Mono-, Di-, and Trihalomethanes

Table 1: ^{35}Cl, ^{79}Br, ^{127}I NQCC tensors (MHz) in mono-, di-, and trihalomethanes. (References are given below.)

X =		Cl	Br	I
CH_3X	χ_{zz}	–74.7514(11)	577.1300(18)	–1934.13022(39)
CH_2X_2	χ_{aa}	–41.7418(11)	335.21(42)[a]	–1180.90(13)
	χ_{bb}	1.8004(12)	–24.93(24)	144.24
	χ_{cc}	39.9414(12)	–310.28(48)	1036.66(9)
	$\lvert\chi_{ab}\rvert$	50.93(23)	402.12(79)	1358.85(54)
	χ_{xx}	35.41(21)	–285.46	993.4(10)
	χ_{yy}	39.9414(12)	–310.28	1036.66(9)
	χ_{zz}	–75.35(21)	595.74	–2030.1(5)
	η	0.060(3)	0.04166	0.0213
CHX_3	χ_{uu}	28.6436(4)	231.9631(33)	
	χ_{vv}	–67.8309(5)	543.8554(53)	
	χ_{ww}	39.1872(5)	–311.8922(53)	
	$\lvert\chi_{uv}\rvert$	34.137(32)	–285.522(13)	
	χ_{xx}	39.501(18)	–310.2161(78)	
	χ_{yy}	39.1872(5)	–311.8922(53)	
	χ_{zz}	–78.688(18)	622.1083(87)	
	η	–0.0040(2)	0.002694(15)	

[a] ^{79}Br in $CH_2{}^{79}Br^{81}Br$

Going from CH_3X to CH_2X_2 to CHX_3,

changes in $|\chi_{zz}|$(Cl) are +0.8 % and +4.4 %

changes in $|\chi_{zz}|$(Br) are +3.2 % and +4.4 %

changes in $|\chi_{zz}|$(I) are +5.0 % and

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