Methylated Halomethanes

Table 1: ^{35}Cl, ^{79}Br, and ^{127}I NQCC tensors (MHz) in methyl, ethyl, isopropyl, and tert-butyl halides. (References are given below.)

X =		Cl	Br	I
CH_3X	χ_{zz}	-74.7514(11)	577.1300(18)	-1934.13022(39)
CH_3CH_2X	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)	913.50(26)
	χ_{yy}	35.64(8)	-273.71(17)	901.71(81)
	χ_{zz}	-70.98(38)	544.03(168)	-1815.22(85)
	η	0.004(5)	0.0062(34)	-0.0065(6)
$(CH_3)_2CHX$	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)[b]	176.89(16)	534.73(58)
	χ_{xx}	33.79(21)	-264.9423(48)	883.81(98)
	χ_{yy}	34.708(9)	-257.3916(764)	857.67(120)
	χ_{zz}	-68.50(21)	522.3339(765)	-1741.47(75)
	η	0.013	-0.01446(15)	-0.0150(12)
$(CH_3)_3CX$	χ_{zz}	–67.3155(28)	511.9797(19)	-1708.2657(24)

[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 calculated on r_m^{ρ} structure of M.Meyer, J-U.Grabow, H.Dreizler, and H.D.Rudolph, J.Mol. Spectrosc. 151,217(1992). The estimated uncertainty is 2× the root mean square difference between calculated and experimental diagonal components.

NOTE: Going from methyl to ethyl to isopropyl to tert-butyl,
changes in $|\chi_{zz}|$(Cl) are –5.0 %, –3.5 %, and –1.7 %,
changes in $|\chi_{zz}|$(Br) are –5.7 %, –4.0 %, and –2.0 %,
changes in $|\chi_{zz}|$(I) are –6.1 %, –4.1 %, and –1.9 %.

References

CH_3Cl	G.Wlodarczak, D.Boucher, R.Bocquet, and J.Demaison, J. Mol. Spectrosc 116,251(1986).
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CH_3I	B.D.Osipov and M.N.Grabois, J. Mol. Spectrosc. 111,344(1985).
CH_3CH_2Cl	M.Hayashi and T.Inagusa, J.Mol.Struct. 220,103(1990).
CH_3CH_2Br	T.Inagusa and M.Hayashi, J.Mol.Spectrosc. 129,160(1988).
CH_3CH_2I	T.Inagusa, M.Fujitake, and M.Hayashi, J.Mol.Spectrosc. 128,456(1988).
$CH_3CHClCH_3$	M.Meyer, J-U.Grabow, H.Dreizler, and H.D.Rudolph, J.Mol. Spectrosc. 151,217(1992).
$CH_3CHBrCH_3$	M.Meyer, W.Stahl, and H.Dreizler, J.Mol. Spectrosc. 151,243(1992).
CH_3CHICH_3	C.Ikeda, T.Inagusa, and M.Hayashi, J.Mol.Spectrosc. 135,334(1989).
$(CH_3)_3CCl$	Z.Kisiel, E.Białkowska-Jaworska, O.Desyatnyk, B.A.Pietrewicz, and L.Pszcółkowski, J.Mol.Spectrosc. 208,113(2001).
$(CH_3)_3CBr$	ibid.
$(CH_3)_3CI$	ibid.