Nuclear Quadrupole Coupling Constants

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Alkyl Monohalides

Table 1: χ_{zz}(MHz) for ^{35}Cl, ^{79}Br, and ^{127}I in Alkyl Monohalides. This Table is a summary of the data collected below in Table 2.

	Cl	Br	I
Methyl	–74.7514(11)	577.1300(18)	–1934.13022(39)
Ethyl	–70.98(38)	544.03(168)	–1815.22(85)
t-1-Propyl	–70.68(11)		–1814.55(55)
g-1-Propyl	–69.8(18)	528.7(46)	–1805.16(56)
2-Propyl	–68.50(21)	522.3339(765)	–1741.47(75)
1-Butyl, AA		543.45(32)	–1815.72(6)
1-Butyl, GA	–70.82(25)	539.71(63)	–1804.133(35)
1-Butyl, GG	–70.2(16)	536.17(46)	–1758.57(14)
2-Butyl, G+/G		518.84(5)	–1731.291(23)
2-Butyl, A		521.32(4)	–1737.458(21)
2-Butyl, G–/G'		518.24(67)	–1730.09(4)
g-Isobutyl[a]	–73.6(79)	531.1(105)	–1793.0(77)
tert-Butyl	–67.3155(28)	511.9797(19)	–1708.2657(24)

[a] gauche-1-Halo-2-methylpropane

Table 2: ^{35}Cl, ^{79}Br, and ^{127}I NQCC tensors (MHz) in Alkyl Monohalides. (References are given below.)

		Cl	Br	I
Methyl	χ_{zz}	–74.7514(11)	577.1300(18)	–1934.13022(39)
Ethyl	χ_{aa}	–49.29(9)	417.75(20)	–1478.06(39)
	χ_{bb}	13.65(8)	–144.04	564.56
	χ_{cc}	35.64(8)	–273.71(17)	913.50(26)
	$\lvert\chi_{ab}\rvert$	42.85(46)[a]	294.77(205)	895.75(121)
	χ_{xx}	35.34(38)	–270.32(166)	901.71(81)
	χ_{yy}	35.64(8)	–273.71(17)	913.50(26)
	χ_{zz}	–70.98(38)	544.03(168)	–1815.22(85)
	η	0.004(5)	0.0062(34)	0.0065(6)
t-1-Propyl	χ_{aa}	–54.7357(57)		–1515.33(67)
	χ_{bb}	19.062(21)		601.22(57)
	χ_{cc}	35.674(21)		914.12(44)
	$\lvert\chi_{ab}\rvert$	37.83(15)		850.21(25)
	χ_{xx}	35.01(11)		900.44(47)
	χ_{yy}	35.674(21)		914.12(44)
	χ_{zz}	–70.68(11)		–1814.55(55)
	η	0.0094(19)		0.0075(5)
g-1-Propyl	χ_{aa}	–19.4384(46)	256.9(11)	–1012.92(24)
	χ_{bb}	10.711(13)	–9.5(5)	189.32(18)
	χ_{cc}	35.150(13)	–247.4(13)	823.59(14)
	$\lvert\chi_{ab}\rvert$	49.5(13)[b]	380.0(43)[c]	1176.14(15)[b]
	$\lvert\chi_{ac}\rvert$	15.12(88)	114.7(192)[a]	361.67(75)
	$\lvert\chi_{bc}\rvert$	17.6(45)	89.0(192)[a]	245.43(288)
	χ_{xx}	41.3(33)	–124.8(192)	923.88(250)
	χ_{yy}	33.5(24)	–403.9(192)	881.28(205)
	χ_{zz}	–69.8(18)	528.7(46)	–1805.16(56)
	η	–0.111(59)	0.527(52)	–0.0236(25)

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

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		Cl	Br	I
2-Propyl	χ_{aa}	–61.496(6)	479.8908(57)	–1626.36(49)
	χ_{bb}	34.708(9)	–264.9423(48)	883.81(98)
	χ_{cc}	26.788(9)	–214.9485(48)	742.55
	$\lvert\chi_{ac}\rvert$	25.83(42)[a]	176.89(16)	534.73(58)
	χ_{xx}	33.79(21)	–257.3916(764)	857.67(120)
	χ_{yy}	34.708(9)	–264.9423(48)	883.81(98)
	χ_{zz}	–68.50(21)	522.3339(765)	–1741.47(75)
	η	0.013	0.01446(15)	0.0150(12)
1-Butyl, AA	χ_{aa}		363.04(34)	–1294.041(34)
	χ_{bb}		–89.07(59)	380.05(6)
	χ_{cc}		–273.97(59)	913.99(7)
	$\lvert\chi_{ab}\rvert$		337.81(13)	1070.28(6)
	χ_{xx}		–269.48(48)	901.73(7)
	χ_{yy}		–273.97(59)	913.99(7)
	χ_{zz}		543.45(32)	–1815.72(6)
	η			0.00675(6)
1-Butyl, GA	χ_{aa}	1.06(52)	87.17(10)	–521.973(12)
	χ_{bb}	–33.06(27)	166.53(6)	–337.242(15)
	χ_{cc}	32.00(59)	–253.70(6)	859.216(19)
	$\lvert\chi_{ab}\rvert$	48.38(8)[a,b]	394.70(44)[c]	1331.251(23)[b]
	$\lvert\chi_{ac}\rvert$	10.50(8)[a]	72.26(236)	226.66(13)
	$\lvert\chi_{bc}\rvert$	15.88(8)[a]	87.38(18)	235.95(6)
	χ_{xx}	34.80(36)	–264.89(197)	884.09(11)
	χ_{yy}	36.01(37)	–274.83(154)	920.04(9)
	χ_{zz}	–70.82(25)	539.71(63)	–1804.133(35)
	η	0.0170(72)		0.01993(8)

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		Cl	Br	I
1-Butyl, GG	χ_{aa}	–6.5(4)	157.83(11)	–752.593(28)
	χ_{bb}	–6.1(2)	–7.93(28)	157.01(5)
	χ_{cc}	12.6(5)	–149.90(28)	595.58(6)
	$\lvert\chi_{ab}\rvert$	41.5(14)[a,b]	336.11(28)[c]	1116.74(13)[b]
	$\lvert\chi_{ac}\rvert$	30.2(14)[a]	221.62(31)	692.17(19)
	$\lvert\chi_{bc}\rvert$	30.7(14)[a]	172.68(76)	460.66(12)
	χ_{xx}	34.7(15)	–264.88(54)	576.17(16)
	χ_{yy}	35.5(15)	–271.29(39)	1182.40(19)
	χ_{zz}	–70.2(16)	536.17(46)	–1758.57(14)
	η	0.012(30)		0.34473(15)
2-Butyl, G+/G	χ_{aa}		300.1367(2)	–1329.651(2)
	χ_{bb}		–82.2620(2)	582.497(14)
	χ_{cc}		–217.8747(2)	747.154(14)
	$\lvert\chi_{ab}\rvert$		321.18(6)[c]	822.076(20)[b]
	$\lvert\chi_{ac}\rvert$		140.93(2)	456.84(5)
	$\lvert\chi_{bc}\rvert$		82.16(1)	176.840(32)
	χ_{xx}		–253.72(1)	842.907(28)
	χ_{yy}		–265.12(5)	888.384(20)
	χ_{zz}		518.84(5)	–1731.291(23)
	η		0.02196(10)	0.026268(20)
2-Butyl, A	χ_{aa}		446.043(9)	–1550.634(13)
	χ_{bb}		–219.206(5)	779.401(12)
	χ_{cc}		–226.837(5)	771.233(17)
	$\lvert\chi_{ab}\rvert$		179.19(4)[c]	497.892(35)[b]
	$\lvert\chi_{ac}\rvert$		145.47(9)	452.170(28)
	$\lvert\chi_{bc}\rvert$		36.62(3)	92.25(7)
	χ_{xx}		–256.91(4)	856.121(20)
	χ_{yy}		–264.40(2)	881.337(18)
	χ_{zz}		521.32(4)	–1737.458(21)
	η		0.01436(7)	0.014513(16)

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		Cl	Br	I
2-Butyl, G-/G'	χ_{aa}		317.134(1)	–1256.176(6)
	χ_{bb}		–127.125(2)	569.007(11)
	χ_{cc}		–190.009(2)	687.169(12)
	$\lvert\chi_{ab}\rvert$		274.8(6)[c]	792.17(4)[b]
	$\lvert\chi_{ac}\rvert$		200.6(9)	615.34(6)
	$\lvert\chi_{bc}\rvert$		96.21(90)	227.51(4)
	χ_{xx}		–259.98(61)	867.14(5)
	χ_{yy}		–258.26(61)	862.95(4)
	χ_{zz}		518.24(67)	–1730.09(4)
	η		–0.0033(17)	–0.00242(4)
g-Isobutyl	χ_{aa}	–51.6(54)	380.0(22)	–1371.1(38)
	χ_{bb}	16.9(28)	–144.8(41)	590.8(42)
	χ_{cc}	34.7(60)	–235.2(46)	780.3(56)
	$\lvert\chi_{ab}\rvert$	37.3(80)[a,b]	282.5(17)[c]	841.7(19)[b]
	$\lvert\chi_{ac}\rvert$	22.3(80)[a]	159.(30)[a]	494.8(174)[a]
	$\lvert\chi_{bc}\rvert$	10.7(80)[a]	69.(30)[a]	198.1(174)[a]
	χ_{xx}	33.2(68)	–203.1(68)	881.6(168)
	χ_{yy}	40.4(68)	–328.0(165)	911.4(161)
	χ_{zz}	–73.6(79)	531.1(105)	–1793.0(77)
	η	0.10(13)	0.235(34)	0.016(13)
tert-Butyl	χ_{zz}	–67.3155(28)	511.9797(19)	–1708.2657(24)

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