Calculation of Nuclear Quadrupole Coupling Constants on Approximate Equilibrium Molecular Structures VII. Chloropropenes

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Abstract

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

trans-1-Chloropropene

cis-1-Chloropropene

2-Chloropropene

cis-3-Chloropropene

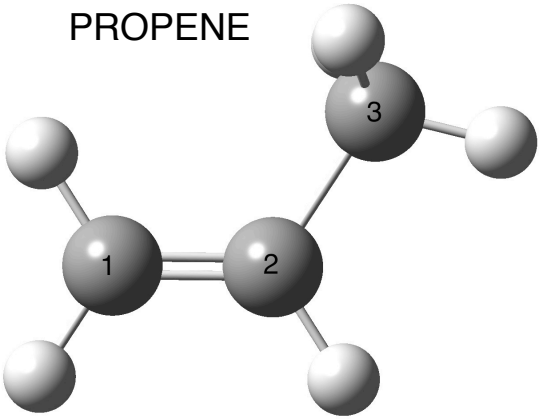
skew 3-Chloropropene

1-Chloro-2-Fluoropropene

1-Chloro-2-Methylpropene

anti-2,3-Dichloropropene

gauche-2,3-Dichloropropene



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.

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 optimization - with and without empirically corrected bond lengths - of the molecular structures of several substituted propenes for calculation of Cl nqcc tensor.

All calculations were made on a Mac Pro from Apple Inc. using the G09M quantum chemistry package of Gaussian Inc. [10].

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 level of theory, the C-C, C=C, 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,

C=C $\sim r_e$ (Å) = 0.98508 × r_{opt} + 0.01614, RSD = 0.0021 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.

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 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.

(Note: The G09M 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 G09M 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

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

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

where q_{ij} are the calculated efg's. The RSD, as above, 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 - 9.

In Tables 1 - 9, r_{opt}, $\sim r_e$, 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-Chloropropene, t-CH_3-C(H)=C(H)Cl (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}	$\sim r_e$		Expt. [a]
ClC(1)	1.7311	1.7279		
C(1)=C(2)	1.3317	1.3279		
C(2)C(3)	1.4951	1.4942		
ClC(1)C(2)	122.93	122.93		
C(1)C(2)C(3)	122.65	122.65		
A	41701.	41800.		
B	2454.	2463.		
C	2351.	2359.		
χ_{aa} (^{35}Cl)	–60.82	–60.64		–60.3
χ_{bb}	28.84	28.78		28.7
χ_{cc}	31.98	31.86		31.6
$\lvert\chi_{ab}\rvert$	31.33	31.27		
RMS	0.3_8 (0.9 %)	0.2_5 (0.6 %)		
χ_{xx}	38.70	38.63		
χ_{yy}	31.98	31.86		

χ_{zz}	–70.69	–70.49		
η	–0.095	–0.096		
$\varphi_{z,a}$	17.48	17.48		
$\varphi_{a,CCl}$	17.27	17.24		
$\varphi_{z,CCl}$	0.21	0.24		
χ_{aa} (^{37}Cl)	–47.98	–43.50		
χ_{bb}	22.77	15.22		
χ_{cc}	25.21	28.28		
$\lvert\chi_{ab}\rvert$	24.63	29.82		
RMS				

[a] R. A. Beaudet, J. Chem. Phys. 37, 2398 (1962). Back to Top

Table 2. *cis*-1-Chloropropene, c-CH_3-C(H)=C(H)Cl (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}	$\sim r_e$		Expt. [a]
ClC(1)	1.7324	1.7292		
C(1)=C(2)	1.3336	1.3299		
C(2)C(3)	1.4906	1.4899		
ClC(1)C(2)	123.77	123.77		
C(1)C(2)C(3)	126.76	126.76		

A	14321.	14346.		14194.33
B	3634.	3649.		3637.76
C	2951.	2962.		2945.92
χ_{aa} (^{35}Cl)	–20.31	–20.15		–19.66
χ_{bb}	–10.49	–10.52		–11.39
χ_{cc}	30.80	30.67		31.05
$\lvert\chi_{ab}\rvert$	53.84	53.72		
RMS	0.66 (3.2 %)	0.62 (3.0 %)		
χ_{xx}	38.67	38.60		
χ_{yy}	30.80	30.67		
χ_{zz}	–69.47	–69.27		
η	–0.113	–0.114		
$\varphi_{z,a}$	42.39	42.44		
$\varphi_{a,CCl}$	42.99	43.02		
$\varphi_{z,CCl}$	0.60	0.58		
χ_{aa} (^{37}Cl)	–16.54	–16.41		
χ_{bb}	–7.74	–7.76		
χ_{cc}	24.28	24.17		
$\lvert\chi_{ab}\rvert$	42.38	42.29		

RMS				

[a] R. A. Beaudet, J. Chem. Phys. 40, 2705 (1964). Experimental values of χ_{aa} and χ_{bb} have been here interchanged. This makes much more sense. Back to Top

Table 3. 2-Chloropropene, CH_3-C(Cl)=CH_2 (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]
C(1)=C(2)	1.3329	1.3291		
C(2)Cl	1.7446	1.7413		
C(2)C(3)	1.4903	1.4896		
ClC(2)C(1)	119.71	119.71		
ClC(2)C(3)	113.85	113.85		
A	9318.	9346.		9271.706(79)
B	4995.	5011.		4983.816(45)
C	3318.	3329.		3304.414(45)
χ_{aa} (^{35}Cl)	–68.39	–68.19		–68.072
χ_{bb}	37.83	37.74		37.097
χ_{cc}	30.56	30.45		30.975
$\lvert\chi_{ab}\rvert$	9.60	9.72		
RMS	0.52 (1.2 %)	0.49 (1.1 %)		

χ_{xx}	38.69	38.63		
χ_{yy}	30.56	30.45		
χ_{zz}	–69.25	–69.08		
η	–0.117	–0.118		
$\varphi_{z,a}$	5.12	5.20		
$\varphi_{a,CCl}$	4.95	5.05		
$\varphi_{z,CCl}$	0.18	0.15		
χ_{aa} (^{37}Cl)	–53.93	–53.78		–53.763
χ_{bb}	29.85	29.78		29.370
χ_{cc}	24.08	24.00		24.394
$\lvert\chi_{ab}\rvert$	7.37	7.48		
RMS	0.34 (1.0 %)	0.33 (0.92 %)		

[a] E. Fliege and H. Dreizler, Z. Naturforsch. 38a, 1231 (1983). Back to Top

Table 4. *cis*-3-Chloropropene, CH_2=C(H)-CH_2Cl (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}	$\sim r_e$		Expt. [a]
C(1)=C(2)	1.3327	1.3289		

C(2)C(3)	1.4941	1.4932		
C(3)Cl	1.7817	1.7784		
C(1)C(2)C(3)	126.65	126.65		
C(2)C(3)Cl	113.92	113.92		
A	13589.	13640.		13582.14(16)
B	3861.	3870.		3816.633(17)
C	3064.	3072.		3035.143(13)
χ_{aa} (^{35}Cl)	–18.62	–18.59		–18.4(4)
χ_{bb}	–18.26	–18.23		–17.98(22)
χ_{cc}	36.89	36.82		36.4(5)
$\lvert\chi_{ab}\rvert$	54.47	54.37		
RMS	0.3_5 (1.4 %)	0.3_0 (1.2 %)		
χ_{xx}	36.02	35.96		
χ_{yy}	36.89	36.82		
χ_{zz}	–72.91	–72.78		
ETA	0.0119	0.0118		
$\varphi_{z,a}$	44.90	44.90		
$\varphi_{a,CCl}$	45.42	45.42		
$\varphi_{z,CCl}$	0.52	0.52		

[a] E. B. Kent, M. N. McCabe, M. A. Phillips, B. P. Gorden, and S. T. Shipman, 66th OSU International Symposium on Molecular Spectroscopy, 2011, Abstract RH01.

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Table 5. skew-3-Chloropropene, CH_2=C(H)-CH_2Cl (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]
C(1)=C(2)	1.3349	1.3311		
C(2)C(3)	1.4862	1.4857		
C(3)Cl	1.7988	1.7956		
C(1)C(2)C(3)	122.83	122.83		
C(2)C(3)Cl	110.41	110.41		
CCCCl	118.23	118.23		
A	21316.	21365.		21669.64(8)
B	2831.	2840.		2800.800(11)
C	2744.	2752.		2714.182(11)
χ_{aa} (^{35}Cl)	–39.23	–39.13		–39.5(5)
χ_{bb}	3.00	2.95		3.5(4)
χ_{cc}	36.23	36.18		36.1(6)
$\lvert\chi_{ab}\rvert$	50.44	50.38		
$\lvert\chi_{ac}\rvert$	2.67	2.75		
$\lvert\chi_{bc}\rvert$	0.55	0.60		

RMS	0.3_4 (1.3 %)	0.3_8 (1.5 %)		
χ_{xx}	37.46	37.40		
χ_{yy}	35.40	35.35		
χ_{zz}	–72.86	–72.75		
η	–0.283	–0.283		
$\varphi_{z,CCl}$	0.34	0.35		
χ_{aa} (^{37}Cl)	–31.21	–31.13		–31.6(8)
χ_{bb}	2.65	2.61		3.1(10)
χ_{cc}	28.56	28.52		28.5(13)
$\lvert\chi_{ab}\rvert$	39.64	39.59		
$\lvert\chi_{ac}\rvert$	1.91	1.98		
$\lvert\chi_{bc}\rvert$	0.30	0.34		
RMS	0.3_4 (1.6 %)	0.3_9 (1.9 %)		

[a] E. B. Kent, M. N. McCabe, M. A. Phillips, B. P. Gorden, and S. T. Shipman, 66th OSU International Symposium on Molecular Spectroscopy, 2011, Abstract RH01. Back to Top

Table 6. *cis*-1-Chloro-2-Fluoropropene, *cis*-C(H)Cl=C(F)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]
C(1)=C(2)	1.3331	1.3293		
C(2)C(3)	1.4826	1.4823		
C(1)C(2)C(3)	126.42	126.42		
ClC(1)	1.7176	1.7144		
ClC(1)C(2)	123.09	123.09		
C(2)F	1.3450	1.3388		
C(1)C(2)F	120.10	120.10		
A	9950.	10016.		9958.22(5)
B	2286.	2294.		2285.88(2)
C	1880.	1888.		1879.89(2)
χ_{aa} (^{35}Cl)	–52.95	–52.86		–53.09(20)
χ_{bb}	19.67	19.69		19.45(5)
χ_{cc}	33.28	33.16		33.64(20)
$\lvert\chi_{ab}\rvert$	44.75	44.54		43.5(30)
RMS	0.24 (0.7 %)	0.34 (1.0 %)		

χ_{xx}	40.99	40.86		39.84
χ_{yy}	33.28	33.16		33.64
χ_{zz}	–74.27	–74.02		–73.49
η	–0.104	–0.104		–0.0844
$\varphi_{z,a}$	25.47	25.42		
$\varphi_{a,CCl}$	26.12	26.06		
$\varphi_{z,CCl}$	0.65	0.64		
χ_{aa} (^{37}Cl)	–41.70	–41.62		–41.70(20)
χ_{bb}	15.47	15.49		15.17(20)
χ_{cc}	26.23	26.13		26.53(20)
$\lvert\chi_{ab}\rvert$	35.29	35.13		
RMS	0.24 (0.9 %)	0.30 (1.0 %)		

[a] R. G. Stone, S. I. Srivastava, and W. H. Flygare, J. Chem. Phys. 48, 1890 (1968).

Table 7. 1-Chloro-2-Methylpropene, *cis*-C(H)Cl=C(CH_3)$_2$ (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]
C(1)=C(2)	1.3366	1.3328		
C(2)C(3)	1.5002	1.4991		
C(1)C(2)C(3)	119.07	119.07		

ClC(1)	1.7330	1.7298		
ClC(1)C(2)	124.33	124.33		
C(2)C(4)	1.4942	1.4933		
C(1)C(2)C(4)	124.40	124.40		
A	8472.	8458.		8400.0178(5)
B	2269.	2261.		2257.7687(2)
C	1830.	1824.		1818.7071(2)
χ_{aa} (^{35}Cl)	–52.90	–52.75		–52.591(1)
χ_{bb}	21.40	21.39		21.086(2)
χ_{cc}	31.49	31.36		31.505(1)
$\lvert\chi_{ab}\rvert$	39.08	38.99		39.037(99)
RMS	0.25 (0.7 %)	0.21 (0.6 %)		
χ_{xx}	38.18	38.12		37.922(73)
χ_{yy}	31.49	31.36		31.505(2)
χ_{zz}	–69.67	–69.48		–69.427(72)
η	–0.0959	–0.0972		–0.092
$\varphi_{z,a}$	23.23	23.22		23.330(37)
$\varphi_{a,CCl}$	23.86	23.83		
$\varphi_{z,CCl}$	0.63	0.61		
χ_{aa} (^{37}Cl)	–41.66	–41.54		–41.429(3)

χ_{bb}	16.84	16.83		16.595(3)
χ_{cc}	24.82	24.72		24.833(4)
$\lvert\chi_{ab}\rvert$	30.83	30.75		30.659(31)
RMS	0.20 (0.7 %)	0.16 (0.6 %)		

[a] T. Bruhn and W. Stahl, J. Mol. Spectrosc. 202, 272 (2000). Back to Top

Table 8. 2,3-Dichloropropene, *anti*-CH_2=C(^{35}Cl)-$CH_2{}^{35}$Cl (C_s). Heavy atom structure parameters (Å and degrees). Rotational constants (MHz). 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]
C(1)=C(2)	1.3301	1.3264		
C(2)C(3)	1.4957	1.4948		
C(1)C(2)C(3)	128.32	128.32		
C(2)Cl	1.7414	1.7382		
C(1)C(2)Cl	121.10	121.10		
C(3)Cl	1.7769	1.7736		
C(2)C(3)Cl	113.16	113.16		
A	8338.	8368.		
B	1510.	1515.		
C	1289.	1293.		

χ_{aa} Cl(2)	–54.52	–54.35		--53.985(20)
χ_{bb}	21.98	21.93		21.266(28)
χ_{cc}	32.54	32.42		32.718(28)
$\lvert\chi_{ab}\rvert$	38.63	38.56		39.3(4)
RMS	0.52 (1.5 %)	0.47 (1.3 %)		
χ_{xx}	38.09	38.02		38.05(29)
χ_{yy}	32.54	32.42		32.718(28)
χ_{zz}	–70.63	–70.44		--70.77(29)
η	–0.0785	–0.0795		
$\varphi_{z,a}$	22.64	22.66		
$\varphi_{a,CCl}$	22.97	23.00		
$\varphi_{z,CCl}$	0.33	0.34		
χ_{aa} Cl(3)	–61.81	–61.63		--61.298(19)
χ_{bb}	23.59	23.49		23.629(35)
χ_{cc}	38.22	38.13		37.669(35)
$\lvert\chi_{ab}\rvert$	35.24	35.23		35.1(4)
RMS	0.52 (1.3 %)	0.34 (0.8 %)		
χ_{xx}	36.25	36.18		36.26(26)
χ_{yy}	38.22	38.13		37.669(35)

χ_{zz}	–74.47	–74.31		--73.93(25)
η	0.0264	0.0263		
$\varphi_{z,a}$	19.77	19.81		
$\varphi_{a,CCl}$	20.39	20.42		
$\varphi_{z,CCl}$	0.62	0.61		

[a] A. S. Dikkumbura, E. R. Webster, R. E. Dorris, R. A. Peebles, S. A. Peebles, N. A. Seifert, and B. Pate, Abstract MI13, 71st International Symposium on Molecular Spectroscopy, Champaign-Urbana, Ill. 2016. Back to Top

Table 9. 2,3-Dichloropropene, *gauche*-CH_2=C(^{35}Cl)$CH_2{}^{35}$Cl (C_1). Heavy atom structure parameters (Å and degrees). Rotational constants (MHz). 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]
C(1)=C(2)	1.3340	1.3302		
C(2)C(3)	1.4876	1.4870		
C(1)C(2)C(3)	123.98	123.98		
C(2)Cl	1.7335	1.7303		
C(1)C(2)Cl	121.11	121.11		
C(1)C(3)C(2)Cl	–179.16	–179.16		
C(3)Cl	1.7895	1.7862		
C(2)C(3)Cl	111.28	111.28		

C(1)C(2)C(3)Cl	113.11	113.11		
A	4819.	4838.		4825.77581(18)
B	2044.	2049.		2027.99973(16)
C	1570.	1574.		1559.15872(16)
χ_{aa} Cl(2)	16.15	16.05		15.695(2)
χ_{bb}	–49.06	–48.86		--48.901(2)
χ_{cc}	32.92	32.81		33.206(2)
χ_{ab}	–44.20	–44.14		43.68(8)
χ_{ac}	0.23	0.26		0.47(15)
χ_{bc}	–5.89	–5.86		--5.62(29)
RMS	0.32(1.0 %)	0.31(1.0 %)		
χ_{xx}	39.72	39.64		38.58(14)
χ_{yy}	31.92	31.80		32.60(12)
χ_{zz}	–71.64	–71.44		--71.19(7)
η	–0.109	–0.110		--0.0841(3)
$\varphi_{z,CCl}$	0.54	0.55		
χ_{aa} Cl(3)	–15.36	–15.29		--15.504(2)
χ_{bb}	12.29	12.25		12.302(3)
χ_{cc}	3.07	3.04		3.202(3)

χ_{ab}	36.81	36.75		--36.79(11)
χ_{ac}	42.21	42.13		--41.80(10)
χ_{bc}	–30.54	–30.51		--30.07(13)
RMS	0.11 (1.1 %)	0.16 (1.5 %)		
χ_{xx}	36.82	36.75		36.58(11)
χ_{yy}	38.61	38.55		38.30(12)
χ_{zz}	–75.43	–75.30		--74.88(12)
η	0.0237	0.0238		0.0230(21)
$\varphi_{z,CCl}$	0.60	0.61		

[a] A. S. Dikkumbura, E. R. Webster, R. E. Dorris, R. A. Peebles, S. A. Peebles, N. A. Seifert, and B. Pate, Abstract MI13, 71st International Symposium on Molecular Spectroscopy, Champaign-Urbana, Ill. 2016. 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 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, which is for ^{35}Cl, 0.49 MHz.

Table 10. Root mean square (RMS) differences (MHz) between calculated and experimental ^{35}Cl diagonal nqcc's (Percent of average experimental nqcc.).

Molecule	r_{opt}	$\sim r_e$
trans-1-Chloropropene	0.3_8 (0.9 %)	0.2_5 (0.6 %)
cis-1-Chloropropene	0.66 (3.2 %)	0.62 (3.0 %)
2-Chloropropene	0.52 (1.2 %)	0.49 (1.1 %)
cis-3-Chloropropene	0.3_5 (1.4 %)	0.3_0 (1.2 %)
skew-3-Chloropropene	0.3_4 (1.3 %)	0.3_8 (1.5 %)
1-Chloro-2-Fluoropropene	0.24 (0.7 %)	0.34 (1.0 %)
1-Chloro-2-Methylpropene	0.25 (0.7 %)	0.21 (0.6 %)
anti-2,3-Dichloropropene Cl(2)	0.52 (1.5 %)	0.47 (1.3 %)
Cl(3)	0.52 (1.3 %)	0.34 (0.8 %)
gau-2,3-Dichloropropene Cl(2)	0.32 (1.0 %)	0.31 (1.0 %)
Cl(3)	0.11 (1.1 %)	0.16 (1.5 %)

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