

Perfluorohaloalkanes

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

X =		H	F
CX ₃ Cl	χ_{zz}	-74.7514(11)	-77.902(30)
CX ₃ CX ₂ Cl	χ_{aa}	-49.29(9)	-25.7949(19)
	χ_{bb}	13.65(8)	12.8998(29)
	χ_{cc}	35.64(8)	38.6937(22)
	$ \chi_{ab} $	42.85(46) ^a	56.90(20)
	χ_{xx}	35.34(38)	37.92(20)
	χ_{yy}	35.64(8)	38.6937(22)
	χ_{zz}	-70.98(38)	-76.61(20)
	η	0.004(5)	0.0101(26)
t-CX ₃ CX ₂ CX ₂ Cl	χ_{aa}	-54.7357(57)	
	χ_{bb}	19.062(21)	
	χ_{cc}	35.674(21)	
	$ \chi_{ab} $	37.83(15)	
	χ_{xx}	35.01(11)	
	χ_{yy}	35.674(21)	
	χ_{zz}	-70.68(11)	
	η	0.0094(19)	

^a *Ab initio* value. The estimated uncertainty is $2\times$ the root mean square difference between calculated and experimental diagonal components.

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

X =		H	F
CX ₃ Br	χ_{zz}	577.1300(18)	618.2628(21)
CX ₃ CX ₂ Br	χ_{aa}	417.75(20)	430.6937(53)
	χ_{bb}	-144.04	-121.7548(85)
	χ_{cc}	-273.71(17)	-308.9389(66)
	$ \chi_{ab} $	-294.77(205)	364.06(12)
	χ_{xx}	-270.32(166)	-302.520(96)
	χ_{yy}	-273.71(17)	-308.9389(66)
	χ_{zz}	544.03(168)	611.459(96)
	η	0.0062(34)	0.0105(2)

^a *Ab initio* value. The estimated uncertainty is $2\times$ the root mean square difference between calculated and experimental diagonal components.

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

X =		H	F
CX ₃ I	χ_{zz}	-1934.13022(39)	-2144.9949(28)
CX ₃ CX ₂ I	χ_{aa}	-1478.06(39)	-1739.8608(95)
	χ_{bb}	564.56	663.0608(29)
	χ_{cc}	913.50(26)	1076.8007(110)
	$ \chi_{ab} $	895.75(121)	1052.618(21)
	χ_{xx}	901.71(81)	1058.945(48)
	χ_{yy}	913.50(26)	1076.801(11)
	χ_{zz}	-1815.22(85)	-2135.746(41)
	η	0.0065(6)	0.00836(3)
t-CX ₃ CX ₂ CX ₂ I	χ_{aa}	-1515.33(67)	-1798.4013(58)
	χ_{bb}	601.22(57)	716.0883(62)
	χ_{cc}	914.12(44)	1082.3130(11)
	$ \chi_{ab} $	850.21(25)	991.7058(35)
	χ_{xx}	900.44(47)	1060.1382(60)
	χ_{yy}	914.12(44)	1082.3130(11)
	χ_{zz}	-1814.55(55)	-2142.4512(49)
	η	0.0075(5)	0.01035(7)
CX ₃ CX ₂ CX ₂ CX ₂ I	χ_{aa}		-1484.247(73) ^a
	χ_{bb}		407.64(22)
	χ_{cc}		1076.60(22)
	χ_{ab}		-1284.0(31)
	χ_{ac}		-155.(27)
	χ_{bc}		-60.5(16)
	χ_{xx}		
	χ_{yy}		
	χ_{zz}		-2141.7(35)
	η		

^a CF₃CF₂CF₂CF₂I is transoidal, C₁ symmetry.

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