GAMESS

Calculation of Cl Nuclear Quadrupole Coupling Constants

on Approximate Equilibrium Molecular Structures

F, Cl - Methanes

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Abstract

Calculations were made of Cl nuclear quadrupole coupling constants on approximate equilibrium molecular structures of F, Cl substituted methanes derived by MP2/aug-cc-pVTZ(GMS) optimization with empirically corrected bond lengths. The molecules are

Methyl Chloride, CH_3Cl Chlorofluoromethane, CH_2FCl

Chlorodifluoromethane, CHF_2Cl Chlorotrifluoromethane, CF_3Cl

Dichloromethane, CH_2Cl_2 Dichlorofluoromethane, $CHFCl_2$

Dichlorodifluoromethane, CF_2Cl_2 Trichloromethane (Chloroform), $CHCl_3$

Trichlorofluoromethane, $CFCl_3$ Carbon Tetrachloride, CCl_4

Excellent agreement between calculated and experimental coupling constants is obtained; which agreement validates, at least in part, the derived structures. The results are as good on the r_{opt} structures as on the r_c structures, for which the bond lengths are corrected.

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[1] Modified November 2007. Updated experimental nqcc's for dichlorofluoromethane [21].

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].

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(GMS) optimization, with and without empirically corrected bond lengths, of the molecular structures of the following molecules for calculation of the Cl nqcc tensors.

Methyl Chloride, CH_3Cl	Chlorofluoromethane, CH_2FCl
Chlorodifluoromethane, CHF_2Cl	Chlorotrifluoromethane, CF_3Cl
Dichloromethane, CH_2Cl_2	Dichlorofluoromethane, $CHFCl_2$
Dichlorodifluoromethane, CF_2Cl_2	Trichloromethane (Chloroform), $CHCl_3$
Trichlorofluoromethane, $CFCl_3$	Carbon Tetrachloride, CCl_4

Carbon tetrachloride, which is not amenable to microwave studies, is included for completeness.

All calculations were made on a Mac G5 from Apple Inc. using the GAMESS (v. 7 Sept 06, R4) quantum chemistry package. Implementation in this package of the aug-cc-pVTZ bases for Al-Ar include one additional tight d-function. This modification is denoted by the appendage GMS. For all calculations, the program deaults for convergence criteria and integration grid were used.

Molecular Structures

Molecular structures were optimized at the MP2/aug-cc-pVTZ(GMS) level of theory, the CF and CCl optimized r_{opt} bond lengths then corrected via the following equations:

CF r_c (Å) = 0.97814 × r_{opt} + 0.02332, RSD = 0.0014 Å,

CCl r_c (Å) = 0.99708 × r_{opt} + 0.00679, RSD = 0.0020 Å.

RSD is the standard deviation of the residuals which may be taken as an estimate of the uncertainty in the corrected bond length, r_c. Derivation of these equations is discussed here; CCl, CF.

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 ij 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.

Calibration of the B3LYP/TZV(3df,2p) model for calculation of the chlorine nqcc's yields

$$\chi_{ij} \, (^{35}Cl) = (-19.185 \text{ MHz/a.u.}) \, q_{ij}, \quad RSD = 0.68 \text{ MHz},$$

$$\chi_{ij} \, (^{37}Cl) = (-15.120 \text{ MHz/a.u.}) \, q_{ij}, \quad RSD = 0.60 \text{ MHz},$$

where q_{ij} are the calculated efg's. The numerical factors contain the constants e, Q, and h, and unit conversions. For ^{35}Cl, Q = -81.65(80) mb, and for ^{37}Cl, Q = -64.35(64) mb [11]. Derivation of these equations is discussed here.

Results

The results of this investigation - structure parameters and nuclear quadrupole coupling constants - are collected below in Tables 1 - 10.

In Tables 1 - 10; r_{opt}, r_c, and experimental structure 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. Methyl Chloride, CH_3Cl. Structure parameters (Å and degrees). 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_c	r_e [a]	Expt. [b]
CH	1.0840	1.0840	1.0872	
CCl	1.7754	1.7770	1.7756	
HCH	110.49	110.49	110.35	
χ_{zz} (^{35}Cl)	-74.95	-75.01	-75.04	-74.7514(11)
χ_{zz} (^{37}Cl)	-59.07	-59.12	-59.14	-58.9166(34)

[a] Ref. [12]. [b] Ref. [13]. Back to Top

Table 2. Chlorofluoromethane, CH_2FCl. Structure parameters (Å and degrees). 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_c	r_o [a]	Expt. [a]
CH	1.0847	1.0847	1.09	
CCl	1.7625	1.7641	1.7621	
CF	1.3656	1.3590	1.370	
ClCH	108.03	108.03	109.4	
ClCF	110.11	110.11	110.1	
HCH	112.68	112.68	110.4	

χ_{aa} (^{35}Cl)	-52.75	-52.76	-52.94	-52.570(26)
χ_{bb}	13.34	13.47	13.26	13.469(20)
χ_{cc}	39.40	39.28	39.68	39.059(18)
$|\chi_{ab}|$	40.04	39.95	40.82	43.7(23)
RMS	0.27 (0.8 %)	0.17 (0.5 %)	0.43 (1.2 %)	
χ_{xx}	32.22	32.24	32.72	35.20(186)
χ_{yy}	39.40	39.28	39.68	39.059(18)
χ_{zz}	-71.62	-71.53	-72.40	-74.30(187)
η	0.1003	0.0984	0.0961	0.0519
$\varphi_{z,a}$	25.24	25.17	25.48	26(3)
$\varphi_{a,CCl}$	24.75	24.60	24.8	24.8
$\varphi_{z,CCl}$	0.48	0.57	0.7	
χ_{aa} (^{37}Cl)	-41.74	-41.75	-41.90	-41.566(32)
χ_{bb}	10.69	10.79	10.63	10.774(27)
χ_{cc}	31.05	30.96	31.27	30.788(27)
$|\chi_{ab}|$	31.42	31.34	32.03	
RMS	0.19 (0.7 %)	0.14 (0.5 %)	0.35 (1.2 %)	

[a] Ref. [14].   Back to Top

Table 3. Chlorodifluoromethane, CHF_2Cl. Structure parameters (Å and degrees). 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_c	r_s [a]	Expt. [a,b]
CH	1.0852	1.0852	1.098	
CCl	1.7543	1.7560	1.742	
CF	1.3422	1.3362	1.346	
ClCH	109.60	109.60	110.8	
ClCF	109.65	109.65	110.5	
FCF	108.05	108.05	107.5	
χ_{aa} (^{35}Cl)	-65.33	-65.13	-65.84	-65.0239(65) [b]
χ_{bb}	35.55	35.49	35.59	35.467(14)
χ_{cc}	29.78	29.64	30.25	29.566(14)
$|\chi_{ac}|$	26.88	26.80	26.46	24.0(5)
RMS	0.22 (0.5 %)	0.08 (0.2 %)	0.62 (1.4 %)	
χ_{xx}	36.85	36.70	37.05	35.3(25)
χ_{yy}	35.55	35.49	35.59	35.467(14)
χ_{zz}	-72.40	-72.19	-72.64	-70.8(25)
η	-0.0179	-0.0167	-0.0202	0.0024(390)
$\varphi_{z,a}$	14.74	14.74	14.42	13.4(25)
$\varphi_{a,CCl}$	14.39	14.32	14.3	
$\varphi_{z,CCl}$	0.35	0.41	0.1	

χ_{aa} (^{37}Cl)	-51.54	-51.38	-51.93	-51.342(31) [a]
χ_{bb}	28.02	27.97	28.05	27.920
χ_{cc}	23.51	23.41	23.89	23.422
$|\chi_{ac}|$	21.10	21.03	20.77	
RMS	0.14 (0.4 %)	0.04 (0.1 %)	0.44 (1.3 %)	

[a] Ref. [15]. [b] Ref. [16].   Back to Top

Table 4. Trifluoromethyl Chloride, CF$_3$Cl. Structure parameters (Å and degrees). 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_c	r_{av} [a]	Expt. [b]
CF	1.3273	1.3216	1.3248	
CCl	1.7464	1.7481	1.7522	
FCF	108.57	108.57	108.57	
χ_{zz} (^{35}Cl)	-78.16	-77.86	-78.28	-77.902(30)
χ_{zz} (^{37}Cl)	-61.60	-61.37	-61.69	-61.496(166)

[a] Ref. [17]. [b] Ref. [18].   Back to Top

Table 5. Dichloromethane, $CH_2{}^{35}Cl_2$. Structure parameters (Å and degrees). 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_c	$r_m{}^\rho$ [a]	Expt. [b]
CCl	1.7628	1.7645	1.7636	
CH	1.0829	1.0829	1.0851	
ClCCl	112.25	112.25	112.25	
HCH	111.70	111.70	111.90	
χ_{aa} (^{35}Cl)	-42.19	-42.26	-42.23	-41.7418(11)
χ_{bb}	2.07	2.09	2.09	1.8004(12)
χ_{cc}	40.12	40.17	40.13	39.9414(12)
$|\chi_{ab}|$	51.20	51.24	51.21	50.93(23)
RMS	0.32 (1.2 %)	0.37 (1.3 %)	0.34 (1.2 %)	
χ_{xx}	35.72	35.75	35.73	35.41(21)
χ_{yy}	40.12	40.17	40.14	39.9414(12)
χ_{zz}	-75.84	-75.92	-75.87	-75.35(21)
η	0.058	0.058	0.058	0.060(3)
$\varphi_{z,a}$	33.31	33.30	33.30	33.43(5)
$\varphi_{a,CCl}$	33.87	33.87	33.88	
$\varphi_{z,CCl}$	0.56	0.57	0.58	

[a] Ref. [19]. [b] Ref. [20]. Back to Top

The following three Tables - 6(a), 6(b), and 6(c) - are respectively $CHF^{35}Cl_2$, $CHF^{35}Cl^{37}Cl$, and $CHF^{37}Cl_2$.

Table 6(a). Dichlorofluoromethane, $CHF^{35}Cl_2$. Structure parameters (Å and degrees). 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_c	r_o-like [a]	Expt. [a]
CCl	1.7549	1.7567	1.764(2)	
CF	1.3515	1.3453	1.335(5)	
CH	1.0840	1.0840	[1.09]	
HCF	109.40	109.40	[110.0]	
FCCl	109.25	109.25	109.6(2)	
ClCCl	111.42	111.42	111.0(2)	
χ_{aa} (^{35}Cl)	-41.23	-41.32	-40.95	-40.8921(19)
χ_{bb}	11.50	11.60	10.92	11.4127(30)
χ_{cc}	29.73	29.72	30.03	29.4794(30)
$|\chi_{ab}|$ [b]	45.03	44.96	45.53	44.63(43)
$|\chi_{ac}|$	26.41	26.34	25.82	26.18(96)
$|\chi_{bc}|$	13.87	13.87	13.88	13.63(51)
RMS	0.25 (0.9 %)	0.30 (1.1 %)	0.43 (1.6 %)	
χ_{xx}	36.60	36.64	36.76	36.19(92)
χ_{yy}	38.89	38.80	38.79	38.6(12)
χ_{zz}	-75.49	-75.44	-75.54	-74.81(91)

η	0.030	0.029	0.029	0.032(28)
$\varphi_{z,CCl}$	1.09	1.17	1.10	

[a] Ref. [21]. Values in square brackets are assumed. [b] The product $\chi_{ab}\,\chi_{ac}\,\chi_{bc}$ is negative.

Table 6(b). Dichlorofluoromethane, $CHF^{35}Cl^{37}Cl$. Chlorine nuclear quadrupole coupling constants (MHz). Coupling constants in a given column were calculated on the molecular structure given in the same column. Structure parameters are given in Table 6(a).

Parameter	r_{opt}	r_c	r_o-like [a]	Expt. [a]
χ_{aa} (^{35}Cl)	-39.63	-39.73	-39.34	-39.3009(67)
χ_{bb}	9.93	10.04	9.33	9.849(15)
χ_{cc}	29.70	29.69	30.00	29.452(15)
$|\chi_{ab}|$ [b]	45.91	45.84	46.39	
$|\chi_{ac}|$	26.20	26.14	25.61	
$|\chi_{bc}|$	14.35	14.36	14.34	
RMS	0.24 (0.9 %)	0.30 (1.2 %)	0.44 (1.7 %)	
χ_{aa} (^{37}Cl)	-33.74	-33.79	-33.52	-33.4548(78)
χ_{bb}	10.24	10.31	9.79	10.165(15)
χ_{cc}	23.50	23.48	23.73	23.290(15)
$|\chi_{ab}|$ [b]	34.79	34.74	35.20	
$|\chi_{ac}|$	20.91	20.86	20.44	
$|\chi_{bc}|$	10.53	10.53	10.54	

RMS	0.21 (0.9 %)	0.24 (1.1 %)	0.34 (1.5 %)	

[a] Ref. [21]. [b] The product $\chi_{ab} \chi_{ac} \chi_{bc}$ is negative.

Table 6(c). Dichlorofluoromethane, $CHF^{37}Cl_2$. Chlorine nuclear quadrupole coupling constants (MHz). Coupling constants in a given column were calculated on the molecular structure given in the same column. Structure parameters are given in Table 6(a).

Parameter	r_{opt}	r_c	r_o-like [a]	Expt. [a]
χ_{aa} (^{37}Cl)	-32.50	-32.56	-32.27	-32.2262(20)
χ_{bb}	9.03	9.10	8.57	8.9588(33)
χ_{cc}	23.47	23.46	23.70	23.2674(33)
$\|\chi_{ab}\|$ [b]	35.52	35.47	35.92	35.36(41)
$\|\chi_{ac}\|$	20.75	20.70	20.29	19.3(12)
$\|\chi_{bc}\|$	10.91	10.91	10.91	10.51(70)
RMS	0.20 (0.9 %)	0.24 (1.1 %)	0.34 (1.6 %)	

[a] Ref. [21]. [b] The product $\chi_{ab} \chi_{ac} \chi_{bc}$ is negative. <u>Back to Top</u>

Table 7. Dichlorodifluoromethane, $CF_2^{35}Cl_2$. Structure parameters (Å and degrees). 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_c	r_s [a]	Expt. [b]
CCl	1.7512	1.7528	1.744	

CF	1.3347	1.3283	1.347	
ClCCl	111.65	111.59	112.6	
FCF	107.72	107.76	106.2	
χ_{aa} (^{35}Cl)	-43.86	-43.96	-45.02	-43.688(33)
χ_{bb}	4.84	4.98	6.06	4.6905
χ_{cc}	39.02	38.99	38.96	38.9975
$|\chi_{ab}|$	54.36	54.16	54.08	52.7(46)
RMS	0.13 (0.4 %)	0.23 (0.8 %)	1.10 (3.8 %)	
χ_{xx}	40.06	39.94	40.33	38.5 [c]
χ_{yy}	39.02	38.99	38.96	38.9975
χ_{zz}	-79.08	-78.93	-79.29	-77.5
η	-0.013	-0.012	-0.017	-0.006
$\varphi_{z,a}$	32.94	32.84	32.36	32.67
$\varphi_{a,CCl}$	34.18	34.18	33.7	
$\varphi_{z,CCl}$	1.24	1.34	1.3	

[a] Ref. [22]. [b] Ref. [23]. [c] Calculated here from experimental data. Back to Top

In Tables 8 and 9 below, χ_{uu} is the component of the nqcc tensor along the threefold symmetry axis; χ_{vv} and χ_{ww} are the components along the v- and w- axes for the Cl atom in the uv-plane.

Table 8. Trichloromethane (Chloroform), $CH^{35}Cl_3$. Structure parameters (Å and degrees). 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_c	r_e [a]	Expt. [b]
CCl	1.7587	1.7604	1.760	
CH	1.0827	1.0827	1.080	
ClCCl	110.92	110.92	110.68	
HCCl	107.97	107.97	108.23	
χ_{uu} (^{35}Cl)	29.03	29.09	28.56	28.6436(4)
χ_{vv}	-68.27	-68.36	-67.86	-67.8309(5)
χ_{ww}	39.24	39.27	39.30	39.1872(5)
$|\chi_{uv}|$	33.69	33.71	34.38	34.137(32)
RMS	0.34 (0.7 %)	0.40 (0.9 %)	0.08 (0.2 %)	
χ_{xx}	39.56	39.61	39.56	39.501(18)
χ_{yy}	39.24	39.27	39.30	39.1872(5)
χ_{zz}	-78.80	-78.88	-78.86	-78.688(18)
η	-0.0041	-0.0043	-0.0033	-0.0040(2)
$\varphi_{z,u}$	72.65	72.66	72.25	72.357(13)
$\varphi_{u,CCl}$	72.03	72.03	71.77	71.77(2) [c]
$\varphi_{z,CCl}$	0.38	0.33	0.58	0.59(2) [c]

[a] Ref. [2]. [b] Ref. [24]. [c] r_e structure.   <u>Back to Top</u>

Table 9. Trichlorofluoromethane, $CF^{35}Cl_3$. Structure parameters (Å and degrees). 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_c	avg. r_o [a]	Expt. [b]
CCl	1.7569	1.7585	1.757	
CF	1.3442	1.3381	1.346	
ClCCl	110.46	110.46	110.35	
FCCl	108.46	108.46		
χ_{uu} (^{35}Cl)	29.04	29.18	28.77	28.98(4)
χ_{vv}	-70.33	-70.41	-70.12	-70.28 [c]
χ_{ww}	41.29	41.23	41.34	41.30 [c]
$|\chi_{uv}|$	34.10	33.96	34.48	
RMS	0.04 (0.1 %)	0.14 (0.3 %)	0.15 (0.3 %)	
χ_{xx}	39.62	39.66	39.61	
χ_{yy}	41.29	41.23	41.34	
χ_{zz}	-80.91	-80.89	-80.95	
η	0.021	0.019	0.021	
$\varphi_{z,u}$	72.77	72.85	72.55	
$\varphi_{u,CCl}$	71.54	71.54	71.42	
$\varphi_{z,CCl}$	1.23	1.31	1.13	

[a] Average of two quite different r_o structures [25, 26]. See Ref. [1]. [b] Ref. [27].
[c] Calculated here from χ_{uu} and $\eta_Q = (\chi_{vv} - \chi_{ww})/\chi_{uu}$ = -3.85(20) MHz [27]. <u>Back to Top</u>

Table 10. Carbon Tetrachloride, CCl_4. Structure parameters (Å and degrees). 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_c		
CCl	1.7620	1.7636		
χ_{zz} (^{35}Cl)	-83.27	-83.37		
χ_{zz} (^{37}Cl)	-65.63	-65.70		

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Discussion

Comparison of r_c and r_e molecular structure parameters of CH_3Cl and $CHCl_3$ are made in Tables 1 and 8, and comparison of r_c and r_m^ρ parameters of CH_2Cl_2 in Table 5. For these, the average CCl difference is 0.0009 Å while the largest difference is 0.0014 Å in CH_3Cl; the average CH difference is 0.0027 Å, the largest difference, 0.0032 Å also in CH_3Cl.   For the angles, the average difference is 0.17°; the largest difference is 0.26° for HCCl in $CHCl_3$. The r_c structures of these molecules approximate the equilibrium structures. This, along with the results of calculations of the nqcc's, leads us to believe that the r_c structures of the other molecules in this series also approximate equilibrium structures.

For CH_2Cl_2, in addition to the r_m^ρ structure, two r_e structures have been reported [28, 29]. These three structures are somewhat different. Whereas the r_c structure is in better agreement with the r_m^ρ structure, nqcc's calculated on the r_e structures are in better agreement with the experimental nqcc's (Visit this link).

Excellent agreement between calculated and experimental coupling constants is obtained on both r_c and r_{opt} structures. On the r_c structures, the average RMS difference between calculated and experimental ^{35}Cl diagonal inertia axes nqcc's is 0.23 MHz; the largest differences are 0.37 and 0.40 MHz for CH_2Cl_2 and $CHCl_3$ respectively. On the r_{opt} structures, this average RMS difference is also 0.22 MHz; the largest differences are 0.32 and 0.34 MHz for CH_2Cl_2 and $CHCl_3$ respectively. These all lie well within the estimated uncertainty in the calculated nqcc's of 0.60 MHz. The results are as good on the r_{opt} structures as on the r_c structures, for which the bond lengths are corrected.

In $CHCl_3$, it is perhaps instructive to note the differences between nqcc's calculated on the r_c and r_e structures. Let us note first that the calculated values of χ_{ww}, χ_{xx}, χ_{yy}, and χ_{zz} are essentially the same for both structures, and in good agreement with the experimental values (Table 8). As the CCl bond lengths are nearly the same in both structures, the relatively large differences between χ_{uu} and χ_{vv} calculated on r_c compared with those calculated on r_e - respectively, 0.53 and 0.50 MHz - are due to the 0.25° angular difference in the two structures between CCl and the u- and v- axes.

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