Calculation of Nuclear Quadrupole Coupling Constants on Approximate Equilibrium Molecular Structures

V. F, Cl, Br - Propanes

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Abstract

Calculations were made of Cl and Br nuclear quadrupole coupling constants on approximate equilibrium molecular structures of several halogen substituted propanes. Equilibrium structures were derived by MP2/aug-cc-pVTZ(G03) optimization with empirically corrected bond lengths. The molecules are

trans-1-Chloropropane	*gauche*-1-Chloropropane
2-Chloropropane	2,2-Dichloropropane
2,2-Chlorofluoropropane	*trans*-1-Bromopropane
gauche-1-Bromopropane	2-Bromopropane

Excellent agreement between calculated and experimental chlorine coupling constants is obtained; which agreement validates, at least in part, the derived structures. Less satisfactory results are obtained for bromine.

Introduction

The nuclear quadrupole coupling constant tensor is the spectroscopic measurement of the energy of interaction of the electric quadrupole moment of the nucleus of an atom with the gradient of the molecular electric field at the site of the nucleus.

Quantum chemistry calculation of the electric field gradient (efg) tensor permits calculation of the nuclear quadrupole coupling constant (nqcc) tensor, the latter being directly proportional to the former. Techniques for this have been developed for a number of quadrupolar nuclei [1], including Cl and Br.

The accuracy of calculated nqcc's is, of course, sensitive to molecular structure. For calculation of near equilibrium structures, Demaison et al. [2 - 9] have shown in a series of publications that errors in quantum chemistry calculation of bond lengths at the MP2 level of theory are largely systematic and can be empirically corrected and that, with sufficiently large bases, accurate interatomic angles may be obtained *ab initio*.

Thus, we investigate here the efficacy of MP2/aug-cc-pVTZ(G03) optimization, with and without empirically corrected bond lengths, of the molecular structures of several substituted propanes for calculation of Cl and Br nqcc tensors.

All calculations were made on a Mac G5 from Apple Inc. using the G03M quantum chemistry package of Gaussian Inc. [10]. This package contains Dunning bases that have been modified somewhat for computational efficiency. That these bases are not exactly the originals is denoted here by the appendage G03.

Molecular Structures

The structures of these several molecules were derived as described in some detail in Ref. [1]. Briefly, the structures were optimized at the MP2/aug-cc-pVTZ(G03) level of theory, the CF and CCl optimized r_{opt} bond lengths then corrected via the following equations:

C-C $\sim r_e$ (Å) = 0.95547 × r_{opt} + 0.06568, RSD = 0.0012 Å,

CF $\sim r_e$ (Å) = 0.97993 × r_{opt} + 0.02084, RSD = 0.0014 Å,

CCl $\sim r_e$ (Å) = 0.99872 × r_{opt} − 0.00097, RSD = 0.0022 Å.

CBr $\sim r_e$ (Å) = 0.99078 × r_{opt} + 0.02591, RSD = 0.0003 Å,

RSD is the standard deviation of the residuals which may be taken as an estimate of the uncertainty in the corrected bond length, $\sim r_e$.

Nuclear Quadrupole Coupling Constants

The components of the nqcc tensor χ are related to those of the efg tensor q by

$$\chi_{ij} = (eQ/h)\, q_{ij}$$

where e is the fundamental electric charge, Q is the electric quadrupole moment of the nucleus, and h is Planck's constant. Subscripts i j refer to coordinate axes. Experimental nqcc's are measured in the principal axes system of the molecular inertia tensor. These axes are associated with the rotational constants A, B, and C; and are labeled a, b, and c. Principal axes of the nqcc tensor are here labeled x, y, and z.

(Note: The G03M code calculates the efg tensor in a coordinate system other than the inertia system. A fortran program used here for transformation of the efg tensor from G03M axes to a,b,c and x,y,z principal axes is available in Ref. [1].)

Calibration of the B1LYP/TZV(3df,2p) model for calculation of the chlorine nqcc's [1] yields

$$\chi_{ij}\,(^{35}\mathrm{Cl}) = -19.185\ \mathrm{MHz/a.u.} \times q_{ij},\quad \mathrm{RSD} = 0.49\ \mathrm{MHz},$$

$$\chi_{ij}\,(^{37}\mathrm{Cl}) = -15.120\ \mathrm{MHz/a.u.} \times q_{ij},\quad \mathrm{RSD} = 0.44\ \mathrm{MHz};$$

calibration of the B1LYP/TZV(3df,3p) model for calculation of the bromine nqcc's [1] yields

$$\chi_{ij}\,(^{79}\mathrm{Br}) = 77.628(43)\ \mathrm{MHz/a.u.} \times q_{ij},\quad \mathrm{RSD} = 1.58\ \mathrm{MHz},$$

$$\chi_{ij}\,(^{81}\mathrm{Br}) = 64.853(40)\ \mathrm{MHz/a.u.} \times q_{ij},\quad \mathrm{RSD} = 1.44\ \mathrm{MHz};$$

where q_{ij} are the calculated efg's. The RMS differences may be taken as estimates of the uncertainty in the calculated nqcc's.

Results

The results of this investigation - structure parameters (heavy atom) and nuclear quadrupole coupling constants - are collected below in Tables 1 - 8.

In Tables 1 - 8; r_{opt}, ~ r_e, and experimental structure (where available) parameters are compared. Coupling constants calculated on each structure are compared with experimental nqcc's. RMS is the root mean square difference between calculated and experimental diagonal nqcc's (percent of average experimental nqcc). $\eta = (\chi_{xx} - \chi_{yy})/\chi_{zz}$ and φ (degrees) is the angle between its subscripted parameters.

Table 1. *trans*-1-Chloropropane, t-CH_2Cl-CH_2-CH_3 (C_s). Heavy atom structure parameters (Å and degrees). Rotational constants (MHz), ^{35}Cl species. Chlorine nuclear quadrupole coupling constants (MHz). Coupling constants in a given column were calculated on the molecular structure given in the same column.

Parameter	r_{opt}	~ r_e		Expt. [a]
ClC(1)	1.7889	1.7856		
C(1)C(2)	1.5137	1.5120		
C(2)C(3)	1.5251	1.5228		
ClC(1)C(2)	111.35	111.35		
C(1)C(2)C(3)	110.60	110.60		
A	26050.3	26085.7		25753.4
B	2396.9	2404.0		2379.7
C	2288.3	2295.1		2271.7
χ_{aa} (^{35}Cl)	-55.22	-55.10		-54.7357(57)
χ_{bb}	19.28	19.22		19.062(21)
χ_{cc}	35.94	35.88		35.674(21)
$\lvert\chi_{ab}\rvert$	37.96	37.93		37.83(15)
RMS	0.34 (0.9 %)	0.26 (0.7 %)		
χ_{xx}	35.21	35.16		35.01(11)
χ_{yy}	35.94	35.88		35.674(21)
χ_{zz}	-71.16	-71.04		-70.68(11)

η	0.0102	0.0100		0.0094(19)
$\varphi_{z,a}$	22.77	22.79		22.85(6)
$\varphi_{a,CCl}$	21.95	21.96		
$\varphi_{z,CCl}$	0.81	0.83		
χ_{aa} (^{37}Cl)	-43.60	-43.50		-43.2170(60)
χ_{bb}	15.27	15.22		15.100(15)
χ_{cc}	28.32	28.28		28.117(15)
$\lvert\chi_{ab}\rvert$	29.84	29.82		32.0(16)
RMS	0.27(0.9 %)	0.20 (0.7 %)		

[a] A. de Luis, M. E. Sanz, F. J. Lorenzo, J. C. López, and J. L. Alonso, J. Mol. Spectrosc. 184, 60 (1997). Rotational constants are rounded-off. Back to Top

Table 2. *gauche*-1-Chloropropane, g-CH_2Cl-CH_2-CH_3 (C_1). Heavy atom structure parameters (Å and degrees). Rotational constants (MHz), ^{35}Cl species. Chlorine nuclear quadrupole coupling constants (MHz). Coupling constants in a given column were calculated on the molecular structure given in the same column.

Parameter	r_{opt}	~ r_e		Expt. [a]
ClC(1)	1.7923	1.7890		
C(1)C(2)	1.5152	1.5134		
C(2)C(3)	1.5197	1.5218		
ClC(1)C(2)	111.53	111.53		
C(1)C(2)C(3)	113.13	113.13		
ClCCC [b]	64.60	64.60		

A	11857.6	11886.1		11829.8
B	3371.9	3381.3		3322.6
C	2890.6	2898.8		2853.0
χ_{aa} (^{35}Cl)	-19.31	-19.23		-19.4384(46)
χ_{bb}	-11.01	-11.02		-10.711(13)
χ_{cc}	30.32	30.25		30.150(13)
$\lvert\chi_{ab}\rvert$	50.33 [c]	50.26 [c]		49.5(13)
$\lvert\chi_{ac}\rvert$	16.01	16.00		15.12(88)
$\lvert\chi_{bc}\rvert$	15.68	15.68		17.6(45)
RMS	0.21 (1.0 %)	0.22 (1.1 %)		
χ_{xx}	34.64	34.59		
χ_{yy}	35.99	35.94		
χ_{zz}	-70.64	-70.53		
η	0.0191	0.0191		
$\phi_{z,CCl}$	0.70	0.71		
χ_{aa} (^{37}Cl)	-15.75	-15.69		-15.8473(44)
χ_{bb}	-8.20	-8.20		-7.970(13)
χ_{cc}	23.95	23.89		23.817(13)
$\lvert\chi_{ab}\rvert$	39.65 [c]	39.60 [c]		39.7(18)
$\lvert\chi_{ac}\rvert$	12.61	12.60		12.0(12)

$\lvert\chi_{bc}\rvert$	12.20	12.20		12.5(66)
RMS	0.16 (1.0 %)	0.17 (1.0 %)		

[a] A. de Luis, M. E. Sanz, F. J. Lorenzo, J. C. López, and J. L. Alonso, J. Mol. Spectrosc. 184, 60 (1997). Rotational constants are rounded-off. [b] Dihedral angle ClC(1)C(2)C(3). [c] The algebraic sign of the product $\chi_{ab}\ \chi_{ac}\ \chi_{bc}$ is negative. Back to Top

Table 3. 2-Chloropropane (Isopropyl chloride), CH_3-CHCl-CH_3 (C_s). Heavy atom structure parameters (Å and degrees). Rotational constants (MHz), ^{35}Cl species. Chlorine nuclear quadrupole coupling constants (MHz). Coupling constants in a given column were calculated on the molecular structure given in the same column.

Parameter	r_{opt}	~ r_e	r_m^{ρ} [a]	Expt. [a]
C(2)Cl	1.8027	1.7994	1.7964(40)	
C(2)C(1,3)	1.5141	1.5124	1.5176(38)	
C(1)C(2)C(3)	112.87	112.87	112.52(35)	
C(1,3)C(2)Cl	108.96	108.96	109.28(15)	
A	8150.9	8166.9		
B	4603.2	4617.2		
C	3237.9	3247.0		
χ_{aa} (^{35}Cl)	-61.76	-61.66	-61.78	-61.496(6)
χ_{bb}	34.87	34.83	34.92	34.708(9)
χ_{cc}	26.90	26.83	26.86	26.788(9)
$\lvert\chi_{ac}\rvert$	25.92	25.91	25.83	

RMS	0.19 (0.5 %)	0.12 (0.3 %)	0.21 (0.5 %)	
χ_{xx}	33.92	33.86	33.84	
χ_{yy}	34.87	34.83	34.92	
χ_{zz}	-68.78	-68.69	-68.76	
η	0.0138	0.0142	0.016	
$\phi_{z,a}$	15.16	15.17	15.12	
$\phi_{a,CCl}$	14.43	14.44	14.36	
$\phi_{z,CCl}$	0.73	0.74	0.75	
χ_{aa} (^{37}Cl)	-48.72	-48.64	-48.74	-48.510(6)
χ_{bb}	27.48	27.45	27.52	27.349(8)
χ_{cc}	21.24	21.19	21.22	21.161(8)
$\lvert\chi_{ac}\rvert$	20.34	20.34	20.28	
RMS	0.15 (0.5 %)	0.10 (0.3 %)	0.17 (0.5 %)	

[a] M. Meyer, J.-U. Grabow, H. Dreizler, and H. D. Rudolph, J. Mol. Spectrosc. 151, 217 (1992). Back to Top

Table 4. 2,2-Dichloropropane, CH_3-CCl_2-CH_3 (C_{2v}). Heavy atom structure parameters (Å and degrees). Rotational constants (MHz), ^{35}Cl species. Chlorine nuclear quadrupole coupling constants (MHz). Coupling constants in a given column were calculated on the molecular structure given in the same column.

Parameter	r_{opt}	~ r_e	r_s [a]	Expt. [a]
C(2)Cl	1.7936	1.7903	1.785	

C(2)C(1,3)	1.5125	1.5108	1.528	
ClC(2)Cl	108.30	108.30	108.9	
C(1)C(2)C(3)	113.41	113.41	112.4	
A	3699.5	3709.2		3660.674(7)
B	2462.7	2470.7		2457.884(19)
C	2165.1	2172.5		2158.301(1)
χ_{aa} (^{35}Cl)	-37.97	-37.88	-38.59	-36.7(5)
χ_{bb}	0.27	0.25	0.88	-0.2(5)
χ_{cc}	37.70	37.63	37.70	36.9(5)
$\lvert\chi_{ab}\rvert$	51.06	51.00	50.86	
RMS	0.9 (3.7 %)	0.8 (3.4 %)	1.3 (5.4 %)	
χ_{xx}	35.68	36.63	35.70	
χ_{yy}	37.70	37.63	37.70	
χ_{zz}	-73.38	-73.26	-73.41	
ETA	0.0275	0.0272	0.027	
$\phi_{z,a}$	34.73	34.75	34.4	
$\phi_{a,CCl}$	35.85	35.85	35.6	
$\phi_{z,CCl}$	1.12	1.10	1.2	

[a] H. Takeo, M. Sugie, and C. Matsumura, J. Mol. Struct. 352/353, 267 (1995).

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Table 5. 2,2-Chlorofluoropropane, CH_3-CClF-CH_3 (C_s). Heavy atom structure parameters (Å and degrees). Rotational constants (MHz), ^{35}Cl species. Chlorine nuclear quadrupole coupling constants (MHz). Coupling constants in a given column were calculated on the molecular structure given in the same column.

Parameter	r_{opt}	~ r_e	r_o/r_s [a]	Expt. [a]
C(2)Cl	1.7961	1.7928	1.775(7)	
C(2)F	1.3818	1.3750	1.387(1)	
C(2)C(1,3)	1.5076	1.5062	1.526(1)	
C(1)C(2)C(3)	114.77	114.77	113.7	
C(1,3)C(2)Cl	109.21	109.21	110.1(1)	
C(1,3)C(2)F	108.30	108.30	105.7(1)	
FC(2)Cl	106.73	106.73	107.8(1)	
A	4859.0	4879.3		4830.856(31)
B	3159.6	3174.4		3151.148(25)
C	3058.4	3067.8		3041.176(25)
χ_{aa} (^{35}Cl)	-69.41	-69.17	-69.75	-69.3(2)
χ_{bb}	36.46	36.31	36.78	36.8(2)
χ_{cc}	32.95	32.86	32.97	32.5(2)
$\lvert\chi_{ac}\rvert$	3.82	3.76	3.14	
RMS	0.3 (0.7 %)	0.4 (0.8 %)	0.4 (0.8 %)	
χ_{xx}	33.09	33.00	33.07	
χ_{yy}	36.46	36.31	36.78	

χ_{zz}	-69.55	-69.31	-69.84	
η	0.048	0.048	0.053	
$\phi_{z,a}$	2.13	2.10	1.75	
$\phi_{a,CCl}$	1.70	1.58	1.50	
$\phi_{z,CCl}$	0.43	0.52	0.24	

[a] H. Takeo, M. Sugie, and C. Matsumura, J. Mol. Struct. 352/353, 267 (1995).

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Table 6. *trans*-1-Bromopropane, t-CH_2Br-CH_2-CH_3 (C_s). Heavy atom structure parameters (Å and degrees). Rotational constants (MHz), ^{79}Br species. Bromine nuclear quadrupole coupling constants (MHz). Coupling constants in a given column were calculated on the molecular structure given in the same column.

Parameter	r_{opt}	~ r_e		Expt.
BrC(1)	1.9352	1.9432		
C(1)C(2)	1.5129	1.5112		
C(2)C(3)	1.5253	1.5231		
BrC(1)C(2)	111.42	111.42		
C(1)C(2)C(3)	110.45	110.45		
A	25501.6	25506.8		
B	1663.2	1658.3		
C	1608.1	1603.5		
χ_{aa} (^{79}Br)	439.33	441.12		
χ_{bb}	-166.29	-167.30		

χ_{cc}	-273.05	-273.82		
$\lvert\chi_{ab}\rvert$	271.1	271.48		
RMS				
χ_{xx}	-269.93	-270.83		
χ_{yy}	-273.05	-273.82		
χ_{zz}	542.98	544.64		
η	0.0057	0.0055		
$\varphi_{z,a}$	20.92	20.87		
$\varphi_{a,CBr}$	20.15	20.85		
$\varphi_{z,CBr}$	0.77	0.77		
χ_{aa} (^{81}Br)	367.17	368.67		
χ_{bb}	-139.05	-139.90		
χ_{cc}	-228.12	-228.76		
$\lvert\chi_{ab}\rvert$	226.38	226.68		
RMS				

Table 7. *gauche*-1-Bromopropane, g-CH_2Br-CH_2-CH_3 (C_1). Heavy atom structure parameters (Å and degrees). Rotational constants (MHz), ^{79}Br species. Bromine nuclear quadrupole coupling constants (MHz). Coupling constants in a given column were calculated on the molecular structure given in the same column.

Parameter	r_{opt}	~ r_e		Expt. [a]
BrC(1)	1.9394	1.9474		
C(1)C(2)	1.5139	1.5122		
C(2)C(3)	1.5213	1.5192		
BrC(1)C(2)	111.69	111.69		
C(1)C(2)C(3)	113.19	113.19		
BrCCC [b]	64.72	64.72		
A	11056.2	11051.4		11034.3
B	2338.5	2331.1		2277.7
C	2072.3	2066.3		2024.5
χ_{aa} (^{79}Br)	240.30	243.31		256.9(11)
χ_{bb}	0.46	-1.52		-9.5(5)
χ_{cc}	-240.76	-241.79		-247.4(13)
$\lvert\chi_{ab}\rvert$	373.46 [c]	374.01 [c]		380.0(43)
$\lvert\chi_{ac}\rvert$	114.71	114.70		
$\lvert\chi_{bc}\rvert$	89.56	89.01		
RMS	11.8 (6.9 %)	9.6 (5.6 %)		
χ_{xx}	-264.75	-265.59		

χ_{yy}	-274.97	-275.73		
χ_{zz}	539.72	541.32		
η	0.0189	0.0187		
$\phi_{z,CBr}$	0.66	0.67		
χ_{aa} (^{81}Br)	201.53	204.04		214.1(11)
χ_{bb}	-0.32	-1.97		-8.1(5)
χ_{cc}	-201.21	-202.07		-206.0(12)
$\lvert\chi_{ab}\rvert$	311.81 [c]	312.27 [c]		311.9(69)
$\lvert\chi_{ac}\rvert$	95.79	95.78		
$\lvert\chi_{bc}\rvert$	74.62	74.16		
RMS	9.0 (6.3 %)	6.3 (4.4 %)		

[a] Y. Niide, I. Ohkoshi, and M. Takano, J. Mol. Spectrosc. 89, 387 (1981). Rotational constants are rounded-off. [b] Dihedral angle BrC(1)C(2)C(3). [c] The algebraic sign of the product $\chi_{ab}\ \chi_{ac}\ \chi_{bc}$ is positive. Back to Top

Table 8. 2-Bromopropane (Isopropyl bromide), CH$_3$-CHBr-CH$_3$ (C$_s$). Heavy atom structure parameters (Å and degrees). Rotational constants (MHz), ^{79}Br species. Bromine nuclear quadrupole coupling constants (MHz). Coupling constants in a given column were calculated on the molecular structure given in the same column.

Parameter	r_{opt}	~ r_e	r_s [a]	Expt. [b]
C(2)Br	1.9495	1.9574	1.962(6)	
C(2)C(1,3)	1.5133	1.5116	1.518(10)	
C(1)C(2)C(3)	112.97	112.97	113.27(165)	
C(1,3)C(2)Br	109.04	109.04	109.25(72)	

A	8134.3	8149.2	8038.9	
B	2965.0	2948.7	2917.8	
C	2332.7	2323.8	2295.3	
χ_{aa} (^{79}Br)	482.21	483.43	487.47	479.8908(57)
χ_{bb}	-266.66	-267.15	-268.13	-264.9423(48)
χ_{cc}	-215.55	-216.28	-219.34	-214.9485(48)
$\|\chi_{ac}\|$	177.29	177.09	175.84	176.89(16)
RMS	1.70 (0.5 %)	2.53 (0.8 %)	5.38 (1.7 %)	
χ_{xx}	-266.66	-267.15	-268.13	-264.9423(48)
χ_{yy}	-258.01	-258.55	-260.67	-257.3916(764)
χ_{zz}	524.67	525.70	528.80	522.3339(765)
η	-0.0165	-0.0164	-0.0141	-0.01446(15)
$\phi_{z,a}$	13.47	13.42	13.23	13.492(11)
$\phi_{a,CBr}$	12.76	12.70	12.60	
$\phi_{z,CBr}$	0.71	0.72	0.63	
χ_{aa} (^{81}Br)	402.93	403.95	407.33	400.9616(59)
χ_{bb}	-222.79	-223.19	-224.01	-221.3304(58)
χ_{cc}	-180.14	-180.76	-183.31	-179.6312(58)
$\|\chi_{ac}\|$	148.00	147.83	146.79	147.93(19)

RMS	1.44 (0.5 %)	2.13 (0.8 %)	4.52 (1.7 %)	

[a] C. Ikeda, T. Inagusa, and M. Hayashi, J. Mol. Spectrosc. 135, 334 (1989). Rotational constants are rounded-off. [b] M. Meyer, W. Stahl, and H. Dreizler, J. Mol. Spectrosc. 151, 243 (1992). Back to Top

Discussion

The above results are summarized below in Table 9, wherein the root mean square (RMS) differences between calculated and experimental ^{35}Cl and ^{79}Br diagonal nqcc's are given. These RMS differences should be compared with the standard deviation of residuals (RSD) for calibration of the models for calculation ot the nqcc's. For ^{35}Cl, the RSD is 0.49 MHz; and for ^{79}Br, 1.58 MHz. As can be seen - with the single exception of 2,2-dichloropropane - agreement between calculated and experimental nqcc's is less than 1*RSD. This is considered excellent agreement. In the case of 2,2-dichloropropane, the RMS difference is 0.8 MHz. We note that for this molecule the estimated uncertainty in the experimental nqcc's is rather large, namely 0.5 MHz.

All-in-all, the results for ^{35}Cl (and ^{37}Cl) are excellent, and we conclude from this that the derived molecular structures are good approximate equilibrium structures.

For ^{79}Br (and ^{81}Br), however, the results are mixed. Agreement between calculated and experimental nqcc's for 2-bromopropane is good; while for *gauche* 1-bromopropane, agreement is poor.

Table 9. Root mean square (RMS) differences (MHz) between calculated and experimental ^{35}Cl and ^{79}Br diagonal nqcc's (Percent of average experimental nqcc.).

Molecule	r_{opt}	~ r_e	Experimental Structure	
t-CH_2Cl-CH_2-CH_3	0.34 (0.9 %)	0.26 (0.7 %)	---	---
g-CH_2Cl-CH_2-CH_3	0.21 (1.0 %)	0.22 (1.1 %)	---	---
CH_3-CHCl-CH_3	0.19 (0.5 %)	0.12 (0.3 %)	r_m^ρ	0.21 (0.5 %)
CH_3-CCl_2-CH_3	0.9 (3.7 %)	0.8 (3.4 %)	r_s	1.3 (5.4 %)
CH_3-CFCl-CH_3	0.3 (0.7 %)	0.4 (0.8 %)	r_o/r_s	0.4 (0.8 %)

t-CH_2Br-CH_2-CH_3	---	---	---	---
g-CH_2Br-CH_2-CH_3	11.8 (6.9 %)	9.6 (5.6 %)	---	---
CH_3-CHBr-CH_3	1.70 (0.5 %)	2.53 (0.8 %)	r_s	5.38 (1.7 %)

References

[1] Calculation of Nuclear Quadrupole Coupling Constants in Gaseous State Molecules, http://homepage.mac.com/wcbailey/nqcc/

[2] J. M. Colmont, D. Priem, P. Dréan, J. Demaison, and J. E. Boggs, J. Mol. Spectrosc. 191, 158 (1998).

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