Fluorinated Haloethanes

Table 1: ^{35}Cl NQCC tensors (MHz) in increasingly fluorinated chloroethane. (References are given below.)

	CH_3CH_2Cl	CH_3CHFCl	CH_3CF_2Cl	t-CH_2FCF_2Cl
χ_{aa}	-49.29(9)	-62.4014(109)	-72.0861(57)	-57.958(10)
χ_{bb}	13.65(8)	34.2641(138)	36.719(13)	21.231(11)
χ_{cc}	35.64(8)	28.1373(138)	35.368(13)	36.727(11)
$\lvert\chi_{ab}\rvert$	42.85(46)[a]	0.66(34)[b,c]	0.50(20)[b]	36.54(30)[b]
$\lvert\chi_{ac}\rvert$		25.5(64)		
$\lvert\chi_{bc}\rvert$		1.97(34)[b]		
χ_{xx}	35.34(38)	32.45(139)	36.721(13)	35.52(20)
χ_{yy}	35.64(8)	36.64(182)	35.368(13)	36.727(11)
χ_{zz}	-70.98(38)	-69.09(314)	-72.088(6)	-72.24(20)
η	0.004(5)	0.060(33)	–0.0188(3)	0.0168(28)
	CF_3CH_2Cl	CF_3CHFCl	CF_3CF_2Cl	
χ_{aa}	-45.9651(10)	-34.247(44)	-25.7949(19)	
χ_{bb}	5.5538(11)	4.487(47)	12.8998(29)	
χ_{cc}	40.4113(11)	29.760(44)	38.6937(22)	
$\lvert\chi_{ab}\rvert$	52.103(13)	47.46(38)[b,c]	56.90(20)	
$\lvert\chi_{ac}\rvert$		27.49(38)[b]		
$\lvert\chi_{bc}\rvert$		16.46(38)[b]		
χ_{xx}	37.917(12)	35.70(37)	37.92(20)	
χ_{yy}	40.4113(11)	40.14(32)	38.6937(22)	
χ_{zz}	-78.329(12)	-75.84(38)	-76.61(20)	
η	0.03184(15)	0.0585(65)	0.0101(26)	

[a] *Ab initio* value calculated on substitution structure of M.Hayashi and T.Inagusa, J. Mol. Struct. 220,103(1990). The estimated uncertainty is 2× the root mean square difference between calculated and experimental diagonal components.
[b] *Ab initio* value. See http://nqcc.wcbailey.net/ClFEthanes.pdf. The estimated uncertainty is 2× the root mean square difference between calculated and experimental diagonal components.
[c] The product $\chi_{ab}\chi_{ac}\chi_{bc}$ is negative.

NOTE: Going from CH_3CH_2Cl to CF_3CF_2Cl, $|\chi_{zz}|$ increases by 7.9%

Table 2: ^{79}Br NQCC tensors (MHz) in increasingly fluorinated bromoethane. (References are given below.)

	CH_3CH_2Br	CH_3CHFBr	g-CH_2FCH_2Br	CF_3CF_2Br
χ_{aa}	417.75(20)	493.49(29)	266.4(17)	430.6937(53)
χ_{bb}	-144.04	-266.19(31)	-11.8(9)	-121.7548(85)
χ_{cc}	-273.71(17)	-227.30(31)	-254.6(19)	-308.9389(66)
$\lvert\chi_{ab}\rvert$	294.77(205)	2.84(180)[a,b]	392.7(43)[b]	364.06(12)
$\lvert\chi_{ac}\rvert$		180.57(180)[a]	117.84(40)[c]	
$\lvert\chi_{bc}\rvert$		11.80(180)[a]	91.51(40)[c]	
χ_{xx}	-270.32(166)	-264.00(76)	-293.1(29)	-302.520(96)
χ_{yy}	-273.71(17)	-319.73(105)	-277.7(18)	-308.9389(66)
χ_{zz}	544.03(168)	533.73(81)	570.8(41)	611.459(96)
η	0.0062(34)	0.1044(24)	-0.027(6)	0.0105(2)

[a] *Ab initio* value. See http://nqcc.wcbailey.net/BrFHCCH3.html. The estimated uncertainty is 2× the root mean square difference between calculated and experimental diagonal components.
[b] The product $\chi_{ab}\chi_{ac}\chi_{bc}$ is positive.
[c] *Ab initio* value. See http://nqcc.wcbailey.net/gCH2BrCH2F.html. The estimated uncertainty is 2× the root mean square difference between calculated and experimental diagonal components.

NOTE: Going from CH_3CH_2Br to CF_3CF_2Br, $|\chi_{zz}|$ increases by 12.4%

Table 3: ^{127}I NQCC tensors (MHz) in increasingly fluorinated iodoethane. (References are given below.)

	CH_3CH_2I	g-CH_2FCH_2I	CF_3CF_2I
χ_{aa}	-1478.06(39)	-1043.69(87)	-1739.8608(95)
χ_{bb}	564.56	183.72(48)	663.0608(145)
χ_{cc}	913.50(26)	859.97(99)	1076.8007(110)
$\lvert\chi_{ab}\rvert$	895.75(121)	1250.9(12)[a]	1052.618(21)
$\lvert\chi_{ac}\rvert$		384.0(14)	
$\lvert\chi_{bc}\rvert$		288.1(14)	
χ_{xx}	901.71(81)	910.9	1058.945(48)
χ_{yy}	913.50(26)	995.1	1076.801(11)
χ_{zz}	-1815.22(85)	-1906.0	-2135.746(41)
η	0.0065(6)	0.04417	0.00836(3)

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

NOTE

Going from CH_3CH_2Cl to CF_3CF_2Cl, $|\chi_{zz}|$ increases by 7.9%

Going from CH_3CH_2Br to CF_3CF_2Br, $|\chi_{zz}|$ increases by 12.4%

Going from CH_3CH_2I to CF_3CF_2I, $|\chi_{zz}|$ increases by 17.7%

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