Mono-, 1,1-Di-, and 1,1,1-Trichloroethane

Table 1: ^{35}Cl NQCC tensors (MHz) in chloro-, 1,1-dichloro-, and 1,1,1-trichloroethane.

	CH_3CH_2Cl[a]	CH_3CHCl_2[b]	CH_3CCl_3[c]
χ_{aa}	–49.29(9)	–39.0405(22)	–65.5378(12)
χ_{bb}	13.65(8)	10.6742(30)	38.6472(12)
χ_{cc}	35.64(8)	28.3663(30)	26.8907(9)
$\lvert\chi_{ab}\rvert$	42.85(46)[d]	44.22(36)[e]	
$\lvert\chi_{ac}\rvert$		24.08(74)	36.510(23)
$\lvert\chi_{bc}\rvert$		16.27(29)	
χ_{xx}	35.34(38)	34.79(93)	39.571(14)
χ_{yy}	35.64(8)	38.41(57)	38.6472(12)
χ_{zz}	–70.98(38)	–73.19(71)	–78.218(14)
η	0.004(5)	0.049(21)	–0.0118(2)

[a] M.Hayashi and T.Inagusa, J. Mol. Struct. 220,103(1990).
[b] A. de Luis, J.C.López, and J.L.Alonso, Chem. Phys. 248,247(1999).
[c] L.Dore and Z.Kisiel, J. Mol. Spectrosc. 189,228(1998).
[d] *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.
[e] The product $\chi_{ab}\chi_{ac}\chi_{bc}$ is negative.

Going from CH_3CH_2Cl to CH_3CHCl_2 to CH_3CCl_3,
changes in $|\chi_{zz}|$ are +3.1 % and +6.9 %