}$	[b])	358 275.433
$25 \leftarrow 24$	$24\frac{1}{2} \leftarrow 23\frac{1}{2}$	[b])	373 097.295
	$25\frac{1}{2} \leftarrow 24\frac{1}{2}$	[b])	373 170.128

[a]) Coupling scheme: $\boldsymbol{J} = \boldsymbol{N} + \boldsymbol{S}$; $\boldsymbol{F} = \boldsymbol{J} + \boldsymbol{I}_1$ where $\boldsymbol{I}_1$ is the ^{1}H nuclear spin.
[b]) Hyperfine structure not resolved.

Microwave data for $^{88}Sr^{16}O^1H$

Transition			ν	Ref.
rotational $N' - N''$	rotational $J' - J''$	parity e/f [a])	[MHz]	
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (0,1^1,0), $^2\Pi$ vibronic component				
$21 \leftarrow 20$	$20\frac{1}{2} \leftarrow 19\frac{1}{2}$	*e*	312 464.538	96Zi
		f	312 962.023	
	$21\frac{1}{2} \leftarrow 20\frac{1}{2}$	*e*	312 537.268	
		f	313 033.734	
$22 \leftarrow 21$	$21\frac{1}{2} \leftarrow 20\frac{1}{2}$	*e*	327 320.513	
		f	327 841.571	
	$22\frac{1}{2} \leftarrow 21\frac{1}{2}$	*e*	327 393.256	
		f	327 913.292	
$23 \leftarrow 22$	$22\frac{1}{2} \leftarrow 21\frac{1}{2}$	*e*	342 172.981	
		f	342 717.620	
	$23\frac{1}{2} \leftarrow 22\frac{1}{2}$	*e*	342 245.744	

		f	342 789.330	
24 ← 23	$23\frac{1}{2} \leftarrow 22\frac{1}{2}$	*e*	357 021.822	
		f	357 589.994	
	$24\frac{1}{2} \leftarrow 23\frac{1}{2}$	*e*	357 094.594	
		f	357 661.716	
25 ← 24	$24\frac{1}{2} \leftarrow 23\frac{1}{2}$	*e*	371 866.844	
		f	372 458.544	
	$25\frac{1}{2} \leftarrow 24\frac{1}{2}$	*e*	371 939.625	
		f	372 530.295	
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational $(0,2^0,0)$, $^2\Sigma$ vibronic component				
21 ← 20	$20\frac{1}{2} \leftarrow 19\frac{1}{2}$	*f*	312 230.547	96Zi
	$21\frac{1}{2} \leftarrow 20\frac{1}{2}$	*e*	312 302.245	
22 ← 21	$21\frac{1}{2} \leftarrow 20\frac{1}{2}$	*f*	327 074.286	
	$22\frac{1}{2} \leftarrow 21\frac{1}{2}$	*e*	327 146.013	
23 ← 22	$22\frac{1}{2} \leftarrow 21\frac{1}{2}$	*f*	341 914.400	
	$23\frac{1}{2} \leftarrow 22\frac{1}{2}$	*e*	341 986.139	
24 ← 23	$23\frac{1}{2} \leftarrow 22\frac{1}{2}$	*f*	356 750.707	
	$24\frac{1}{2} \leftarrow 23\frac{1}{2}$	*e*	356 822.451	
25 ← 24	$24\frac{1}{2} \leftarrow 23\frac{1}{2}$	*f*	371 583.047	
	$25\frac{1}{2} \leftarrow 24\frac{1}{2}$	*e*	371 654.821	
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational $(0,2^2,0)$, $^2\Delta$ vibronic component				
21 ← 20	$20\frac{1}{2} \leftarrow 19\frac{1}{2}$	*e*	311 915.648	96Zi
		f	311 921.687	
	$21\frac{1}{2} \leftarrow 20\frac{1}{2}$	*e*	311 987.218	
		f	311 993.217	
22 ← 21	$21\frac{1}{2} \leftarrow 20\frac{1}{2}$	*e*	326 745.038	
		f	326 751.996	
	$22\frac{1}{2} \leftarrow 21\frac{1}{2}$	*e*	326 816.637	
		f	326 823.565	
23 ← 22	$22\frac{1}{2} \leftarrow 21\frac{1}{2}$	*e*	341 570.881	
		f	341 578.850	
	$23\frac{1}{2} \leftarrow 22\frac{1}{2}$	*e*	341 642.493	
		f	341 650.407	
24 ← 23	$23\frac{1}{2} \leftarrow 22\frac{1}{2}$	*e*	356 393.034	
		f	356 402.981	
	$24\frac{1}{2} \leftarrow 23\frac{1}{2}$	*e*	356 464.656	
		f	356 473.633	
25 ← 24	$24\frac{1}{2} \leftarrow 23\frac{1}{2}$	*e*	371 211.302	
		f	371 221.538	
	$25\frac{1}{2} \leftarrow 24\frac{1}{2}$	*e*	371 282.944	
		f	371 293.174	
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational $(0,3^1,0)$, $^2\Pi$ vibronic component				
21 ← 20	$20\frac{1}{2} \leftarrow 19\frac{1}{2}$	*e*	311 230.959	96Zi
		f	312 277.882	
	$21\frac{1}{2} \leftarrow 20\frac{1}{2}$	*e*	311 302.799	
		f	312 348.142	
22 ← 21	$21\frac{1}{2} \leftarrow 20\frac{1}{2}$	*e*	326 027.213	
		f	327 123.741	
	$22\frac{1}{2} \leftarrow 21\frac{1}{2}$	*e*	326 099.270	

		f	327 194.004	
23 ← 22	$22\frac{1}{2} \leftarrow 21\frac{1}{2}$	e	340 819.878	
		f	341 965.941	
	$23\frac{1}{2} \leftarrow 22\frac{1}{2}$	e	340 891.849	
		f	342 036.245	
24 ← 23	$23\frac{1}{2} \leftarrow 22\frac{1}{2}$	e	355 608.757	
		f	356 804.311	
	$24\frac{1}{2} \leftarrow 23\frac{1}{2}$	e	355 680.789	
		f	356 874.630	
25 ← 24	$24\frac{1}{2} \leftarrow 23\frac{1}{2}$	e	370 393.777	
		f	371 638.683	
	$25\frac{1}{2} \leftarrow 24\frac{1}{2}$	e	370 465.729	
		f	371 709.031	
State: electronic $\widetilde{X}\,^2\Sigma^+$; vibrational (1,0,0), $^2\Pi$ vibronic component				
21 ← 20	$20\frac{1}{2} \leftarrow 19\frac{1}{2}$	f	311 651.803	96Zi
	$21\frac{1}{2} \leftarrow 20\frac{1}{2}$	e	311 723.992	
22 ← 21	$21\frac{1}{2} \leftarrow 20\frac{1}{2}$	f	326 469.343	
	$22\frac{1}{2} \leftarrow 21\frac{1}{2}$	e	326 541.547	
23 ← 22	$22\frac{1}{2} \leftarrow 21\frac{1}{2}$	f	341 283.421	
	$23\frac{1}{2} \leftarrow 22\frac{1}{2}$	e	341 355.628	
24 ← 23	$23\frac{1}{2} \leftarrow 22\frac{1}{2}$	f	356 093.904	
	$24\frac{1}{2} \leftarrow 23\frac{1}{2}$	e	356 166.122	
25 ← 24	$24\frac{1}{2} \leftarrow 23\frac{1}{2}$	f	370 900.605	
	$25\frac{1}{2} \leftarrow 24\frac{1}{2}$	e	370 972.835	

[a]) States with parity equal to ± $(-1)^{J-0.5}$ are labeled *e* and *f* respectively.

Molecular parameters for $^{88}Sr^{16}O\,^1H$

Parameter		Value	Method	Ref.
State: electronic $\widetilde{X}\,^2\Sigma^+$; vibrational (0,0,0)				
B	[MHz]	7 470.822 5(6) [a])	MW	92An, 95 Fl
D	[kHz]	6.518 6(7)		
γ	[MHz]	72.774(16)		
$b_F(^1H)$	[MHz]	1.713(3)	MODR	93Fl
$c(^1H)$	[MHz]	1.673(15)		
μ	[D]	1.900(42)	OS	92St
State: electronic $\widetilde{X}\,^2\Sigma^+$; vibrational (0,1^1,0), $^2\Pi$ vibronic component				
B	[MHz]	7 452.243 0(20)[a])	MW	95Fl
D	[kHz]	6.623 8(19)		
γ	[MHz]	72.240(22)		
q	[MHz]	– 11.854 6(41)		
q_D	[kHz]	0.024 7(37)		
p_Π [b])	[MHz]	– 1.03(4)		
State: electronic $\widetilde{X}\,^2\Sigma^+$; vibrational (0,2^0,0), $^2\Sigma$ vibronic component				
B	[MHz]	7 440.989 7(29) [a])	MW	95Fl
D	[kHz]	6.725 5(27)		
γ	[MHz]	71.736(32)		
State: electronic $\widetilde{X}\,^2\Sigma^+$; vibrational (0,2^2,0), $^2\Delta$ vibronic component				
B	[MHz]	7 433.286 6(20) [a])	MW	95Fl
D	[kHz]	6.718 3(19)		

γ	[MHz]	71.589(22)		
q	[MHz]	– 11.934(16)		
State: electronic $\widetilde{X}\,^2\Sigma^+$; vibrational (0,3^1,0), $^2\Pi$ vibronic component				
B	[MHz]	7 429.630 7(20)	MW	95Fl
D	[kHz]	6.886 8(19)		
γ	[MHz]	71.135(22)		
q	[MHz]	– 12.484 0(20)		
q_D	[kHz]	0.034 2(19)		
p_Π [b])	[MHz]	– 1.67(4)		
State: electronic $\widetilde{X}\,^2\Sigma^+$; vibrational (1,0,0), $^2\Sigma$ vibronic component				
B	[MHz]	7 426.907 1(29) [a])	MW	95Fl
D	[kHz]	6.538 1(26)		
γ	[MHz]	72.210(32)		

[a]) The numbers in parenthesis are 3 standard deviations of the least-squares fit, in units of the last quoted decimal place.
[b]) This parameter takes care of the different spin-rotation splittings in the l-type doubling components.

Microwave data for $^{86}Sr^{16}O\,^1H$

Transition			ν	Ref.
rotational $N' - N''$	fine structure $J' - J''$	parity [a])	[MHz]	
State: electronic $\widetilde{X}\,^2\Sigma^+$; vibrational (0,0,0)				
14 ← 13	$13\frac{1}{2} \leftarrow 12\frac{1}{2}$	*f*	209 851.313	92An
	$14\frac{1}{2} \leftarrow 13\frac{1}{2}$	*e*	209 924.327	
15 ← 14	$14\frac{1}{2} \leftarrow 13\frac{1}{2}$	*f*	224 831.861	
	$15\frac{1}{2} \leftarrow 14\frac{1}{2}$	*e*	224 904.896	
16 ← 15	$15\frac{1}{2} \leftarrow 14\frac{1}{2}$	*f*	239 810.054	
	$16\frac{1}{2} \leftarrow 15\frac{1}{2}$	*e*	239 883.074	
17 ← 16	$16\frac{1}{2} \leftarrow 15\frac{1}{2}$	*f*	254 785.727	
	$17\frac{1}{2} \leftarrow 16\frac{1}{2}$	*e*	254 858.772	
18 ← 17	$17\frac{1}{2} \leftarrow 16\frac{1}{2}$	*f*	269 758.723	
	$18\frac{1}{2} \leftarrow 17\frac{1}{2}$	*e*	269 831.781	
19 ← 18	$18\frac{1}{2} \leftarrow 17\frac{1}{2}$	*f*	284 728.887	
	$19\frac{1}{2} \leftarrow 18\frac{1}{2}$	*e*	284 801.936	
20 ← 19	$19\frac{1}{2} \leftarrow 18\frac{1}{2}$	*f*	299 696.037	
	$20\frac{1}{2} \leftarrow 19\frac{1}{2}$	*e*	299 769.119	
21 ← 20	$20\frac{1}{2} \leftarrow 19\frac{1}{2}$	*f*	314 660.042	
	$21\frac{1}{2} \leftarrow 20\frac{1}{2}$	*e*	314 733.117	
22 ← 21	$21\frac{1}{2} \leftarrow 20\frac{1}{2}$	*f*	329 620.758	
	$22\frac{1}{2} \leftarrow 21\frac{1}{2}$	*e*	329 693.829	
23 ← 22	$22\frac{1}{2} \leftarrow 21\frac{1}{2}$	*f*	344 577.976	
	$23\frac{1}{2} \leftarrow 22\frac{1}{2}$	*e*	344 651.071	
24 ← 23	$23\frac{1}{2} \leftarrow 22\frac{1}{2}$	*f*	359 531.588	
	$24\frac{1}{2} \leftarrow 23\frac{1}{2}$	*e*	359 604.688	
25 ← 24	$24\frac{1}{2} \leftarrow 23\frac{1}{2}$	*f*	374 481.408	
	$25\frac{1}{2} \leftarrow 24\frac{1}{2}$	*e*	374 554.513	

[a]) States with parity equal to $\pm(-1)^{J-0.5}$ are labeled *e* and *f* respectively.

Molecular parameters for $^{86}Sr^{16}O^{1}H$

Parameter		Value	Method	Ref.
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (0,0,0)				
B	[MHz]	7 498.567 6(6) [a])	MW	92An
D	[kHz]	6.566 7(7)		
γ	[MHz]	73.063(14)		

[a]) The numbers in parenthesis are 3 standard deviations of the least-squares fit, in units of the last quoted decimal.

Microwave data for $^{86}Sr^{16}O^{2}H$ (SrOD)

Transition			ν	Ref.
rotational $N' - N''$	fine structure $J' - J''$	parity [a])	[MHz]	
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (0,0,0)				
15 ← 14	$14\frac{1}{2} \leftarrow 13\frac{1}{2}$	*f*	202 543.882	92An
	$15\frac{1}{2} \leftarrow 14\frac{1}{2}$	*e*	202 609.846	
16 ← 15	$15\frac{1}{2} \leftarrow 14\frac{1}{2}$	*f*	216 039.087	
	$16\frac{1}{2} \leftarrow 15\frac{1}{2}$	*e*	216 105.073	
17 ← 16	$16\frac{1}{2} \leftarrow 15\frac{1}{2}$	*f*	229 523.398	
	$17\frac{1}{2} \leftarrow 16\frac{1}{2}$	*e*	229 598.373	
18 ← 17	$17\frac{1}{2} \leftarrow 16\frac{1}{2}$	*f*	243 023.653	
	$18\frac{1}{2} \leftarrow 17\frac{1}{2}$	*e*	243 089.661	
19 ← 18	$18\frac{1}{2} \leftarrow 17\frac{1}{2}$	*f*	256 412.776	
	$19\frac{1}{2} \leftarrow 18\frac{1}{2}$	*e*	256 578.748	
20 ← 19	$19\frac{1}{2} \leftarrow 18\frac{1}{2}$	*f*	269 999.517	
	$20\frac{1}{2} \leftarrow 19\frac{1}{2}$	*e*	270 065.587	
21 ← 20	$20\frac{1}{2} \leftarrow 19\frac{1}{2}$	*f*	283 484.033	
	$21\frac{1}{2} \leftarrow 20\frac{1}{2}$	*e*	283 550.032	
22 ← 21	$21\frac{1}{2} \leftarrow 20\frac{1}{2}$	*f*	296 965.962	
	$22\frac{1}{2} \leftarrow 21\frac{1}{2}$	*e*	297 031.952	
23 ← 22	$22\frac{1}{2} \leftarrow 21\frac{1}{2}$	*f*	310 445.235	
	$23\frac{1}{2} \leftarrow 22\frac{1}{2}$	*e*	310 511.286	
24 ← 23	$23\frac{1}{2} \leftarrow 22\frac{1}{2}$	*f*	323 921.757	
	$24\frac{1}{2} \leftarrow 23\frac{1}{2}$	*e*	323 987.767	
25 ← 24	$24\frac{1}{2} \leftarrow 23\frac{1}{2}$	*f*	337 395.410	
	$25\frac{1}{2} \leftarrow 24\frac{1}{2}$	*e*	337 461.441	
26 ← 25	$25\frac{1}{2} \leftarrow 24\frac{1}{2}$	*f*	350 866.067	
	$26\frac{1}{2} \leftarrow 25\frac{1}{2}$	*e*	350 932.105	

[a]) States with parity equal to $\pm(-1)^{J-0.5}$ are labeled *e* and *f* respectively.

Molecular parameters for $^{86}Sr^{16}O^{2}H$ (Sr OD)

Parameter		Value	Method	Ref.
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (0,0,0)				
B	[MHz]	6 754.808 3(8) [a])	MW	92An
D	[kHz]	4.991 8(9)		
γ	[MHz]	66.008(18)		

[a]) The numbers in parenthesis are 3 standard deviations of the least-squares fit, in units of the last quoted decimal place.

References for SrOH

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96Zi Ziurys, L.M., Fletcher, D.A., Anderson, M.A., Barclay, W.L. : Astrophys. J. Supp. **102** (1996) 425.

3.2.1.2.38 BaOH

Microwave data for $^{138}Ba^{16}O^{1}H$

Transition			ν	Ref.
rotational $N' - N''$	rotational $J' - J''$	parity e/f [a])	[MHz]	
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (0,0,0)				
6 ← 5	$5\frac{1}{2} \leftarrow 4\frac{1}{2}$	*f*	77 885.432	93An
	$6\frac{1}{2} \leftarrow 5\frac{1}{2}$	*e*	77 956.778	
7 ← 6	$6\frac{1}{2} \leftarrow 5\frac{1}{2}$	*f*	90 870.430	
	$7\frac{1}{2} \leftarrow 6\frac{1}{2}$	*e*	90 870.430	
8 ← 7	$7\frac{1}{2} \leftarrow 6\frac{1}{2}$	*f*	103 854.631	
	$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	*e*	103 925.993	
10 ← 9	$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	*f*	129 820.097	
	$10\frac{1}{2} \leftarrow 9\frac{1}{2}$	*e*	129 891.492	
11 ← 10	$10\frac{1}{2} \leftarrow 9\frac{1}{2}$	*f*	142 801.118	
	$11\frac{1}{2} \leftarrow 10\frac{1}{2}$	*e*	142 872.557	
12 ← 11	$11\frac{1}{2} \leftarrow 10\frac{1}{2}$	*f*	155 780.835	
	$12\frac{1}{2} \leftarrow 11\frac{1}{2}$	*e*	155 852.264	
13 ← 12	$12\frac{1}{2} \leftarrow 11\frac{1}{2}$	*f*	168 759.137	
	$13\frac{1}{2} \leftarrow 12\frac{1}{2}$	*e*	168 830.594	
14 ← 13	$13\frac{1}{2} \leftarrow 12\frac{1}{2}$	*f*	181 735.933	
	$14\frac{1}{2} \leftarrow 13\frac{1}{2}$	*e*	181 807.374	
15 ← 14	$14\frac{1}{2} \leftarrow 13\frac{1}{2}$	*f*	194 710.993	
	$15\frac{1}{2} \leftarrow 14\frac{1}{2}$	*e*	194 782.497	
16 ← 15	$15\frac{1}{2} \leftarrow 14\frac{1}{2}$	*f*	207 684.390	
	$16\frac{1}{2} \leftarrow 15\frac{1}{2}$	*e*	207 755.864	
17 ← 16	$16\frac{1}{2} \leftarrow 15\frac{1}{2}$	*f*	220 655.848	
	$17\frac{1}{2} \leftarrow 16\frac{1}{2}$	*e*	220 727.352	
18 ← 17	$17\frac{1}{2} \leftarrow 16\frac{1}{2}$	*f*	233 625.234	
	$18\frac{1}{2} \leftarrow 17\frac{1}{2}$	*e*	233 696.794	
19 ← 18	$18\frac{1}{2} \leftarrow 17\frac{1}{2}$	*f*	246 592.547	
	$19\frac{1}{2} \leftarrow 18\frac{1}{2}$	*e*	246 664.114	
20 ← 19	$19\frac{1}{2} \leftarrow 18\frac{1}{2}$	*f*	259 557.599	
	$20\frac{1}{2} \leftarrow 19\frac{1}{2}$	*e*	259 629.194	
21 ← 20	$20\frac{1}{2} \leftarrow 19\frac{1}{2}$	*f*	272 520.302	
	$21\frac{1}{2} \leftarrow 20\frac{1}{2}$	*e*	272 591.937	
22 ← 21	$21\frac{1}{2} \leftarrow 20\frac{1}{2}$	*f*	285 480.518	
	$22\frac{1}{2} \leftarrow 21\frac{1}{2}$	*e*	285 552.165	

$23 \leftarrow 22$	$22\frac{1}{2} \leftarrow 21\frac{1}{2}$	*f*	298 438.128	
	$23\frac{1}{2} \leftarrow 22\frac{1}{2}$	*e*	298 509.819	
$24 \leftarrow 23$	$23\frac{1}{2} \leftarrow 22\frac{1}{2}$	*f*	311 393.024	
	$24\frac{1}{2} \leftarrow 23\frac{1}{2}$	*e*	311 464.740	
$25 \leftarrow 24$	$24\frac{1}{2} \leftarrow 23\frac{1}{2}$	*f*	324 345.069	
	$25\frac{1}{2} \leftarrow 24\frac{1}{2}$	*e*	324 416.834	
$26 \leftarrow 25$	$25\frac{1}{2} \leftarrow 24\frac{1}{2}$	*f*	337 294.177	
	$26\frac{1}{2} \leftarrow 25\frac{1}{2}$	*e*	337 365.979	
$27 \leftarrow 26$	$26\frac{1}{2} \leftarrow 25\frac{1}{2}$	*f*	350 240.214	
	$27\frac{1}{2} \leftarrow 26\frac{1}{2}$	*e*	350 312.037	
$28 \leftarrow 27$	$27\frac{1}{2} \leftarrow 26\frac{1}{2}$	*f*	363 183.031	
	$28\frac{1}{2} \leftarrow 27\frac{1}{2}$	*e*	363 254.912	
$29 \leftarrow 28$	$28\frac{1}{2} \leftarrow 27\frac{1}{2}$	*f*	376 122.568	
	$29\frac{1}{2} \leftarrow 28\frac{1}{2}$	*e*	376 194.485	
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (0,1^1,0), $^2\Pi$ vibronic component				
$24 \leftarrow 23$	$23\frac{1}{2} \leftarrow 22\frac{1}{2}$	*e*	310 753.499	96Zi
		f	311 209.221	
	$24\frac{1}{2} \leftarrow 23\frac{1}{2}$	*e*	310 824.320	
		f	311 277.356	
$25 \leftarrow 24$	$24\frac{1}{2} \leftarrow 23\frac{1}{2}$	*e*	323 678.514	
		f	324 153.044	
	$25\frac{1}{2} \leftarrow 24\frac{1}{2}$	*e*	323 749.374	
		f	324 221.265	
$26 \leftarrow 25$	$25\frac{1}{2} \leftarrow 24\frac{1}{2}$	*e*	336 600.516	
		f	337 093.864	
	$26\frac{1}{2} \leftarrow 25\frac{1}{2}$	*e*	336 671.478	
		f	337 162.165	
$27 \leftarrow 26$	$26\frac{1}{2} \leftarrow 25\frac{1}{2}$	*e*	349 519.401	
		f	350 031.528	
	$27\frac{1}{2} \leftarrow 26\frac{1}{2}$	*e*	349 590.476	
		f	350 099.916	
$28 \leftarrow 27$	$27\frac{1}{2} \leftarrow 26\frac{1}{2}$	*e*	362 435.060	
		f	362 965.956	
	$28\frac{1}{2} \leftarrow 27\frac{1}{2}$	*e*	362 506.173	
		f	363 934.406	
$29 \leftarrow 28$	$28\frac{1}{2} \leftarrow 27\frac{1}{2}$	*e*	375 347.344	
		f	375 897.009	
	$29\frac{1}{2} \leftarrow 28\frac{1}{2}$	*e*	375 418.518	
		f	375 965.531	
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (0,2^0,0), $^2\Sigma$ vibronic component				
$24 \leftarrow 23$	$23\frac{1}{2} \leftarrow 22\frac{1}{2}$	*f*	310 837.301	96Zi
	$24\frac{1}{2} \leftarrow 23\frac{1}{2}$	*e*	310 905.900	
$25 \leftarrow 24$	$24\frac{1}{2} \leftarrow 23\frac{1}{2}$	*f*	323 764.784	
	$25\frac{1}{2} \leftarrow 24\frac{1}{2}$	*e*	323 833.392	
$26 \leftarrow 25$	$25\frac{1}{2} \leftarrow 24\frac{1}{2}$	*f*	336 689.121	
	$26\frac{1}{2} \leftarrow 25\frac{1}{2}$	*e*	336 757.782	
$27 \leftarrow 26$	$26\frac{1}{2} \leftarrow 25\frac{1}{2}$	*f*	349 610.213	
	$27\frac{1}{2} \leftarrow 26\frac{1}{2}$	*e*	349 678.921	

28 ← 27	$27\frac{1}{2} \leftarrow 26\frac{1}{2}$	*f*	362 527.938	
	$28\frac{1}{2} \leftarrow 27\frac{1}{2}$	*e*	362 596.695	
29 ← 28	$28\frac{1}{2} \leftarrow 27\frac{1}{2}$	*f*	375 442.126	
	$29\frac{1}{2} \leftarrow 28\frac{1}{2}$	*e*	375 510.957	
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (0,2^2,0), $^2\Delta$ vibronic component				
24 ← 23	$23\frac{1}{2} \leftarrow 22\frac{1}{2}$	*e*	310 553.616	96Zi
		f	310 559.318	
	$24\frac{1}{2} \leftarrow 23\frac{1}{2}$	*e*	310 619.553	
		f	310 625.171	
25 ← 24	$24\frac{1}{2} \leftarrow 23\frac{1}{2}$	*e*	323 469.720	
		f	323 476.135	
	$25\frac{1}{2} \leftarrow 24\frac{1}{2}$	*e*	323 535.819	
		f	323 542.185	
26 ← 25	$25\frac{1}{2} \leftarrow 24\frac{1}{2}$	*f*	336 389.965	
	$26\frac{1}{2} \leftarrow 25\frac{1}{2}$	*f*	336 456.178	
27 ← 26	$26\frac{1}{2} \leftarrow 25\frac{1}{2}$	*e*	349 292.571	
		f	349 300.691	
	$27\frac{1}{2} \leftarrow 26\frac{1}{2}$	*e*	349 359.057	
		f	349 367.077	
28 ← 27	$27\frac{1}{2} \leftarrow 26\frac{1}{2}$	*e*	362 199.103	
		f	362 208.173	
	$28\frac{1}{2} \leftarrow 27\frac{1}{2}$	*e*	362 265.766	
		f	362 274.727	
29 ← 28	$28\frac{1}{2} \leftarrow 27\frac{1}{2}$	*e*	375 102.235	
		f	375 112.365	
	$29\frac{1}{2} \leftarrow 28\frac{1}{2}$	*e*	375 169.101	
		f	375 178.992	
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (0,3^3,0), $^2\Phi$ vibronic component				
24 ← 23	$23\frac{1}{2} \leftarrow 22\frac{1}{2}$	*e,f*	310 202.674	96Zi
	$24\frac{1}{2} \leftarrow 23\frac{1}{2}$	*e,f*	310 271.127	
25 ← 24	$24\frac{1}{2} \leftarrow 23\frac{1}{2}$	*e,f*	323 103.752	
	$25\frac{1}{2} \leftarrow 24\frac{1}{2}$	*e,f*	323 172.260	
26 ← 25	$25\frac{1}{2} \leftarrow 24\frac{1}{2}$	*e,f*	336 001.673	
	$26\frac{1}{2} \leftarrow 25\frac{1}{2}$	*e,f*	336 070.346	
27 ← 26	$26\frac{1}{2} \leftarrow 25\frac{1}{2}$	*e,f*	348 896.386	
	$27\frac{1}{2} \leftarrow 26\frac{1}{2}$	*e,f*	348 965.081	
28 ← 27	$27\frac{1}{2} \leftarrow 26\frac{1}{2}$	*e,f*	361 787.793	
	$28\frac{1}{2} \leftarrow 27\frac{1}{2}$	*e,f*	361 856.519	
29 ← 28	$28\frac{1}{2} \leftarrow 27\frac{1}{2}$	*e,f*	374 675.667	
	$29\frac{1}{2} \leftarrow 28\frac{1}{2}$	*e,f*	374 744.587	
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (1,0,0), $^2\Sigma$ vibronic component				
24 ← 23	$23\frac{1}{2} \leftarrow 22\frac{1}{2}$	*f*	309 802.953	96Zi
	$24\frac{1}{2} \leftarrow 23\frac{1}{2}$	*e*	309 874.286	
25 ← 24	$24\frac{1}{2} \leftarrow 23\frac{1}{2}$	*f*	322 688.681	
	$25\frac{1}{2} \leftarrow 24\frac{1}{2}$	*e*	322 760.029	
26 ← 25	$25\frac{1}{2} \leftarrow 24\frac{1}{2}$	*f*	335 571.436	
	$26\frac{1}{2} \leftarrow 25\frac{1}{2}$	*e*	335 642.829	

27 ← 26	$26\frac{1}{2} \leftarrow 25\frac{1}{2}$	*f*	348 451.084
	$27\frac{1}{2} \leftarrow 26\frac{1}{2}$	*e*	348 522.552
28 ← 27	$27\frac{1}{2} \leftarrow 26\frac{1}{2}$	*f*	361 327.565
	$28\frac{1}{2} \leftarrow 27\frac{1}{2}$	*e*	361 399.045
29 ← 28	$28\frac{1}{2} \leftarrow 27\frac{1}{2}$	*f*	374 200.77
	$29\frac{1}{2} \leftarrow 28\frac{1}{2}$	*e*	374 272.245

[a]) States with parity equal to ± $(-1)^{J-0.5}$ are labeled *e* and *f* respectively.

Molecular parameters for $^{138}Ba^{16}O^{1}H$

Parameter		Value	Method	Ref.
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (0,0,0)				
B	[MHz]	6 493.775 1(5) [a])	MW	93An, 95 Fl
D	[kHz]	4.924(4)		
γ	[MHz]	71.325(27)		
γ_D	[kHz]	0.231(20)		
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (0,1^1,0), $^2\Pi$ vibronic component				
B	[MHz]	6 485.264 0(15) [a])	MW	95Fl
D	[kHz]	5.010 3(11)		
γ	[MHz]	68.65(16)		
γ_D	[kHz]	0.48(8)		
q	[MHz]	– 9.493 2(31)		
q_D	[kHz]	0.023 3(21)		
p_Π [b])	[MHz]	– 2.66(4)		
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (0,2^0,0), $^2\Sigma$ vibronic component				
B	[MHz]	6 482.486 9(22) [a])	MW	95Fl
D	[kHz]	5.204 0(15)		
γ	[MHz]	68.06(23)		
γ_D	[kHz]	0.031(11)		
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (0,2^2,0), $^2\Delta$ vibronic component				
B	[MHz]	6 476.377 0(16) [a])	MW	95Fl
D	[kHz]	5.038 39(11)		
γ	[MHz]	64.04(16)		
γ_D	[kHz]	1.08(8)		
q	[kHz]	0.102 69(28)		
p_Δ [b])	[MHz]	– 0.055(20)		
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (0,3^3,0), $^2\Pi$ vibronic component				
B	[MHz]	6 469.245 0(22) [a])	MW	95Fl
D	[kHz]	5.187 9(15)		
γ	[MHz]	67.52(23)		
γ_D	[kHz]	0.54(11)		
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (1,0,0), $^2\Sigma$ vibronic component				
B	[MHz]	6 460.661 9(22) [a])	MW	95Fl
D	[kHz]	4.939 8(15)		
γ	[MHz]	70.89(23)		
γ_D	[kHz]	0.025(11)		

[a]) The numbers in parentheses are 3 standard deviations of the least-squares fit, in units of the last quoted decimal place.

[b]) This parameter takes care of the different spin-rotation splittings in the l-type doubling components.

Microwave data for $^{136}Ba^{16}O^{1}H$

Transition rotational $N' - N''$	fine structure $J' - J''$	parity [a])	ν [MHz]	Ref.
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (0,0,0)				
20 ← 19	$19\frac{1}{2} \leftarrow 18\frac{1}{2}$	*f*	259 971.690	93An
	$20\frac{1}{2} \leftarrow 19\frac{1}{2}$	*e*	260 043.407	
21 ← 20	$20\frac{1}{2} \leftarrow 19\frac{1}{2}$	*f*	272 955.053	
	$21\frac{1}{2} \leftarrow 20\frac{1}{2}$	*e*	273 026.770	
22 ← 21	$21\frac{1}{2} \leftarrow 20\frac{1}{2}$	*f*	285 935.908	
	$22\frac{1}{2} \leftarrow 21\frac{1}{2}$	*e*	286 007.680	
23 ← 22	$22\frac{1}{2} \leftarrow 21\frac{1}{2}$	*f*	298 914.143	
	$23\frac{1}{2} \leftarrow 22\frac{1}{2}$	*e*	298 985.943	
24 ← 23	$23\frac{1}{2} \leftarrow 22\frac{1}{2}$	*f*	311 889.673	
	$24\frac{1}{2} \leftarrow 23\frac{1}{2}$	*e*	311 961.509	
25 ← 24	$24\frac{1}{2} \leftarrow 23\frac{1}{2}$	*f*	324 862.336	
	$25\frac{1}{2} \leftarrow 24\frac{1}{2}$	*e*	324 934.217	
26 ← 25	$25\frac{1}{2} \leftarrow 24\frac{1}{2}$	*f*	337 832.069	
	$26\frac{1}{2} \leftarrow 25\frac{1}{2}$	*e*	337 903.944	
27 ← 26	$26\frac{1}{2} \leftarrow 25\frac{1}{2}$	*f*	350 798.671	
	$27\frac{1}{2} \leftarrow 26\frac{1}{2}$	*e*	350 870.623	
28 ← 27	$27\frac{1}{2} \leftarrow 26\frac{1}{2}$	*f*	363 762.090	
	$28\frac{1}{2} \leftarrow 27\frac{1}{2}$	*e*	363 834.065	
29 ← 28	$28\frac{1}{2} \leftarrow 27\frac{1}{2}$	*f*	376 722.214	
	$29\frac{1}{2} \leftarrow 28\frac{1}{2}$	*e*	376 794.274	

[a]) States with parity equal to $\pm(-1)^{J-0.5}$ are labeled *e* and *f* respectively.

Molecular parameters for $^{136}Ba^{16}O^{1}H$

Parameter		Value	Method	Ref.
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (0,0,0)				
B	[MHz]	6 504.140 90(63) [a])	MW	93An
D	[kHz]	4.940 22(48)		
γ	[MHz]	71.415(58)		
γ_D	[kHz]	− 0.243(30)		

[a]) The numbers in parenthesis are 3 standard deviations of the least-squares fit, in units of the last quoted decimal place.

Microwave data for $^{137}Ba^{16}O^{1}H$

Transition rotational $N' - N''$	fine structure $J' - J''$	Hyperfine [a]) $F' - F''$	ν [MHz]	Ref.
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (0,0,0)				
26← 25	$25\frac{1}{2} \leftarrow 24\frac{1}{2}$	24 ← 23	337 560.942	93An
		27 ← 26	337 570.607	
		26 ← 25	337 582.491	
		25 ← 24	337 594.512	
	$26\frac{1}{2} \leftarrow 25\frac{1}{2}$	25 ← 24	337 599.096	
		26 ← 25	337 611.153	

		$27 \leftarrow 26$	337 623.093
		$28 \leftarrow 27$	337 632.855
$27 \leftarrow 26$	$26\frac{1}{2} \leftarrow 25\frac{1}{2}$	$25 \leftarrow 24$	350 517.238
		$28 \leftarrow 27$	350 526.626
		$27 \leftarrow 26$	350 538.288
		$26 \leftarrow 25$	350 551.465
	$27\frac{1}{2} \leftarrow 26\frac{1}{2}$	$26 \leftarrow 25$	350 554.665
		$27 \leftarrow 26$	350 567.870
		$28 \leftarrow 27$	350 579.550
		$29 \leftarrow 28$	350 589.045
$28 \leftarrow 27$	$27\frac{1}{2} \leftarrow 26\frac{1}{2}$	$26 \leftarrow 25$	363 470.233
		$29 \leftarrow 28$	363 479.233
		$28 \leftarrow 27$	363 490.888
		$27 \leftarrow 26$	363 505.206
	$28\frac{1}{2} \leftarrow 27\frac{1}{2}$	$27 \leftarrow 26$	363 506.746
		$28 \leftarrow 27$	363 521.388
		$29 \leftarrow 28$	363 532.855
		$30 \leftarrow 29$	363 542.131

[a]) Coupling scheme: $\boldsymbol{J} = \boldsymbol{N} + \boldsymbol{S}$; $\boldsymbol{F} = \boldsymbol{J} + \boldsymbol{I}_1$ where $\boldsymbol{I}_1$ is the ^{137}Ba nuclear spin.
[b]) Hyperfine structure not resolved.

Molecular parameters for $^{137}Ba^{16}O^{1}H$

Parameter		Value	Method	Ref.
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (0,0,0)				
B	[MHz]	6 498.926(15) [a])	MW	93An
D	[kHz]	4.939 6(99)		
γ	[MHz]	72.01(13)		
$b(^{137}Ba)$	[MHz]	2 200.2(59)		
$c(^{137}Ba)$	[MHz]	0.0 [b])		
$C_I(^{137}Ba)$ [c])	[MHz]	– 0.101(46)		
eQq_0	[MHz]	– 394.2(12)		

[a]) The numbers in parenthesis are 3 standard deviations of the least-squares fit, in units of the last quoted decimal place.
[b]) Parameter constrained to zero in the least squares fit.
[c]) Nuclear spin-rotation constant, see Vol. II24/C

Microwave data for $^{138}Ba^{16}O^{2}H$ (BaOD)

Transition: rotational $N' - N''$	fine structure $J' - J''$	Parity [a])	ν [MHz]	Ref.
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (0,0,0)				
$20 \leftarrow 19$	$19\frac{1}{2} \leftarrow 18\frac{1}{2}$	f	234 586.020	93An
	$20\frac{1}{2} \leftarrow 19\frac{1}{2}$	e	234 651.120	
$21 \leftarrow 20$	$20\frac{1}{2} \leftarrow 19\frac{1}{2}$	f	246 303.890	
	$21\frac{1}{2} \leftarrow 20\frac{1}{2}$	e	246 368.995	
$22 \leftarrow 21$	$21\frac{1}{2} \leftarrow 20\frac{1}{2}$	f	258 019.876	
	$22\frac{1}{2} \leftarrow 21\frac{1}{2}$	e	258 085.008	
$23 \leftarrow 22$	$22\frac{1}{2} \leftarrow 21\frac{1}{2}$	f	269 733.837	
	$23\frac{1}{2} \leftarrow 22\frac{1}{2}$	e	269 799.003	
$24 \leftarrow 23$	$23\frac{1}{2} \leftarrow 22\frac{1}{2}$	f	281 445.729	
	$24\frac{1}{2} \leftarrow 23\frac{1}{2}$	e	281 510.879	

25 ← 24	$24\frac{1}{2} \leftarrow 23\frac{1}{2}$	*f*	293 155.391
	$25\frac{1}{2} \leftarrow 24\frac{1}{2}$	*e*	293 220.601
26 ← 25	$25\frac{1}{2} \leftarrow 24\frac{1}{2}$	*f*	304 862.804
	$26\frac{1}{2} \leftarrow 25\frac{1}{2}$	*e*	304 928.047
27 ← 26	$26\frac{1}{2} \leftarrow 25\frac{1}{2}$	*f*	316 567.844
	$27\frac{1}{2} \leftarrow 26\frac{1}{2}$	*e*	316 633.148
28 ← 27	$27\frac{1}{2} \leftarrow 26\frac{1}{2}$	*f*	328 270.440
	$28\frac{1}{2} \leftarrow 27\frac{1}{2}$	*e*	328 335.749
29 ← 28	$28\frac{1}{2} \leftarrow 27\frac{1}{2}$	*f*	339 970.503
	$29\frac{1}{2} \leftarrow 28\frac{1}{2}$	*e*	340 035.830
30 ← 29	$29\frac{1}{2} \leftarrow 28\frac{1}{2}$	*f*	351 667.915
	$30\frac{1}{2} \leftarrow 29\frac{1}{2}$	*e*	351 733.286
31 ← 30	$30\frac{1}{2} \leftarrow 29\frac{1}{2}$	*f*	363 62.618
	$31\frac{1}{2} \leftarrow 30\frac{1}{2}$	*e*	363 428.016

[a]) States with parity equal to ± $(-1)^{J-0.5}$ are labeled *e* and *f* respectively

Molecular parameters for $^{138}Ba^{16}O^{2}H$ (BaOD)

Parameter		Value	Method	Ref.
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (0,0,0)				
B	[MHz]	5 868.494 50(42) [a])	MW	93An
D	[kHz]	3.787 62(29)		
γ	[MHz]	63.860(40)		
γ_D	[kHz]	– 0.189(19)		

[a]) The numbers in parenthesis are 3 standard deviations of the least-squares fit, in units of the last quoted decimal place.

References for BaOH

93An Anderson, M.A., Allen, M.D., Barclay, W.L., Ziurys, L.M.: Chem. Phys. Letters. **205** (1993) 415.

95Fl Fletcher, D.A., Anderson, M.A., Barclay, W.L., Ziurys, L.M.: J. Chem. Phys. **102** (1995) 4334.

96Zi Ziurys, L.M., Fletcher, D.A., Anderson, M.A., Barclay, W.L. : Astrophys. J. Supp. **102** (1996) 425.

3.2.1.2.39 MgCN

Microwave data for $^{24}Mg^{12}C^{15}N$

Transition		ν	
rotational $N' - N''$	fine structure $J' - J''$ [a])	[MHz]	Ref.
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (0,0,0)			
9 ← 8	$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	91 690.9	95Zi
	$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	91 705.9	
10 ← 9	$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	101 877.556	94An
	$10\frac{1}{2} \leftarrow 9\frac{1}{2}$	101 892.557	
11 ← 10	$10\frac{1}{2} \leftarrow 9\frac{1}{2}$	112 063.443	
	$11\frac{1}{2} \leftarrow 10\frac{1}{2}$	112 078.440	
13 ← 12	$12\frac{1}{2} \leftarrow 11\frac{1}{2}$	132 433.041	
	$13\frac{1}{2} \leftarrow 12\frac{1}{2}$	132 448.060	

$14 \leftarrow 13$	$13\frac{1}{2} \leftarrow 12\frac{1}{2}$	142 616.595
	$14\frac{1}{2} \leftarrow 13\frac{1}{2}$	142 631.584
$15 \leftarrow 16$	$15\frac{1}{2} \leftarrow 14\frac{1}{2}$	152 799.206
	$16\frac{1}{2} \leftarrow 15\frac{1}{2}$	152 814.172
$16 \leftarrow 15$	$16\frac{1}{2} \leftarrow 15\frac{1}{2}$	162 980.808
	$17\frac{1}{2} \leftarrow 16\frac{1}{2}$	162 995.839
$17 \leftarrow 16$	$16\frac{1}{2} \leftarrow 15\frac{1}{2}$	173 161.328
	$17\frac{1}{2} \leftarrow 16\frac{1}{2}$	173 176.328
$18 \leftarrow 17$	$17\frac{1}{2} \leftarrow 16\frac{1}{2}$	183 340.745
	$18\frac{1}{2} \leftarrow 17\frac{1}{2}$	183 355.678
$19 \leftarrow 18$	$18\frac{1}{2} \leftarrow 17\frac{1}{2}$	193 518.946
	$19\frac{1}{2} \leftarrow 18\frac{1}{2}$	193 533.904
$20 \leftarrow 19$	$19\frac{1}{2} \leftarrow 18\frac{1}{2}$	203 695.952
	$20\frac{1}{2} \leftarrow 19\frac{1}{2}$	203 710.802
$21 \leftarrow 20$	$20\frac{1}{2} \leftarrow 19\frac{1}{2}$	213 871.497
	$21\frac{1}{2} \leftarrow 20\frac{1}{2}$	213 886.491
$22 \leftarrow 21$	$21\frac{1}{2} \leftarrow 20\frac{1}{2}$	224 045.684
	$22\frac{1}{2} \leftarrow 21\frac{1}{2}$	224 060.674
$23 \leftarrow 22$	$22\frac{1}{2} \leftarrow 21\frac{1}{2}$	234 218.443
	$23\frac{1}{2} \leftarrow 22\frac{1}{2}$	234 233.459
$24 \leftarrow 23$	$23\frac{1}{2} \leftarrow 22\frac{1}{2}$	244 389.675
	$24\frac{1}{2} \leftarrow 23\frac{1}{2}$	244 404.674
$25 \leftarrow 24$	$24\frac{1}{2} \leftarrow 23\frac{1}{2}$	254 559.227
	$25\frac{1}{2} \leftarrow 24\frac{1}{2}$	254 574.229
$26 \leftarrow 25$	$25\frac{1}{2} \leftarrow 24\frac{1}{2}$	264 727.276
	$26\frac{1}{2} \leftarrow 25\frac{1}{2}$	264 742.177
$27 \leftarrow 26$	$26\frac{1}{2} \leftarrow 25\frac{1}{2}$	274 893.432
	$27\frac{1}{2} \leftarrow 26\frac{1}{2}$	274 908.361
$28 \leftarrow 27$	$27\frac{1}{2} \leftarrow 26\frac{1}{2}$	285 057.868
	$28\frac{1}{2} \leftarrow 27\frac{1}{2}$	285 072.811
$29 \leftarrow 28$	$28\frac{1}{2} \leftarrow 27\frac{1}{2}$	295 220.418
	$29\frac{1}{2} \leftarrow 28\frac{1}{2}$	295 235.384
$30 \leftarrow 29$	$29\frac{1}{2} \leftarrow 28\frac{1}{2}$	305 381.094
	$30\frac{1}{2} \leftarrow 29\frac{1}{2}$	305 395.999
$31 \leftarrow 30$	$30\frac{1}{2} \leftarrow 29\frac{1}{2}$	315 539.740
	$31\frac{1}{2} \leftarrow 30\frac{1}{2}$	315 554.633
$32 \leftarrow 31$	$31\frac{1}{2} \leftarrow 30\frac{1}{2}$	325 696.292
	$32\frac{1}{2} \leftarrow 31\frac{1}{2}$	325 711.326
$33 \leftarrow 32$	$32\frac{1}{2} \leftarrow 31\frac{1}{2}$	335 850.803
	$33\frac{1}{2} \leftarrow 32\frac{1}{2}$	335 865.659
$34 \leftarrow 33$	$33\frac{1}{2} \leftarrow 32\frac{1}{2}$	346 002.999
	$35\frac{1}{2} \leftarrow 34\frac{1}{2}$	356 167.920

[a]) Nuclear hyperfine structure not resolved

Molecular parameters for $^{24}Mg^{12}C^{15}N$

Parameter		Value	Method	Ref.
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (0,0,0)				
B	[MHz]	5 094.803 51(62) [a])	MW	94An
D	[kHz]	2.774 21(33)		
γ	[MHz]	15.014(24)		
γ_D	[kHz]	0.032 [b])		

[a]) The numbers in parenthesis are 3 standard deviations of the least-squares fit, in units of the last quoted decimal place.
[b]) Parameter constrained to this value in the least-squares fit.

References for MgCN

94An Anderson, M.A., Steimle, T.C., Ziurys, L.M. : Astrophys. J. **429** (1994) L41.
95Zi Ziurys, L.M., Apponi, A.J., Guélin, M., Cernicharo, J. : Astrophys. J. **445** (1995) L47.

3.2.1.2.40 MgNC

Microwave data for $^{24}Mg^{14}N^{12}C$

Transition			ν [MHz]	Ref.
rotational $N'-N''$	fine structure $J'-J''$	Hyperfine [a]) $F'-F''$		
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (0,0,0)				
1 ← 0	½ ← ½	½ ← 1½	11 922.925 1(15) [b])	98Wa
		1½ ← ½	11 928.645 0(15)	
	1½ ← ½	1½ ← 1½	11 932.241 1(15)	
		½ ← ½	11 935.773 5(15)	
		2½ ← 1½	11 941.214 4(15)	
2 ← 1	1½ ← ½	2½ ← 1½	23 861.228 6(15)	
	2½ ← 1½	1½ ← 1½	23 863.075 0(15)	
	1½ ← 1½	1½ ← ½	23 863.779 5(15)	
	2½ ← 1½	2½ ← 2½	23 864.654 2(15)	
	2½ ← ½	1½ ← ½	23 872.388 7(15)	
	2½ ← 1½	2½ ← 1½	23 873.727 8(15)	
		3½ ← 2½	23 875.039 6(15)	
7 ← 6	6½ ← 5½	[c])	83 522.9	86Gu
	7½ ← 6½	[c])	83 538.0	
8 ← 7	7½ ← 6½	[c])	95 454.4	
	8½ ← 7½	[c])	95 469.3	
9 ← 8	8½ ← 7½	[c])	107 384.6	
	9½ ← 8½	[c])	107 399.8	
21 ← 20	20½ ← 19½	[c])	250 445.992(20)	93Ka
	21½ ← 20½	[c])	250 461.245(20)	
22 ← 21	21½ ← 20½	[c])	262 356.464(20)	
	22½ ← 21½	[c])	262 371.679(20)	
23 ← 22	22½ ← 21½	[c])	274 264.702(20)	
	23½ ← 22½	[c])	274 279.991(20)	
24 ← 23	23½ ← 22½	[c])	286 170.795(20)	

	$24\frac{1}{2} \leftarrow 23\frac{1}{2}$	[c])	286 186.023(20)	
$26 \leftarrow 25$	$25\frac{1}{2} \leftarrow 24\frac{1}{2}$	[c])	309 975.563(20)	
	$26\frac{1}{2} \leftarrow 25\frac{1}{2}$	[c])	309 990.788(20)	
$27 \leftarrow 26$	$26\frac{1}{2} \leftarrow 25\frac{1}{2}$	[c])	321 874.135(20)	
	$27\frac{1}{2} \leftarrow 26\frac{1}{2}$	[c])	321 889.423(20)	
$28 \leftarrow 27$	$27\frac{1}{2} \leftarrow 26\frac{1}{2}$	[c])	333 769.950(20)	
	$28\frac{1}{2} \leftarrow 27\frac{1}{2}$	[c])	333 785.266(20)	
$29 \leftarrow 28$	$28\frac{1}{2} \leftarrow 27\frac{1}{2}$	[c])	345 663.196(20)	
	$29\frac{1}{2} \leftarrow 28\frac{1}{2}$	[c])	345 678.383(20)	
$30 \leftarrow 29$	$29\frac{1}{2} \leftarrow 28\frac{1}{2}$	[c])	357 553.444(20)	
	$30\frac{1}{2} \leftarrow 29\frac{1}{2}$	[c])	357 568.654(20)	
$31 \leftarrow 30$	$30\frac{1}{2} \leftarrow 29\frac{1}{2}$	[c])	369 440.810(20)	
	$31\frac{1}{2} \leftarrow 30\frac{1}{2}$	[c])	369 455.973(20)	

[a]) Coupling scheme: $\boldsymbol{J} = \boldsymbol{N} + \boldsymbol{S}$; $\boldsymbol{F} = \boldsymbol{J} + \boldsymbol{I}_1$ where $\boldsymbol{I}_1$ is the ^{14}N nuclear spin.
[b]) The figures in parenthesis are the authors' estimate of the experimental uncertainty, in units of the last quoted decimal place.
[c]) ^{14}N hyperfine splitting not resolved.

Microwave data for ^{24}Mg^{14}N^{12}C

Transition			ν [MHz]	Ref.
rotational $N' - N''$	fine structure $J' - J''$	parity [a])		
State: electronic $\widetilde{X}\,^2\Sigma^+$; vibrational $(0,1^1,0)$				
$27 \leftarrow 26$	$26\frac{1}{2} \leftarrow 25\frac{1}{2}$	*e*	325 379.604	96Ka
		f	326 792.823	
	$27\frac{1}{2} \leftarrow 26\frac{1}{2}$	*e*	325 364.084	
		f	326 777.540	
$28 \leftarrow 27$	$27\frac{1}{2} \leftarrow 26\frac{1}{2}$	*e*	337 398.199	
		f	338 858.647	
	$28\frac{1}{2} \leftarrow 27\frac{1}{2}$	*e*	337 382.780	
		f	338 843.375	
$29 \leftarrow 28$	$28\frac{1}{2} \leftarrow 27\frac{1}{2}$	*e*	349 413.424	
		f	350 920.456	
	$29\frac{1}{2} \leftarrow 28\frac{1}{2}$	*e*	349 298.150	
		f	350 905.183	
$30 \leftarrow 29$	$29\frac{1}{2} \leftarrow 28\frac{1}{2}$	*e*	361 425.196	
		f	362 978.288	
	$30\frac{1}{2} \leftarrow 29\frac{1}{2}$	*e*	361 409.819	
		f	362 962.968	
$31 \leftarrow 30$	$30\frac{1}{2} \leftarrow 29\frac{1}{2}$	*e*	373 433.211	
		f	375 031.871	
	$31\frac{1}{2} \leftarrow 30\frac{1}{2}$	*e*	373 417.909	
		f	375 016.631	
State: electronic $\widetilde{X}\,^2\Sigma^+$; vibrational $(0,2^0,0)$				
$26 \leftarrow 25$	$26\frac{1}{2} \leftarrow 25\frac{1}{2}$	*e*	318 634.446	96Ka
	$27\frac{1}{2} \leftarrow 26\frac{1}{2}$	*f*	318 619.079	
$27 \leftarrow 26$	$26\frac{1}{2} \leftarrow 25\frac{1}{2}$	*f*	330 866.822	
	$27\frac{1}{2} \leftarrow 26\frac{1}{2}$	*e*	330 851.451	

$29 \leftarrow 28$	$28\frac{1}{2} \leftarrow 27\frac{1}{2}$	*f*	355 323.149	
	$29\frac{1}{2} \leftarrow 28\frac{1}{2}$	*e*	355 307.777	
$30 \leftarrow 29$	$29\frac{1}{2} \leftarrow 28\frac{1}{2}$	*e*	367 546.866	
	$30\frac{1}{2} \leftarrow 29\frac{1}{2}$	*f*	367 531.448	
$31 \leftarrow 30$	$30\frac{1}{2} \leftarrow 29\frac{1}{2}$	*f*	379 767.244	
	$31\frac{1}{2} \leftarrow 30\frac{1}{2}$	*e*	379 751.929	

State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational $(0,2^2,0)$

$26 \leftarrow 25$	$26\frac{1}{2} \leftarrow 25\frac{1}{2}$	*e*	318 358.109	96Ka
		f	318 374.740	
	$27\frac{1}{2} \leftarrow 26\frac{1}{2}$	*e*	318 342.740	
		f	318 359.111	
$27 \leftarrow 26$	$26\frac{1}{2} \leftarrow 25\frac{1}{2}$	*e*	330 559.497	
		f	330 553.521	
	$27\frac{1}{2} \leftarrow 26\frac{1}{2}$	*e*	330 544.084	
		f	330 537.822	
$29 \leftarrow 28$	$28\frac{1}{2} \leftarrow 27\frac{1}{2}$	*e*	354 947.924	
		f	354 890.175	
	$29\frac{1}{2} \leftarrow 28\frac{1}{2}$	*e*	354 932.529	
		f	354 874.547	
$30 \leftarrow 29$	$29\frac{1}{2} \leftarrow 28\frac{1}{2}$	*e*	367 134.793	
		f	367 047.866	
	$30\frac{1}{2} \leftarrow 29\frac{1}{2}$	*e*	367 119.350	
		f	367 032.199	
$31 \leftarrow 30$	$30\frac{1}{2} \leftarrow 29\frac{1}{2}$	*e*	379 316.507	
		f	379 198.297	
	$31\frac{1}{2} \leftarrow 30\frac{1}{2}$	*e*	379 301.077	
		f	379 182.599	

State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational $(0,3^1,0)$

$26 \leftarrow 25$	$26\frac{1}{2} \leftarrow 25\frac{1}{2}$	*e*	321 957.733	96Ka
		f	325 082.381	
	$27\frac{1}{2} \leftarrow 26\frac{1}{2}$	*e*	321 941.713	
		f	325 066.698	
$27 \leftarrow 26$	$26\frac{1}{2} \leftarrow 25\frac{1}{2}$	*e*	334 277.393	
		f	337 502.919	
	$27\frac{1}{2} \leftarrow 26\frac{1}{2}$	*e*	334 261.421	
		f	337 487.202	
$28 \leftarrow 27$	$27\frac{1}{2} \leftarrow 26\frac{1}{2}$	*e*	346 590.469	
		f	349 914.700	
	$28\frac{1}{2} \leftarrow 27\frac{1}{2}$	*e*	346 574.540	
		f	349 899.036	
$29 \leftarrow 28$	$28\frac{1}{2} \leftarrow 27\frac{1}{2}$	*e*	358 896.728	
		f	362 317.367	
	$29\frac{1}{2} \leftarrow 28\frac{1}{2}$	*e*	358 880.839	
		f	362 301.666	
$30 \leftarrow 29$	$29\frac{1}{2} \leftarrow 28\frac{1}{2}$	*e*	371 196.057	
		f	374 710.780	
	$30\frac{1}{2} \leftarrow 29\frac{1}{2}$	*e*	371 180.137	
		f	374 695.090	

State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational $(0,3^3,0)$

$26 \leftarrow 25$	$26\frac{1}{2} \leftarrow 25\frac{1}{2}$	*e*	323 100.410	96Ka

		f	323 119.699	
	$27\frac{1}{2} \leftarrow 26\frac{1}{2}$	*e*	323 082.013	
		f	323 104.287	
27 ← 26	$26\frac{1}{2} \leftarrow 25\frac{1}{2}$	*e*	335 478.794	
		f	335 501.930	
	$27\frac{1}{2} \leftarrow 26\frac{1}{2}$	*e*	335 463.325	
		f	335 486.563	
28 ← 27	$27\frac{1}{2} \leftarrow 26\frac{1}{2}$	*e*	347 851.797	
		f	347 879.437	
	$28\frac{1}{2} \leftarrow 27\frac{1}{2}$	*e*	347 836.350	
		f	347 864.016	
29 ← 28	$28\frac{1}{2} \leftarrow 27\frac{1}{2}$	*e*	360 219.263	
		f	360 252.020	
	$29\frac{1}{2} \leftarrow 28\frac{1}{2}$	*e*	360 203.827	
		f	360 236.307	
30 ← 29	$29\frac{1}{2} \leftarrow 28\frac{1}{2}$	*e*	372 581.005	
		f	372 619.517	
	$30\frac{1}{2} \leftarrow 29\frac{1}{2}$	*e*	372 565.517	
		f	372 604.087	

State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational $(0,4^4,0)$

26 ← 25	$26\frac{1}{2} \leftarrow 25\frac{1}{2}$	[b])	328 108.742	96Ka
	$27\frac{1}{2} \leftarrow 26\frac{1}{2}$	[b])	328 093.253	
30 ← 29	$29\frac{1}{2} \leftarrow 28\frac{1}{2}$	[b])	378 328.921	
	$30\frac{1}{2} \leftarrow 29\frac{1}{2}$	[b])	378 313.042	

State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (0,5,0) [c])

25 ← 24	$24\frac{1}{2} \leftarrow 23\frac{1}{2}$	[b])	320 791.730	96Ka
	$25\frac{1}{2} \leftarrow 24\frac{1}{2}$	[b])	320 776.236	
26 ← 25	$25\frac{1}{2} \leftarrow 24\frac{1}{2}$	[b])	333 546.836	
	$26\frac{1}{2} \leftarrow 25\frac{1}{2}$	[b])	333 531.268	
28 ← 27	$27\frac{1}{2} \leftarrow 26\frac{1}{2}$	[b])	359 030.8	
	$28\frac{1}{2} \leftarrow 27\frac{1}{2}$	[b])	359 015.2	

[a]) States with parity equal to $\pm(-1)^{J-0.5}$ are labeled *e* and *f* respectively.
[b]) Parity doubling not resolved.
[c]) *l*-quantum number not identified

Molecular parameters for $^{24}Mg^{14}N^{12}C$

Parameter		Value	Method	Ref.
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (0,0,0)				
B	[MHz]	5 966.903 49(19) [a])	MW	98Wa
D	[kHz]	4.243 36(43)		
H	[Hz]	0.035 21(30)		
γ	[MHz]	15.332 2(19)		
γ_D	[kHz]	– 0.051 8(45)		
$b_F(^{14}N)$	[MHz]	29.163 7(77)		
$c(^{14}N)$	[MHz]	5.384 0(77)		
$eQq_0(^{14}N)$	[MHz]	– 2.323 1(53)		
μ	[D]	5.308(75)	Opt Stark	01St
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (0,1^1,0)				
B	[MHz]	6 046.887(24) [a])	MW	96Ka
D	[kHz]	5.880(28)		
H	[Hz]	0.104(11)		
γ_e	[MHz]	15.348(31)		
γ_f	[MHz]	15.277(39)		
Q	[MHz]	27.386 3(39)		
q_D	[kHz]	– 0.833 9(23)		
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (0,2^0,0)				
B	[MHz]	6 138.900(12) [a])	MW	96Ka
D	[kHz]	8.478(14)		
H	[Hz]	0.213 3(58)		
γ_e	[MHz]	15.672(16)		
Q	[MHz]	43.168 2(54)		
q_D	[kHz]	– 1.705 0(41)		
$x_{//}$	[GHz]	115.752 [b])		
ΔE	[GHz]	438.478(52)		
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (0,2^2,0)				
B	[MHz]	6 132.432 5(80) [a])	MW	96Ka
D	[kHz]	7.833(10)		
H	[Hz]	0.161 4(41)		
γ_f	[MHz]	15.385(11)		
Q	[MHz]	43.168 2(54)		
q_D	[kHz]	– 1.705 0(41)		
$x_{//}$	[GHz]	115.752 [b])		
ΔE	[GHz]	438.478(52)		
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (0,3^1,0)				
B	[MHz]	6 239.258(14) [a])	MW	96Ka
D	[kHz]	11.877(18)		
H	[Hz]	0.400 2(77)		
γ_e	[MHz]	15.939(20)		
γ_f	[MHz]	15.695(18)		
Q	[MHz]	32.300(15)		
q_D	[kHz]	– 1.640(18)		
q_H	[Hz]	0.107 7(77)		
$x_{//}$	[GHz]	115.752(27)		
ΔE	[GHz]	876.233(73)		
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (0,3^3,0)				
B	[MHz]	6 224.649(13) [a])	MW	96Ka

D	[kHz]	10.443(17)
H	[Hz]	0.302 0(73)
γ_e	[MHz]	15.441(18)
γ_f	[MHz]	15.411(19)
q	[MHz]	32.300(15)
q_D	[kHz]	– 1.640(18)
q_H	[Hz]	0.107 7(77)
x_{ll} [c])	[GHz]	115.752(27)
ΔE	[GHz]	876.233(73)

[a]) The numbers in parenthesis represent 1 standard deviation of the least-squares fit, in units of the last quoted decimal place.
[b]) Parameter constrained to the value determined by the analysis of the (0,3,0) levels.

[c]) Anharmonicity parameter in the vibrational-energy expansion, see Vol. II24/A

Microwave data for $^{25}Mg^{14}N^{12}C$

Transition: rotational $N' - N''$	Transition: fine structure $J' - J''$	Transition: Hyperfine [a]) $F' - F''$	ν [MHz]	Ref.
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (0,0,0)				
30 ← 29	$29\frac{1}{2} \leftarrow 28\frac{1}{2}$	27 ← 26	350 879.420	94An
		28 ← 27	350 880.728	
		29 ← 28	350 882.155	
		30 ← 29	350 883.838	
		31 ← 30	350 885.593 [b])	
		32 ← 31	350 885.593 [b])	
	$30\frac{1}{2} \leftarrow 29\frac{1}{2}$	32 ← 31	350 888.087 [b])	
		31 ← 30	350 888.087 [b])	
		30 ← 29	350 889.895	
		29 ← 28	350 891.560	
		28 ← 27	350 894.032 [b])	
		33 ← 32	350 894.032 [b])	
32 ← 31	$31\frac{1}{2} \leftarrow 30\frac{1}{2}$	29 ← 28	374 208.371	
		30 ← 29	374 209.586	
		31 ← 30	374 211.031	
		32 ← 31	374 212.612	
		33 ← 32	374 214.593 [b])	
		34 ← 33	374 214.593 [b])	
	$32\frac{1}{2} \leftarrow 31\frac{1}{2}$	34 ← 33	374 217.211 [b])	
		33 ← 32	374 217.211 [b])	
		32 ← 31	374 219.314	
		31 ← 30	374 220.920	
		30 ← 29	374 223.273 [b])	
		35 ← 34	374 223.273 [b])	
33 ← 32	$32\frac{1}{2} \leftarrow 31\frac{1}{2}$	30 ← 29	385 868.275	
		31 ← 30	385 869.558	
		32 ← 31	385 870.993	
		33 ← 32	385 872.589	
		34 ← 33	385 874.556 [b])	
		35 ← 34	385 874.556 [b])	
	$33\frac{1}{2} \leftarrow 32\frac{1}{2}$	35 ← 34	385 877.232 [b])	

34 ← 33	385 877.232 [b])
33 ← 32	385 879.321
32 ← 31	385 880.310
31 ← 30	385 882.352
36 ← 35	385 883.379

[a]) Coupling scheme: $\boldsymbol{J} = \boldsymbol{N} + \boldsymbol{S}$; $\boldsymbol{F} = \boldsymbol{J} + \boldsymbol{I}_1$ where $\boldsymbol{I}_1$ is the ^{25}Mg nuclear spin (I = 5/2). ^{14}N hyperfine splitting not resolved.
[b]) Blended lines.

Molecular parameters for ^{25}Mg^{14}N^{12}C

Parameter		Value	Method	Ref.
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (0,0,0)				
B	[MHz]	5 855.312(12) [a])	MW	94An
D	[kHz]	3.998(6)		
γ	[MHz]	14.89(16)		
$b(^{25}$Mg)	[MHz]	– 303(5)		
$c(^{25}$Mg)	[MHz]	14.72 [b])		
$eQq_0(^{25}$Mg)	[MHz]	– 19.5 (10)		

[a]) The numbers in parenthesis represent 1 standard deviation of the least-squares fit, in units of the last quoted decimal place.
[b]) Parameter constrained to this value in the least-squares fit.

Microwave data for ^{26}Mg^{14}N^{12}C

Transition		ν [MHz]	Ref.
rotational $N' - N''$	fine structure $J' - J''$ [a])		
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (0,0,0)			
26 ← 25	$25\frac{1}{2} \leftarrow 24\frac{1}{2}$	298 844.284	94An
	$26\frac{1}{2} \leftarrow 25\frac{1}{2}$	298 858.961	
27 ← 26	$26\frac{1}{2} \leftarrow 25\frac{1}{2}$	310 316.349	
	$27\frac{1}{2} \leftarrow 26\frac{1}{2}$	310 331.025	
28 ← 27	$27\frac{1}{2} \leftarrow 26\frac{1}{2}$	321 785.901	
	$28\frac{1}{2} \leftarrow 27\frac{1}{2}$	321 800.610	
29 ← 28	$28\frac{1}{2} \leftarrow 27\frac{1}{2}$	333 252.907	
	$29\frac{1}{2} \leftarrow 28\frac{1}{2}$	333 267.571	
30 ← 29	$29\frac{1}{2} \leftarrow 28\frac{1}{2}$	344 717.206	
	$30\frac{1}{2} \leftarrow 29\frac{1}{2}$	344 731.878	
31 ← 30	$30\frac{1}{2} \leftarrow 29\frac{1}{2}$	356 178.843	
	$31\frac{1}{2} \leftarrow 30\frac{1}{2}$	356 193.461	
32 ← 31	$31\frac{1}{2} \leftarrow 30\frac{1}{2}$	367 637.561	
	$32\frac{1}{2} \leftarrow 31\frac{1}{2}$	367 652.239	

[a]) Nuclear hyperfine structure not resolved.

Molecular parameters for $^{26}Mg^{14}N^{12}C$

Parameter		Value	Method	Ref.
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (0,0,0)				
B	[MHz]	5 752.379 8(13) [a])	MW	94An
D	[kHz]	3.871 9(7)		
γ	[MHz]	14.671(20)		

[a]) The numbers in parenthesis represent 1 standard deviation of the least-squares fit, in units of the last quoted decimal place.

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3.2.1.2.41 CaNC

Microwave data for $^{40}Ca^{14}N^{12}C$

Transition: rotational $N'-N''$	fine structure $J'-J''$	Hyperfine [a]) $F'-F''$	ν [MHz]	Ref.
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (0,0,0)				
$1 \leftarrow 0$	$1\frac{1}{2} \leftarrow \frac{1}{2}$	$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	8 106.515(4) [b])	94Sc
$2 \leftarrow 1$	$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	16 203.892(10)	
		$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	16 203.886(4)	
		$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	16 204.180(10)	
		$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	16 204.177(4)	
		$1\frac{1}{2} \leftarrow \frac{1}{2}$	16 204.363(10)	
		$1\frac{1}{2} \leftarrow \frac{1}{2}$	16 204.374(4)	
		$2\frac{1}{2} \leftarrow 2\frac{1}{2}$	16 196.471(10)	
		$2\frac{1}{2} \leftarrow 2\frac{1}{2}$	16 196.485(4)	
	$1\frac{1}{2} \leftarrow \frac{1}{2}$	$1\frac{1}{2} \leftarrow 1\frac{1}{2}$	16 190.519(10)	
		$1\frac{1}{2} \leftarrow 1\frac{1}{2}$	16 190.514(4)	
		$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	16 185.536(10)	
		$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	16 185.540(4)	
		$1\frac{1}{2} \leftarrow \frac{1}{2}$	16 185.363(10)	
		$1\frac{1}{2} \leftarrow \frac{1}{2}$	16 185.361(4)	
		$1\frac{1}{2} \leftarrow 1\frac{1}{2}$	16 160.130(10)	
	$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	$2\frac{1}{2} \leftarrow 2\frac{1}{2}$	16 199.185(10)	
$3 \leftarrow 2$	$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	$4\frac{1}{2} \leftarrow 3\frac{1}{2}$	24 301.017(10)	
		$4\frac{1}{2} \leftarrow 3\frac{1}{2}$	24 301.023(4)	
		$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	24 301.141(4)	
		$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	24 301.215(4)	
	$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	24 282.810(10)	

		$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	24 282.840(4)	
		$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	24 282.782(4)	
		$1\frac{1}{2} \leftarrow \frac{1}{2}$	24 282.974(10)	
		$1\frac{1}{2} \leftarrow \frac{1}{2}$	24 282.956(4)	
		$2\frac{1}{2} \leftarrow 2\frac{1}{2}$	24 238.740(10)	
$5 \leftarrow 4$	$5\frac{1}{2} \leftarrow 4\frac{1}{2}$	$6\frac{1}{2} \leftarrow 5\frac{1}{2}$	40 494.096(10)	
$6 \leftarrow 5$	$5\frac{1}{2} \leftarrow 4\frac{1}{2}$	$6\frac{1}{2} \leftarrow 5\frac{1}{2}$	48 571.690(10)	
	$6\frac{1}{2} \leftarrow 5\frac{1}{2}$	$7\frac{1}{2} \leftarrow 6\frac{1}{2}$	48 589.794(10)	
$17 \leftarrow 16$	$16\frac{1}{2} \leftarrow 15\frac{1}{2}$	[c])	137 553.750(80)	93St
	$17\frac{1}{2} \leftarrow 16\frac{1}{2}$	[c])	137 571.734(80)	
$18 \leftarrow 17$	$17\frac{1}{2} \leftarrow 16\frac{1}{2}$	[c])	145 633.943(80)	
	$18\frac{1}{2} \leftarrow 17\frac{1}{2}$	[c])	145 651.922(80)	
$19 \leftarrow 18$	$18\frac{1}{2} \leftarrow 17\frac{1}{2}$	[c])	153 712.328(80)	
	$19\frac{1}{2} \leftarrow 18\frac{1}{2}$	[c])	153 730.281(80)	
$20 \leftarrow 19$	$19\frac{1}{2} \leftarrow 18\frac{1}{2}$	[c])	161 788.578(80)	
	$20\frac{1}{2} \leftarrow 19\frac{1}{2}$	[c])	161 806.594(80)	
$30 \leftarrow 29$	$29\frac{1}{2} \leftarrow 28\frac{1}{2}$	[c])	242 427.891(80)	
	$30\frac{1}{2} \leftarrow 29\frac{1}{2}$	[c])	242 445.813(80)	
$31 \leftarrow 30$	$30\frac{1}{2} \leftarrow 29\frac{1}{2}$	[c])	250 477.953(80)	
	$31\frac{1}{2} \leftarrow 30\frac{1}{2}$	[c])	250 495.938(80)	
$32 \leftarrow 31$	$31\frac{1}{2} \leftarrow 30\frac{1}{2}$	[c])	258 525.513 [d])	
	$32\frac{1}{2} \leftarrow 31\frac{1}{2}$	[c])	258 543.328(80)	
$33 \leftarrow 32$	$32\frac{1}{2} \leftarrow 31\frac{1}{2}$	[c])	266 570.000(80)	
	$33\frac{1}{2} \leftarrow 32\frac{1}{2}$	[c])	266 587.938(80)	
$34 \leftarrow 33$	$33\frac{1}{2} \leftarrow 32\frac{1}{2}$	[c])	274 611.844(80)	
	$34\frac{1}{2} \leftarrow 33\frac{1}{2}$	[c])	274 629.750(80)	
$35 \leftarrow 34$	$34\frac{1}{2} \leftarrow 33\frac{1}{2}$	[c])	282 650.813(80)	
	$35\frac{1}{2} \leftarrow 34\frac{1}{2}$	[c])	282 668.719(80)	
$43 \leftarrow 42$	$42\frac{1}{2} \leftarrow 41\frac{1}{2}$	[c])	346 854.844(80)	
	$43\frac{1}{2} \leftarrow 42\frac{1}{2}$	[c])	346 872.656(80)	
$44 \leftarrow 43$	$43\frac{1}{2} \leftarrow 42\frac{1}{2}$	[c])	354 866.281(80)	
	$44\frac{1}{2} \leftarrow 43\frac{1}{2}$	[c])	354 884.156(80)	
$45 \leftarrow 44$	$44\frac{1}{2} \leftarrow 43\frac{1}{2}$	[c])	362 874.563(80)	
	$45\frac{1}{2} \leftarrow 44\frac{1}{2}$	[c])	362 892.406(80)	
$46 \leftarrow 45$	$45\frac{1}{2} \leftarrow 44\frac{1}{2}$	[c])	370 879.688(80)	
	$46\frac{1}{2} \leftarrow 45\frac{1}{2}$	[c])	370 897.500(80)	

[a]) Coupling scheme: $\boldsymbol{J} = \boldsymbol{N} + \boldsymbol{S}$; $\boldsymbol{F} = \boldsymbol{J} + \boldsymbol{I}_1$ where $\boldsymbol{I}_1$ is the ^{14}N nuclear spin.
[b]) The figures in parenthesis are the authors' estimate of the experimental uncertainty, in units of the last quoted decimal place.
[c]) ^{14}N hyperfine splitting not resolved.
[d]) Overlapped with a line from a contaminating species.

Molecular parameters for $^{40}Ca^{14}N^{12}C$

Parameter		Value	Method	Ref.
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (0,0,0)				
B	[MHz]	4 048.754 332(29) [a])	MW, MODR	94Sc
D	[kHz]	4.96(3)		
γ	[MHz]	18.055 06(23)		
γ_D	[kHz]	− 0.32(13)		
$b_F(^{14}N)$	[MHz]	12.481 49(93)		
$c(^{14}N)$	[MHz]	2.073 5(14)		
$eQq_0(^{14}N)$	[MHz]	− 2.697 4(11)		
μ	[D]	6.895(9)	Opt Stark	92St

[a]) The numbers in parentheses represent 1 standard deviation of the least-squares fit, in units of the last quoted decimal place.

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3.2.1.2.42 MgCCH

Microwave data for $^{24}Mg^{12}C^{12}C^{1}H$

Transition		ν [MHz]	Ref.
rotational $N' - N''$	fine structure $J' - J''$ [a])		
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (0,0,0,0,0)			
32 ← 31	$31\frac{1}{2} \leftarrow 30\frac{1}{2}$	317 480.813	99Br [b])
	$32\frac{1}{2} \leftarrow 31\frac{1}{2}$	317 497.414	
33 ← 32	$32\frac{1}{2} \leftarrow 31\frac{1}{2}$	327 383.235	
	$33\frac{1}{2} \leftarrow 32\frac{1}{2}$	327 399.797	
34 ← 33	$33\frac{1}{2} \leftarrow 32\frac{1}{2}$	337 283.890	
	$34\frac{1}{2} \leftarrow 33\frac{1}{2}$	337 300.444	
35 ← 34	$34\frac{1}{2} \leftarrow 33\frac{1}{2}$	347 182.751	
	$35\frac{1}{2} \leftarrow 34\frac{1}{2}$	347 199.272	
36 ← 35	$35\frac{1}{2} \leftarrow 34\frac{1}{2}$	357 079.709	
	$36\frac{1}{2} \leftarrow 35\frac{1}{2}$	357 096.278	
37 ← 36	$36\frac{1}{2} \leftarrow 35\frac{1}{2}$	366 974.804	
	$37\frac{1}{2} \leftarrow 36\frac{1}{2}$	366 991.309	
38 ← 37	$37\frac{1}{2} \leftarrow 36\frac{1}{2}$	376 867.871	
	$38\frac{1}{2} \leftarrow 37\frac{1}{2}$	376 884.383	
39 ← 38	$38\frac{1}{2} \leftarrow 37\frac{1}{2}$	386 758.930	
	$39\frac{1}{2} \leftarrow 38\frac{1}{2}$	386 775.451	
40 ← 39	$39\frac{1}{2} \leftarrow 38\frac{1}{2}$	396 647.909	
	$40\frac{1}{2} \leftarrow 39\frac{1}{2}$	396 664.421	
41 ← 40	$40\frac{1}{2} \leftarrow 39\frac{1}{2}$	406 534.724	
	$41\frac{1}{2} \leftarrow 40\frac{1}{2}$	406 551.247	
42 ← 41	$41\frac{1}{2} \leftarrow 40\frac{1}{2}$	416 419.411	

	$42\frac{1}{2} \leftarrow 41\frac{1}{2}$	416 435.888
$43 \leftarrow 42$	$42\frac{1}{2} \leftarrow 41\frac{1}{2}$	426 301.796
	$43\frac{1}{2} \leftarrow 42\frac{1}{2}$	426 318.346
$44 \leftarrow 43$	$43\frac{1}{2} \leftarrow 42\frac{1}{2}$	436 181.970
	$44\frac{1}{2} \leftarrow 43\frac{1}{2}$	436 198.470
$45 \leftarrow 44$	$44\frac{1}{2} \leftarrow 43\frac{1}{2}$	446 059.752
	$45\frac{1}{2} \leftarrow 44\frac{1}{2}$	446 076.240
$46 \leftarrow 45$	$45\frac{1}{2} \leftarrow 44\frac{1}{2}$	455 935.155
	$46\frac{1}{2} \leftarrow 45\frac{1}{2}$	455 951.635
$47 \leftarrow 46$	$46\frac{1}{2} \leftarrow 45\frac{1}{2}$	465 808.128
	$47\frac{1}{2} \leftarrow 46\frac{1}{2}$	465 824.563
$48 \leftarrow 47$	$47\frac{1}{2} \leftarrow 46\frac{1}{2}$	475 678.561
	$48\frac{1}{2} \leftarrow 47\frac{1}{2}$	475 695.022
$49 \leftarrow 48$	$48\frac{1}{2} \leftarrow 47\frac{1}{2}$	485 546.464
	$49\frac{1}{2} \leftarrow 48\frac{1}{2}$	485 562.911
$50 \leftarrow 49$	$49\frac{1}{2} \leftarrow 48\frac{1}{2}$	495 411.765
	$50\frac{1}{2} \leftarrow 49\frac{1}{2}$	495 428.094
$51 \leftarrow 50$	$50\frac{1}{2} \leftarrow 49\frac{1}{2}$	505 274.375
	$51\frac{1}{2} \leftarrow 50\frac{1}{2}$	505 290.800
$52 \leftarrow 51$	$51\frac{1}{2} \leftarrow 50\frac{1}{2}$	515 134.329
	$52\frac{1}{2} \leftarrow 51\frac{1}{2}$	515 150.713
$53 \leftarrow 52$	$52\frac{1}{2} \leftarrow 51\frac{1}{2}$	524 991.472
	$53\frac{1}{2} \leftarrow 52\frac{1}{2}$	525 007.857

[a]) Nuclear hyperfine structure not resolved.
[b]) Original measurements and assignments, given by [95An], have been superseded by those given here.

Microwave data for $^{24}Mg^{12}C^{12}C^{1}H$

Transition			ν [MHz]	Ref.
rotational $N' - N''$	parity [a])	fine structure $J' - J''$		
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (0,0,0,0,1[1])				
$32 \leftarrow 31$	*e*	$31\frac{1}{2} \leftarrow 30\frac{1}{2}$	319 555.690	99Br
		$32\frac{1}{2} \leftarrow 31\frac{1}{2}$	319 572.094	
	f	$31\frac{1}{2} \leftarrow 30\frac{1}{2}$	320 321.234	
		$32\frac{1}{2} \leftarrow 31\frac{1}{2}$	320 337.714	
$33 \leftarrow 32$	*e*	$32\frac{1}{2} \leftarrow 31\frac{1}{2}$	329 521.182	
		$33\frac{1}{2} \leftarrow 32\frac{1}{2}$	329 537.744	
	f	$32\frac{1}{2} \leftarrow 31\frac{1}{2}$	330 309.674	
		$33\frac{1}{2} \leftarrow 32\frac{1}{2}$	330 326.131	
$34 \leftarrow 33$	*e*	$33\frac{1}{2} \leftarrow 32\frac{1}{2}$	339 484.813	
		$34\frac{1}{2} \leftarrow 33\frac{1}{2}$	339 501.272	
	f	$33\frac{1}{2} \leftarrow 32\frac{1}{2}$	340 296.114	
		$34\frac{1}{2} \leftarrow 33\frac{1}{2}$	340 312.552	
$35 \leftarrow 34$	*e*	$34\frac{1}{2} \leftarrow 33\frac{1}{2}$	349 446.508	
		$35\frac{1}{2} \leftarrow 34\frac{1}{2}$	349 462.977	

	f	$34\frac{1}{2} \leftarrow 33\frac{1}{2}$	350 280.465	
		$35\frac{1}{2} \leftarrow 34\frac{1}{2}$	350 312.552	
$36 \leftarrow 35$	*e*	$35\frac{1}{2} \leftarrow 34\frac{1}{2}$	359 406.173	
		$36\frac{1}{2} \leftarrow 35\frac{1}{2}$	359 422.576	
	f	$35\frac{1}{2} \leftarrow 34\frac{1}{2}$	360 262.697	
		$36\frac{1}{2} \leftarrow 35\frac{1}{2}$	360 279.131	
$37 \leftarrow 36$	*e*	$36\frac{1}{2} \leftarrow 35\frac{1}{2}$	369 363.604	
		$37\frac{1}{2} \leftarrow 36\frac{1}{2}$	369 380.100	
	f	$36\frac{1}{2} \leftarrow 35\frac{1}{2}$	370 242.777	
		$37\frac{1}{2} \leftarrow 36\frac{1}{2}$	370 259.215	
$38 \leftarrow 37$	*e*	$37\frac{1}{2} \leftarrow 36\frac{1}{2}$	379 319.085	
		$38\frac{1}{2} \leftarrow 37\frac{1}{2}$	379 335.518	
$39 \leftarrow 38$	*e*	$38\frac{1}{2} \leftarrow 37\frac{1}{2}$	389 272.236	
		$39\frac{1}{2} \leftarrow 38\frac{1}{2}$	389 288.658	
$40 \leftarrow 39$	*e*	$39\frac{1}{2} \leftarrow 38\frac{1}{2}$	399 223.271	
		$40\frac{1}{2} \leftarrow 39\frac{1}{2}$	399 239.657	
$41 \leftarrow 40$	*e*	$40\frac{1}{2} \leftarrow 39\frac{1}{2}$	409 171.807	
		$41\frac{1}{2} \leftarrow 40\frac{1}{2}$	409 188.230	
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational $(0,0,0,0,2^0)$				
$32 \leftarrow 31$	*f*	$31\frac{1}{2} \leftarrow 30\frac{1}{2}$	322 477.972	99Br
	e	$32\frac{1}{2} \leftarrow 31\frac{1}{2}$	322 494.218	
$33 \leftarrow 32$	*f*	$32\frac{1}{2} \leftarrow 31\frac{1}{2}$	332 531.907	
	e	$33\frac{1}{2} \leftarrow 32\frac{1}{2}$	332 548.023	
$34 \leftarrow 33$	*f*	$33\frac{1}{2} \leftarrow 32\frac{1}{2}$	342 583.581	
	e	$34\frac{1}{2} \leftarrow 33\frac{1}{2}$	342 599.754	
$35 \leftarrow 34$	*f*	$34\frac{1}{2} \leftarrow 33\frac{1}{2}$	352 633.120	
	e	$35\frac{1}{2} \leftarrow 34\frac{1}{2}$	352 649.249	
$36 \leftarrow 35$	*f*	$35\frac{1}{2} \leftarrow 34\frac{1}{2}$	362 680.097	
	e	$36\frac{1}{2} \leftarrow 35\frac{1}{2}$	362 696.337	
$37 \leftarrow 36$	*f*	$36\frac{1}{2} \leftarrow 35\frac{1}{2}$	372 724.867	
	e	$37\frac{1}{2} \leftarrow 36\frac{1}{2}$	372 741.104	
$38 \leftarrow 37$	*f*	$37\frac{1}{2} \leftarrow 36\frac{1}{2}$	382 767.111	
	e	$38\frac{1}{2} \leftarrow 37\frac{1}{2}$	382 783.463	
$39 \leftarrow 38$	*f*	$38\frac{1}{2} \leftarrow 37\frac{1}{2}$	392 806.919	
	e	$39\frac{1}{2} \leftarrow 38\frac{1}{2}$	392 823.280	
$40 \leftarrow 39$	*f*	$39\frac{1}{2} \leftarrow 38\frac{1}{2}$	402 844.233	
	e	$40\frac{1}{2} \leftarrow 39\frac{1}{2}$	402 860.512	
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational $(0,0,0,0,2^2)$				
$32 \leftarrow 31$	*e*	$31\frac{1}{2} \leftarrow 30\frac{1}{2}$	322 410.880	99Br
		$32\frac{1}{2} \leftarrow 31\frac{1}{2}$	322 427.363	
	f	$31\frac{1}{2} \leftarrow 30\frac{1}{2}$	322 566.780	
		$32\frac{1}{2} \leftarrow 31\frac{1}{2}$	322 583.041	
$33 \leftarrow 32$	*e*	$32\frac{1}{2} \leftarrow 31\frac{1}{2}$	332 456.730	
		$33\frac{1}{2} \leftarrow 32\frac{1}{2}$	332 473.246	
	f	$32\frac{1}{2} \leftarrow 31\frac{1}{2}$	332 628.988	

		$33\frac{1}{2} \leftarrow 32\frac{1}{2}$	332 645.276
$34 \leftarrow 33$	*e*	$33\frac{1}{2} \leftarrow 32\frac{1}{2}$	342 499.957
		$34\frac{1}{2} \leftarrow 33\frac{1}{2}$	342 516.437
	f	$33\frac{1}{2} \leftarrow 32\frac{1}{2}$	342 689.464
		$34\frac{1}{2} \leftarrow 33\frac{1}{2}$	342 705.703
$35 \leftarrow 34$	*e*	$34\frac{1}{2} \leftarrow 33\frac{1}{2}$	352 540.386
		$35\frac{1}{2} \leftarrow 34\frac{1}{2}$	352 556.874
	f	$34\frac{1}{2} \leftarrow 33\frac{1}{2}$	352 748.188
		$35\frac{1}{2} \leftarrow 34\frac{1}{2}$	352 764.423
$36 \leftarrow 35$	*e*	$35\frac{1}{2} \leftarrow 34\frac{1}{2}$	362 577.908
		$36\frac{1}{2} \leftarrow 35\frac{1}{2}$	362 594.384
	f	$35\frac{1}{2} \leftarrow 34\frac{1}{2}$	362 805.058
		$36\frac{1}{2} \leftarrow 35\frac{1}{2}$	362 821.327
$37 \leftarrow 36$	*e*	$36\frac{1}{2} \leftarrow 35\frac{1}{2}$	372 612.518
		$37\frac{1}{2} \leftarrow 36\frac{1}{2}$	372 629.046
	f	$36\frac{1}{2} \leftarrow 35\frac{1}{2}$	372 860.065
		$37\frac{1}{2} \leftarrow 36\frac{1}{2}$	372 876.286
$38 \leftarrow 37$	*e*	$37\frac{1}{2} \leftarrow 36\frac{1}{2}$	382 644.201
		$38\frac{1}{2} \leftarrow 37\frac{1}{2}$	382 660.794
	f	$37\frac{1}{2} \leftarrow 36\frac{1}{2}$	382 913.050
		$38\frac{1}{2} \leftarrow 37\frac{1}{2}$	382 929.413
$39 \leftarrow 38$	*e*	$38\frac{1}{2} \leftarrow 37\frac{1}{2}$	392 672.924
		$39\frac{1}{2} \leftarrow 38\frac{1}{2}$	392 689.457
	f	$38\frac{1}{2} \leftarrow 37\frac{1}{2}$	392 964.236
		$39\frac{1}{2} \leftarrow 38\frac{1}{2}$	392 980.394
$40 \leftarrow 39$	*e*	$39\frac{1}{2} \leftarrow 38\frac{1}{2}$	402 698.463
		$40\frac{1}{2} \leftarrow 39\frac{1}{2}$	402 714.936
	f	$39\frac{1}{2} \leftarrow 38\frac{1}{2}$	403 013.104
		$40\frac{1}{2} \leftarrow 39\frac{1}{2}$	403 029.396

[a]) States with parity equal to $\pm(-1)^{J-0.5}$ are labeled *e* and *f* respectively.

Molecular parameters for $^{24}Mg^{12}C^{12}C^{1}H$

Parameter		Value	Method	Ref.
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (0,0,0,0,0)				
B	[MHz]	4 965.334 6(38) [a])	MW	99Br
D	[kHz]	2.232 4(20)		
H	[Hz]	0.001 44(34)		
γ	[MHz]	16.488(45)		
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (0,0,0,0,1^1)				
B	[MHz]	5 004.250 1(36) [a])	MW	99Br
D	[kHz]	2.484 7(14)		
γ	[MHz]	16.447(53)		
q	[MHz]	– 12.210 6(71)		
q_D	[kHz]	0.121 2(29)		
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (0,0,0,0,2^0)				
B	[MHz]	5 044.516 6(35) [a])	MW	99Br

D	[kHz]	2.769 7(13)		
γ	[MHz]	16.237(71)		
State: electronic $\widetilde{X}\,^2\Sigma^+$; vibrational (0,0,0,0,2^0)				
B	[MHz]	5 044.710 0(25) [a])	MW	99Br
D	[kHz]	2.791 70(93)		
γ	[MHz]	16.383(50)		
q	[kHz]	– 0.952(16)		
q_D	[Hz]	– 0.226(16)		
q_H	[Hz]	$0.517(44)\times10^{-4}$		

[a]) The numbers in parentheses are 3 standard deviations of the least-squares fit, in units of the last quoted decimal place.

References for MgCCH

95And Anderson, M.A., Ziurys, L.M. : Astrophys. J. **439** (1995) L25.
99Br Brewster, M.A., Apponi, A.J., Xin, J., Ziurys, L.M. : Chem. Phys. Letts. **310** (1999) 411.

3.2.1.2.43 CaCCH

Microwave data for $^{40}Ca^{12}C^{12}C^{1}H$

Transition: rotational $N' - N''$	Transition: fine structure $J' - J''$ [a])	ν [MHz]	Ref.
State: electronic $\widetilde{X}\,^2\Sigma^+$; vibrational (0,0,0,0,0)			
34 ← 33	$33\frac{1}{2} \leftarrow 32\frac{1}{2}$	230 748.207	95An
	$34\frac{1}{2} \leftarrow 33\frac{1}{2}$	230 770.046	
35 ← 34	$34\frac{1}{2} \leftarrow 33\frac{1}{2}$	237 522.807	
	$35\frac{1}{2} \leftarrow 34\frac{1}{2}$	237 544.672	
36 ← 35	$35\frac{1}{2} \leftarrow 34\frac{1}{2}$	244 296.354	
	$36\frac{1}{2} \leftarrow 35\frac{1}{2}$	244 318.207	
37 ← 36	$36\frac{1}{2} \leftarrow 35\frac{1}{2}$	251 068.882	
	$37\frac{1}{2} \leftarrow 36\frac{1}{2}$	251 090.749	
38 ← 37	$37\frac{1}{2} \leftarrow 36\frac{1}{2}$	257 840.206	
	$38\frac{1}{2} \leftarrow 37\frac{1}{2}$	257 862.073	
39 ← 38	$38\frac{1}{2} \leftarrow 37\frac{1}{2}$	264 610.432	
	$39\frac{1}{2} \leftarrow 38\frac{1}{2}$	264 632.227	
40 ← 39	$39\frac{1}{2} \leftarrow 38\frac{1}{2}$	271 379.356	
	$40\frac{1}{2} \leftarrow 39\frac{1}{2}$	271 401.185	
41 ← 40	$40\frac{1}{2} \leftarrow 39\frac{1}{2}$	278 147.162	
	$41\frac{1}{2} \leftarrow 40\frac{1}{2}$	278 168.997	
43 ← 42	$42\frac{1}{2} \leftarrow 41\frac{1}{2}$	291 678.989	
	$43\frac{1}{2} \leftarrow 42\frac{1}{2}$	291 700.823	
44 ← 43	$43\frac{1}{2} \leftarrow 42\frac{1}{2}$	298 442.881	
	$44\frac{1}{2} \leftarrow 43\frac{1}{2}$	298 464.707	
45 ← 44	$44\frac{1}{2} \leftarrow 43\frac{1}{2}$	305 205.500	
	$45\frac{1}{2} \leftarrow 44\frac{1}{2}$	305 227.335	
46 ← 45	$45\frac{1}{2} \leftarrow 44\frac{1}{2}$	311 966.739	
	$46\frac{1}{2} \leftarrow 45\frac{1}{2}$	311 988.552	
47 ← 46	$46\frac{1}{2} \leftarrow 45\frac{1}{2}$	318 726.584	

	$47\frac{1}{2} \leftarrow 46\frac{1}{2}$	318 748.420
$48 \leftarrow 47$	$47\frac{1}{2} \leftarrow 46\frac{1}{2}$	325 484.991
	$48\frac{1}{2} \leftarrow 47\frac{1}{2}$	325 506.813
$49 \leftarrow 48$	$48\frac{1}{2} \leftarrow 47\frac{1}{2}$	332 241.995
	$49\frac{1}{2} \leftarrow 48\frac{1}{2}$	332 263.809
$50 \leftarrow 49$	$49\frac{1}{2} \leftarrow 48\frac{1}{2}$	338 997.456
	$50\frac{1}{2} \leftarrow 49\frac{1}{2}$	339 019.224
$51 \leftarrow 50$	$50\frac{1}{2} \leftarrow 49\frac{1}{2}$	345 751.410
	$51\frac{1}{2} \leftarrow 50\frac{1}{2}$	345 773.231
$52 \leftarrow 51$	$51\frac{1}{2} \leftarrow 50\frac{1}{2}$	352 503.838
	$52\frac{1}{2} \leftarrow 51\frac{1}{2}$	352 525.627
$53 \leftarrow 52$	$52\frac{1}{2} \leftarrow 51\frac{1}{2}$	359 254.692
	$53\frac{1}{2} \leftarrow 52\frac{1}{2}$	359 276.486
$54 \leftarrow 53$	$53\frac{1}{2} \leftarrow 52\frac{1}{2}$	366 003.963
	$54\frac{1}{2} \leftarrow 53\frac{1}{2}$	366 025.750
$55 \leftarrow 54$	$54\frac{1}{2} \leftarrow 53\frac{1}{2}$	372 751.592
	$55\frac{1}{2} \leftarrow 54\frac{1}{2}$	372 773.358
$56 \leftarrow 55$	$55\frac{1}{2} \leftarrow 54\frac{1}{2}$	379 497.551
	$55\frac{1}{2} \leftarrow 54\frac{1}{2}$	379 519.360

[a]) Nuclear hyperfine structure not resolved

Molecular parameters for $^{40}Ca^{12}C^{12}C^{1}H$

Parameter		Value	Method	Ref.
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (0,0,0,0,0)				
B	[MHz]	43 396.489 6(13) [a])	MW	95An
D	[kHz]	1.290 44(64)		
H	[Hz]	0.002 456(96)		
γ	[MHz]	21.821(17)		
μ	[D]	2.41(2)	Opt. Stark	95Mar

[a]) The numbers in parentheses are 3 standard deviations of the least-squares fit, in units of the last quoted decimal place.

Reference for CaCCH

95An Anderson, M.A., Ziurys, L.M. : Astrophys. J. **444** (1995) L57.
95Mar Marr, A.J., Perry, J., Steimle, T.C. : J.Chem.Phys. **103** (1995) 3861.

3.2.1.2.44 SrCCH

Microwave data for $^{86}Sr^{12}C^{12}C^{1}H$

Transition		ν [MHz]	Ref.
rotational $N' - N''$	fine structure $J' - J''$ [a])		
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (0,0,0,0,0)			
57 ← 56	$56\frac{1}{2} \leftarrow 55\frac{1}{2}$	284 341.205	95Nu
	$57\frac{1}{2} \leftarrow 56\frac{1}{2}$	284 392.047	
58 ← 57	$57\frac{1}{2} \leftarrow 56\frac{1}{2}$	289 309.021	
	$58\frac{1}{2} \leftarrow 57\frac{1}{2}$	289 360.005	
59 ← 58	$58\frac{1}{2} \leftarrow 57\frac{1}{2}$	294 275.963	
	$59\frac{1}{2} \leftarrow 58\frac{1}{2}$	294 326.862	
60 ← 59	$59\frac{1}{2} \leftarrow 58\frac{1}{2}$	299 241.732	
	$60\frac{1}{2} \leftarrow 59\frac{1}{2}$	299 292.673	
61 ← 60	$60\frac{1}{2} \leftarrow 59\frac{1}{2}$	304 206.450	
	$61\frac{1}{2} \leftarrow 60\frac{1}{2}$	304 257.345	
62 ← 61	$61\frac{1}{2} \leftarrow 60\frac{1}{2}$	309 170.135	
	$62\frac{1}{2} \leftarrow 61\frac{1}{2}$	309 220.911	
63 ← 62	$62\frac{1}{2} \leftarrow 61\frac{1}{2}$	314 132.502	
64 ← 63	$63\frac{1}{2} \leftarrow 62\frac{1}{2}$	319 093.734	
	$64\frac{1}{2} \leftarrow 63\frac{1}{2}$	319 144.628	
65 ← 64	$64\frac{1}{2} \leftarrow 63\frac{1}{2}$	324 053.814	
	$65\frac{1}{2} \leftarrow 64\frac{1}{2}$	324 104.732	
66 ← 65	$65\frac{1}{2} \leftarrow 64\frac{1}{2}$	329 012.757	
	$66\frac{1}{2} \leftarrow 65\frac{1}{2}$	329 063.670	
67 ← 66	$66\frac{1}{2} \leftarrow 65\frac{1}{2}$	333 970.462	
	$67\frac{1}{2} \leftarrow 66\frac{1}{2}$	334 021.353	
69 ← 68	$68\frac{1}{2} \leftarrow 67\frac{1}{2}$	343 882.173	
	$69\frac{1}{2} \leftarrow 68\frac{1}{2}$	343 932.947	
70 ← 69	$46\frac{1}{2} \leftarrow 45\frac{1}{2}$	348 836.241	
	$47\frac{1}{2} \leftarrow 46\frac{1}{2}$	348 887.022	
71 ← 70	$47\frac{1}{2} \leftarrow 46\frac{1}{2}$	353 788.895	
	$48\frac{1}{2} \leftarrow 47\frac{1}{2}$	353 839.741	
72 ← 71	$48\frac{1}{2} \leftarrow 47\frac{1}{2}$	358 740.278	
73 ← 72	$49\frac{1}{2} \leftarrow 48\frac{1}{2}$	363 690.522	
	$50\frac{1}{2} \leftarrow 49\frac{1}{2}$	363 741.270	
74 ← 73	$50\frac{1}{2} \leftarrow 49\frac{1}{2}$	368 639.256	
	$51\frac{1}{2} \leftarrow 50\frac{1}{2}$	368 690.115	

[a]) Nuclear hyperfine structure not resolved

Molecular parameters for $^{86}Sr^{12}C^{12}C^{1}H$

Parameter		Value	Method	Ref.
State: electronic $\tilde{X}\,^2\Sigma^+$; vibrational (0,0,0,0,0)				
B	[MHz]	2 499.604 0(56) [a])	MW	95Nu
D	[kHz]	0.803 6(13)		
H	[Hz]	0.001 9(1)		
γ	[MHz]	50.865(32)		

[a])The numbers in parentheses are 3 standard deviations of the least-squares fit, in units of the last quoted decimal place.

Reference for SrCCH

95Nu Nuccio, B.P., Apponi, A.J., Ziurys, L.M. : Chem. Phys. Letts. **247** (1995) 283.

3.2.1.2.45 ArOH

Microwave data for $^{40}Ar^{16}O^{1}H$

Transition				ν [MHz]	Ref.
rotational $J' - J''$	spin P	parity	hyperfine $F' - F''$		
State: electronic $\tilde{X}\,^2\Pi$; vibrational zero point level					
$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	$1\frac{1}{2} \leftarrow 1\frac{1}{2}$	$+ \leftarrow -$	$2 \leftarrow 1$	15 349.305(5) [a])	91Oh
			$3 \leftarrow 2$	15 336.420(5)	
			$2 \leftarrow 2$	15 310.581(5)	
		$- \leftarrow +$	$2 \leftarrow 1$	15 364.495(5)	94En
			$3 \leftarrow 2$	15 351.583(5)	
			$2 \leftarrow 2$	15 325.777(5)	
$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	$1\frac{1}{2} \leftarrow 1\frac{1}{2}$	$+ \leftarrow -$	$3 \leftarrow 2$	21 469.644(5)	
			$4 \leftarrow 3$	21 463.955(5)	
		$- \leftarrow +$	$3 \leftarrow 2$	21 499.253(5)	
			$4 \leftarrow 3$	21 493.518(5)	
$1\frac{1}{2} \leftarrow 1\frac{1}{2}$	$\frac{1}{2} \leftarrow 1\frac{1}{2}$		[b])	291 000	92Be
			[b])	576 000	
			[b])	639 000	

[a]) The figures in parentheses are the authors' estimates of experimental uncertainty (1σ).
[b]) ^{1}H hyperfine structure not resolved.

Molecular parameters for $^{40}Ar^{16}O^{1}H$

Parameter		Value	Method	Ref.
State: electronic $\tilde{X}^2\Pi$; vibrational zero point level				
B	[MHz]	2 982.15(143) [a])	FTMW	94En
D	[kHz]	– 58.150(122)		
A	[GHz]	– 4 169 [b])		
B_{OH}	[MHz]	555 537 [b])		
γ	[MHz]	– 3 690 [b])		
p	[MHz]	7 052 [b])		
q	[MHz]	– 1 160 [b])		
$h_1(^1H)$	[MHz]	94.230(33)		
$h_2(^1H)$	[MHz]	79.1 [b])		
$b(^1H)$	[MHz]	– 116.7 [b])		
$d(^1H)$	[MHz]	56.65 [b])		
V_1^0 [c])	[GHz]	– 475.00(128)		
V_2^0	[GHz]	– 378.0(25)		
V_3^0	[GHz]	– 194.0(106)		
V_2^2	[GHz]	1 293.0(108)		
V_{2D}	[MHz]	– 2 200 [d])		

[a]) The numbers in parentheses represent 1 standard deviation of the least-squares fit, in units of the last quoted decimal place.
[b]) Constrained to the value for isolated OH. ArOH is a van der Waals complex.
[c]) The parameters V_l^k are the coefficients in the intermolecular potential between OH and the Ar atom.
[d]) The value of this parameter was adjusted manually to minimise the standard deviation of the fit.

Microwave data for $^{40}Ar^{16}O^{2}H$ (ArOD)

Transition				ν [MHz]	Ref.
rotational $J' - J''$	spin P	parity	hyperfine $F' - F''$		
State: electronic $\tilde{X}^2\Pi$; vibrational zero point level					
$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	$1\frac{1}{2} \leftarrow 1\frac{1}{2}$	$+ \leftarrow -$	$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	15 010.020(5) [a])	91Oh
			$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	15 013.551(5)	
			$1\frac{1}{2} \leftarrow \frac{1}{2}$	15 014.943(5)	
			$2\frac{1}{2} \leftarrow 2\frac{1}{2}$	15 004.347(5)	
			$1\frac{1}{2} \leftarrow 1\frac{1}{2}$	15 009.489(5)	

[a]) The figures in parentheses are the authors' estimates of experimental uncertainty (1σ).

Molecular parameters for $^{40}Ar^{16}O^{2}H$ (ArOD)

Parameter		Value	Method	Ref.
State: electronic $\tilde{X}^2\Pi$; vibrational zero point level				
B	[MHz]	3 002.985	FTMW	91Oh
q_J [a])	[MHz]	0.192		
h_1 [b])	[MHz]	9.005		
h_{1J} [b])	[MHz]	0.056		
eQq_0 [c])	[MHz]	0.145		
eQq_{0J} [c])	[MHz]	– 0.010		

[a]) P-doubling parameter, J-dependence assumed as $\pm q_J(J–1/2)(J+1/2)(J+3/2)$
[b]) Magnetic hfs splitting was analyzed with the J-dependence $h_1 + h_{1J}J(J+1)$
[c]) Deuteron nuclear quadrupole hfs was analyzed with the J-dependence $eQq_0 + eQq_{0J}J(J+1)$

References for ArOH

91OH Ohshima, Y., Iida, M., Endo, Y. : J. Chem. Phys. **95** (1991) 7001.
92Be Berry, M.T., Loomis, R.A., Giancarlo, L.C., Lester, M.I. : J. Chem. Phys. **96** (1992) 7890.
94En Endo, Y., Kohguchi, H., Ohshima, Y. : Faraday Discuss. **197** (1994) 341.

3.2.1.2.46 ArSH

Microwave data for $^{40}Ar^{32}S^{1}H$

Transition				ν [MHz]	Ref.
rotational $J' - J''$	spin P	parity	hyperfine $F' - F''$		
State: electronic $\tilde{X}^2\Pi$; vibrational zero point level					
$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	$1\frac{1}{2} \leftarrow 1\frac{1}{2}$	l [a])	$2 \leftarrow 1$	7 846.942(5) [b])	00Su
			$3 \leftarrow 2$	7 844.742(5)	
			$2 \leftarrow 2$	7 839.535(5)	
		u	$2 \leftarrow 1$	7 858.505(5)	
			$3 \leftarrow 2$	7 856.295(5)	
			$2 \leftarrow 2$	7 851.093(5)	
$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	$1\frac{1}{2} \leftarrow 1\frac{1}{2}$	l	$3 \leftarrow 2$	10 985.736(5)	
			$4 \leftarrow 3$	10 984.847(5)	
		u	$3 \leftarrow 2$	11 008.084(5)	
			$4 \leftarrow 3$	11 007.185(5)	
$4\frac{1}{2} \leftarrow 3\frac{1}{2}$	$1\frac{1}{2} \leftarrow 1\frac{1}{2}$	l	$4 \leftarrow 3$	14 128.309(5)	
			$5 \leftarrow 4$	14 127.889(5)	
		u	$4 \leftarrow 3$	14 163.924(5)	
			$5 \leftarrow 4$	14 163.494(5)	
$5\frac{1}{2} \leftarrow 4\frac{1}{2}$	$1\frac{1}{2} \leftarrow 1\frac{1}{2}$	l	$5 \leftarrow 4$	17 275.368(5)	
			$6 \leftarrow 5$	17 275.173(5)	
		u	$5 \leftarrow 4$	17 325.924(5)	
			$6 \leftarrow 5$	17 325.712(5)	
$6\frac{1}{2} \leftarrow 5\frac{1}{2}$	$1\frac{1}{2} \leftarrow 1\frac{1}{2}$	l	$6 \leftarrow 5$	20 427.751(5)	
			$7 \leftarrow 6$	20 427.665(5)	
		u	$6 \leftarrow 5$	20 494.028(5)	
			$7 \leftarrow 6$	20 493.930(5)	
$7\frac{1}{2} \leftarrow 6\frac{1}{2}$	$1\frac{1}{2} \leftarrow 1\frac{1}{2}$	l	$7 \leftarrow 6$	23 586.015(5) [c])	
			$8 \leftarrow 7$	23 586.015(5) [c])	

		u	7← 6	23 667.856(5) [c])	
			8← 7	23 667.856(5) [c])	
$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	$1\frac{1}{2} \leftarrow 1\frac{1}{2}$	l	8← 7	26 750.434(5) [c])	
			9← 8	26 750.434(5) [c])	

[a]) Upper or lower components of parity doubling.
[b]) The figures in parentheses are the authors' estimates of experimental uncertainty (1σ).
[c]) Proton hyperfine structure not resolved.

Microwave data for $^{40}Ar^{32}S^{2}H$ (ArSD)

Transition				ν [MHz]	Ref.
rotational $J' - J''$	spin P	parity	hyperfine $F' - F''$		
State: electronic $\tilde{X}^2\Pi$; vibrational zero point level					
$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	$1\frac{1}{2} \leftarrow 1\frac{1}{2}$	l [a])	$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	7 837.834(5) [b])	00Su
			$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	7.838.438(5)	
			$1\frac{1}{2} \leftarrow \frac{1}{2}$	7 838.629(5)	
			$2\frac{1}{2} \leftarrow 2\frac{1}{2}$	7 836.740(5)	
			$1\frac{1}{2} \leftarrow 1\frac{1}{2}$	7 837.660(5)	
		u	$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	7 843.703(5)	
			$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	7 844.305(5)	
			$1\frac{1}{2} \leftarrow \frac{1}{2}$	7 844.516(5)	
			$2\frac{1}{2} \leftarrow 2\frac{1}{2}$	7 842.615(5)	
			$1\frac{1}{2} \leftarrow 1\frac{1}{2}$	7 843.517(5)	
$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	$1\frac{1}{2} \leftarrow 1\frac{1}{2}$	l	$4\frac{1}{2} \leftarrow 3\frac{1}{2}$	10 975.690(5)	
			$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	10 975.925(5)	
			$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	10 976.026(5)	
		u	$4\frac{1}{2} \leftarrow 3\frac{1}{2}$	10 987.033(5)	
			$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	10 987.270(5)	
			$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	10 987.374(5)	
$4\frac{1}{2} \leftarrow 3\frac{1}{2}$	$1\frac{1}{2} \leftarrow 1\frac{1}{2}$	l	$5\frac{1}{2} \leftarrow 4\frac{1}{2}$	14 116.571(5)	
			$4\frac{1}{2} \leftarrow 3\frac{1}{2}$	14 116.691(5)	
			$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	14 116.725(5)	
		u	$5\frac{1}{2} \leftarrow 4\frac{1}{2}$	14 134.650(5)	
			$4\frac{1}{2} \leftarrow 3\frac{1}{2}$	14 134.764(5)	
			$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	14 134802(5)	
$5\frac{1}{2} \leftarrow 4\frac{1}{2}$	$1\frac{1}{2} \leftarrow 1\frac{1}{2}$	l	$6\frac{1}{2} \leftarrow 5\frac{1}{2}$	17 261.318(5)	
			$5\frac{1}{2} \leftarrow 4\frac{1}{2}$	17 261.346(5)	
			$4\frac{1}{2} \leftarrow 3\frac{1}{2}$	17 261.412(5)	
		u	$6\frac{1}{2} \leftarrow 5\frac{1}{2}$	17 286.962(5)	
			$5\frac{1}{2} \leftarrow 4\frac{1}{2}$	17 287.002(5)	
			$4\frac{1}{2} \leftarrow 3\frac{1}{2}$	17 287.055(5)	
$6\frac{1}{2} \leftarrow 5\frac{1}{2}$	$1\frac{1}{2} \leftarrow 1\frac{1}{2}$	l	$7\frac{1}{2} \leftarrow 6\frac{1}{2}$	20 410.454(5)	
			$6\frac{1}{2} \leftarrow 5\frac{1}{2}$	20 410.512(5) [c])	
			$5\frac{1}{2} \leftarrow 4\frac{1}{2}$	20 410.512(5) [c])	
		u	$7\frac{1}{2} \leftarrow 6\frac{1}{2}$	20 444.081(5)	

			$6\frac{1}{2} \leftarrow 5\frac{1}{2}$	20 444.129(5) [c])
			$5\frac{1}{2} \leftarrow 4\frac{1}{2}$	20 444.129(5) [c])
$7\frac{1}{2} \leftarrow 6\frac{1}{2}$	$1\frac{1}{2} \leftarrow 1\frac{1}{2}$	*l*	$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	23 564.254(5) [c])
			$7\frac{1}{2} \leftarrow 6\frac{1}{2}$	23 564.254(5) [c])
			$6\frac{1}{2} \leftarrow 5\frac{1}{2}$	23 564.254(5) [c])
		u	$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	23 605.795(5) [c])
			$7\frac{1}{2} \leftarrow 6\frac{1}{2}$	23 605.795(5) [c])
			$6\frac{1}{2} \leftarrow 5\frac{1}{2}$	23 605.795(5) [c])
$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	$1\frac{1}{2} \leftarrow 1\frac{1}{2}$	*l*	$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	26 722.586(5) [c])
			$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	26 722.586(5) [c])
			$7\frac{1}{2} \leftarrow 6\frac{1}{2}$	26 722.586(5) [c])
		u	$9\frac{1}{2} \leftarrow 8\frac{1}{2}$	26 771.831(5) [c])
			$8\frac{1}{2} \leftarrow 7\frac{1}{2}$	26 771.831(5) [c])
			$7\frac{1}{2} \leftarrow 6\frac{1}{2}$	26 771.831(5) [c])

[a]) Upper or lower components of parity doubling.
[b]) The figures in parentheses are the authors' estimates of experimental uncertainty (1σ).
[c]) Deuteron hyperfine structure not resolved.

Molecular parameters for $^{40}Ar^{32}S^{1}H$

Parameter		Value	Method	Ref.
State: electronic $\tilde{X}^2\Pi$; vibrational zero point level				
A	[GHz]	– 11 297.1 [a])	FTMW	00Su
B	[GHz]	283.616 9 [a])		
γ	[MHz]	– 4 573.034 [a])		
p	[MHz]	9 006.975 [a])		
q	[MHz]	– 284.52 [a])		
$h_1(^1H)$	[MHz]	17 561(14) [b])		
$h_2(^1H)$	[MHz]	48.08 [c])		
$b(^1H)$	[MHz]	– 74.253 [c])		
$d(^1H)$	[MHz]	27.386 [c])		
ε_0 [d])	[cm^{-1}]	105.7 [e])		
ε_1	[cm^{-1}]	6.588(11)		
ε_2	[cm^{-1}]	12.266 0(44)		
ε_3	[cm^{-1}]	– 10.21 [e])		
R^0_m	[Å]	3.967 98(10)		
R^1_m	[Å]	0.079 [e])		
R^2_m	[Å]	0.052 [e])		
R^3_m	[Å]	0.150 [e])		
m^0	[MHz]	11.808(49)		
m^1	[MHz]	0.829 [e])		
m^2	[MHz]	2.057 [e])		
m^3	[MHz]	1.080 [e])		
γ_ν	[MHz]	10.69 [e])		
V_2^2	[cm^{-1}]	57.352(49)		
β	[Å^{-1}]	3.075 [e])		
κ	[Å^6]	110997.8 [e])		

[a]) Constrained to the value for isolated SH [95Mo]. ArSH is a van der Waals complex.
[b]) The numbers in parentheses represent 1 standard deviation of the least-squares fit, in units of the last quoted decimal place.
[c]) Constrained to the value for isolated SH [75Me].
[d]) ε_0 and all the following parameters are the coefficients in the intermolecular potential between SH and the Ar atom. ArSD data were employed additionally to obtain these values.
[e]) Parameter constrained to this value.

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75Me Meerts, W.L., Dymanus,A. : Can. J. Phys. **53** (1975) 2123.
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3.2.1.2.47 FeCO

Microwave data for $^{54}Fe^{12}C^{16}O$

Transition		ν	Ref.
rotational $J' - J''$	fine structure Ω	[MHz]	
State: electronic $\tilde{X}\,^3\Sigma^-$; vibrational (0,0,0)			
$1 \leftarrow 0$	0	8 681.118 2(10) [a])	95Ka
$2 \leftarrow 1$		17 362.298 7(10)	
$3 \leftarrow 2$		26 043.616 4(10)	

[a]) The figures in parentheses are the authors' estimates of experimental uncertainty (1σ).

Molecular parameters for $^{56}Fe^{12}C^{16}O$

Parameter		Value	Method	Ref.
State: electronic $\tilde{X}\,^3\Sigma^-$; vibrational (0,0,0)				
B	[MHz]	4 408.09(27) [a])	MW	95Ka
D	[kHz]	1.260 5 [b])		
λ	[GHz]	579.9(22)		

[a]) The numbers in parentheses are 1 standard deviation of the least-squares fit, in units of the last quoted decimal place.
[b]) D was constrained to the value calculated from a force constant calculation (93Vi).

Microwave data for $^{56}Fe^{12}C^{16}O$

Transition		ν	Ref.
rotational $J' - J''$	fine structure Ω	[MHz]	
State: electronic $\tilde{X}\,^3\Sigma^-$; vibrational (0,0,0)			
$1 \leftarrow 0$	0	8 585.503 3(10) [a])	95Ka
$2 \leftarrow 1$		17 171.067 9(10)	
$3 \leftarrow 2$		25 756.756 0(10)	
$4 \leftarrow 3$		34 342.631 5(10)	
$15 \leftarrow 14$	0	128 815.447(30)	97Ta
	1^f	130 894.888(30)	
	1^e	132 989.314(30)	
$16 \leftarrow 15$	0	137 407.791(30)	
	1^f	139 618.852(30)	
	1^e	141 845.839(30)	
$17 \leftarrow 16$	0	146 000.952(30)	
	1^f	148 342.217(30)	
$24 \leftarrow 23$	1^f	209 390.752(30)	
	1^e	212 628.172(30)	
$25 \leftarrow 24$	0	214 777.719(30)	
	1^f	218 109.382(30)	
	1^e	221 466.094(30)	
$26 \leftarrow 25$	0	223 378.998(30) [b])	
	1^f	226 827.246(30) [b])	
	1^e	230 301.620(30) [b])	
$27 \leftarrow 26$	0	231 981.227(30) [b])	
	1^f	235 544.415(30) [b])	

	1^e	239 134.667(30) [b])	
28 ← 27	0	240 584.386(30) [b])	
	1^f	244 260.751(30) [b])	
	1^e	247 965.206(30) [b])	
29 ← 28	0	249 188.458	97Ka
	1^f	252 976.291	
	1^e	256 793.202	
30 ← 29	0	257 793.503	
36 ← 35	1^f	313 959.529	
	1^e	318 513.761	
37 ← 36	0	318 052.225	
	1^f	322 667.400	
	1^e	327 319.731	
38 ← 37	0	326 663.691	
	1^f	331 374.224	
	1^e	336 122.932	
39 ← 38	0	335 275.843	
	1^f	340 079.919	
	1^e	344 923.209	
40 ← 39	0	343 888.722	
	1^f	348 784.423	
	1^e	353 720.529	
41 ← 40	1^f	357 487.832	
	1^e	362 514.938	
42 ← 41	0	361 115.933	
	1^f	366 190.037	
	1^e	371 306.387	
43 ← 42	0	369 730.352	

[a]) The figures in parentheses are the authors' estimates of experimental uncertainty (1σ).
[b]) Independent measurement given in 97Ka.

Molecular parameters for $^{56}Fe^{12}C^{16}O$

Parameter		Value	Method	Ref.
State: electronic $\tilde{X}\,^3\Sigma^-$; vibrational (0,0,0)				
B	[MHz]	4 363.891 35(37) [a])	MW	97Ka
D	[kHz]	1.221 361(80)		
λ	[GHz]	678.940(318)		
λ_D	[MHz]	– 0.263 03(27)		
γ	[MHz]	– 1 088.2(23)		
γ_D	[kHz]	1.752(90)		

[a]) The numbers in parentheses are 1 standard deviation of the least-squares fit, in units of the last quoted decimal place.

Microwave data for $^{57}Fe^{12}C^{16}O$

Transition			ν [MHz]	Ref.
rotational $J' – J''$	fine structure Ω	hyperfine $F' – F''$ [a])		
State: electronic $\tilde{X}\,^3\Sigma^-$; vibrational (0,0,0)				
1 ← 0	0	$\frac{1}{2} \leftarrow \frac{1}{2}$	8 540.573 8(10) [b])	95Ka
		$1\frac{1}{2} \leftarrow \frac{1}{2}$	8 539.724 9(10)	
2 ← 1		$1\frac{1}{2} \leftarrow \frac{1}{2}$	17 080.348 8(10)	
		$1\frac{1}{2} \leftarrow 1\frac{1}{2}$	17 081.201 2(10)	
		$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	17 079.784 5(10)	
3 ← 2		$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	25 620.541 8(10)	

		$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	25 619.969 0(10)	

[a]) Hyperfine splitting from the ^{57}Fe nucleus (I = 1/2).
[b]) The figures in parentheses are the authors' estimates of experimental uncertainty (1σ).

Molecular parameters for $^{57}Fe^{12}C^{16}O$

Parameter		Value	Method	Ref.
State: electronic $\tilde{X}\,^3\Sigma^-$; vibrational (0,0,0)				
B	[MHz]	4 335.18(41) [a])	MW	95Ka
D	[kHz]	1.222 1 [b])		
λ	[GHz]	581.0(36)		
γ	[MHz]	0.0 [c])		
$b(^{57}Fe)$	[MHz]	– 37.73(22)		

[a]) The numbers in parentheses are 1 standard deviation of the least-squares fit, in units of the last quoted decimal place.
[b]) D was constrained to the value calculated from a force constant calculation (93Vi).
[c]) γ was constrained to zero in the least-squares fit. The parameter is strongly correlated with λ in a fit of this type of data.

Microwave data for $^{57}Fe^{13}C^{16}O$

Transition			ν [MHz]	Ref.
rotational $J' - J''$	fine structure Ω	hyperfine $F' - F''$ [a])		
State: electronic $\tilde{X}\,^3\Sigma^-$; vibrational (0,0,0)				
$1 \leftarrow 0$	0	$\frac{1}{2} \leftarrow \frac{1}{2}$	8 524.187 0(10) [b])	95Ka
		$1\frac{1}{2} \leftarrow \frac{1}{2}$	8 523.198 0(10)	
$2 \leftarrow 1$		$1\frac{1}{2} \leftarrow \frac{1}{2}$	17 047.442 7(10)	
		$1\frac{1}{2} \leftarrow 1\frac{1}{2}$	17 048.430 4(10)	
		$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	17 046.784 0(10)	
$3 \leftarrow 2$		$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	25 571.146 1(10)	
		$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	25 570.491 8(10)	

[a]) Hyperfine splitting from the ^{57}Fe nucleus (I = 1/2).
[b]) The figures in parentheses are the authors' estimates of experimental uncertainty (1σ).

Molecular parameters for $^{57}Fe^{13}C^{16}O$

Parameter		Value	Method	Ref.
State: electronic $\tilde{X}\,^3\Sigma^-$; vibrational (0,0,0)				
B	[MHz]	4 326.56(11) [a])	MW	95Ka
D	[kHz]	1.228 3 [b])		
λ	[GHz]	582.1(10)		
γ	[MHz]	0.0 [c])		
$b(^{57}Fe)$	[MHz]	– 43.989(72)		

[a]) The numbers in parentheses are 1 standard deviation of the least-squares fit, in units of the last quoted decimal place.
[b]) D was constrained to the value calculated from a force constant calculation (93Vi).
[c]) γ was constrained to zero in the least-squares fit. The parameter is strongly correlated with λ in a fit of this type of data.

Microwave data for $^{57}Fe^{13}C^{18}O$

Transition			ν [MHz]	Ref.
rotational $J' - J''$	fine structure Ω	hyperfine $F' - F''$ [a])		
State: electronic $\tilde{X}\,^3\Sigma^-$; vibrational (0,0,0)				
$1 \leftarrow 0$	0	$\frac{1}{2} \leftarrow \frac{1}{2}$	7 957.496 9(10) [b])	95Ka
		$1\frac{1}{2} \leftarrow \frac{1}{2}$	7 956.573 8(10)	
$2 \leftarrow 1$		$1\frac{1}{2} \leftarrow \frac{1}{2}$	15 914.110 5(10)	
		$1\frac{1}{2} \leftarrow 1\frac{1}{2}$	15 915.032 0(10)	
		$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	15 913.497 6(10)	
$3 \leftarrow 2$		$2\frac{1}{2} \leftarrow 1\frac{1}{2}$	23 871.119 7(10)	
		$3\frac{1}{2} \leftarrow 2\frac{1}{2}$	23 870.503 1(10)	

[a]) Hyperfine splitting from the ^{57}Fe nucleus (I = 1/2).
[b]) The figures in parentheses are the authors' estimates of experimental uncertainty (1σ).

Molecular parameters for $^{57}Fe^{13}C^{18}O$

Parameter		Value	Method	Ref.
State: electronic $\tilde{X}\,^3\Sigma^-$; vibrational (0,0,0)				
B	[MHz]	4 034.80(18) [a])	MW	95Ka
D	[kHz]	1.048 4 [b])		
λ	[GHz]	581.8(18)		
γ	[MHz]	0.0 [c])		
$b(^{57}Fe)$	[MHz]	– 44.02(13)		

[a]) The numbers in parentheses are 1 standard deviation of the least-squares fit, in units of the last quoted decimal place.
[b]) D was constrained to the value calculated from a force constant calculation (93Vi).
[c]) γ was constrained to zero in the least-squares fit. The parameter is strongly correlated with λ in a fit of this type of data.

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