Alkenyl Halides

Table 1: χ_{zz}(MHz) for ^{35}Cl, ^{79}Br, and ^{127}I in Alkenyl Halides.

	Cl	Br	I
Ethylene Halide	-70.75	549.97(328)	-1870.71(207)
t-1-Halo-2-Fluororethylene	-74.88(74)	600.3(37)	
c-1-Halo-2-Fluoroethylene	-74.455(13)	589.14(3)	
1-Halo-1-Fluoroethylene	-73.27(12)	582.15(27)	
1-Halo-2,2-Difluoroethylene	-77.89(10)	615.711(20)	
Halotrifluoroethylene	-77.46(10)		
2-Halopropene	-68.96	538.9(62)	-1828.59(11)
t-1-Halopropene	-70.1		
c-1-Halopropene	-69.40		
c-3-Halopropene	-72.36		
g-3-Halopropene	-72.8(8)	558.7(87)	-1863.
1-Halo-2-Methylpropene	-69.427(72)		
c-1-Halo-2-Fluoropropene	-73.49		
g-3-Halo-3,3-Difluoropropene		563.56(11)	
Haloallene	-75.20	589.02	-2010.15(64)
1-Halo-1-Fluoroallene	-75.04		
2-Halo-1,3-Butadiene	-71.4(7)		
c-1-Halo-1,3-Butadiene	-69.78(64)		

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

		Cl	Br	I
Ethylene Halide	χ_{aa}	-57.21(13)	470.98(9)	-1654.62(23)
	χ_{bb}	25.47	-216.97	769.32
	χ_{cc}	31.74	-254.01(10)	885.30(17)
	$\lvert\chi_{ab}\rvert$	36.10(116)[a]	246.14(564)	755.32(392)
	χ_{xx}	39.01	-295.97(328)	985.42(207)
	χ_{yy}	31.74	-254.01(10)	885.30(17)
	χ_{zz}	-70.75	549.97(328)	-1870.71(207)
	η	-0.103	-0.0763	-0.0535(11)
t-1-Halo-2-Fluoroethylene	χ_{aa}	-63.586(58)	514.499(12)	
	χ_{bb}	27.53(27)	-227.489	
	χ_{cc}	36.05(27)	-287.01(18)	
	$\lvert\chi_{ab}\rvert$	34.01(124)[a]	265.9(75)	
	χ_{xx}	38.82(78)	-313.3(37)	
	χ_{yy}	36.05(27)	-287.01(18)	
	χ_{zz}	-74.88(74)	600.3(37)	
	η	-0.370(11)	-0.0880(1)	
c-1-Halo-2-Fluoroethylene	χ_{aa}	-22.719(14)	278.044(9)	
	χ_{bb}	-10.600(13)	-9.364	
	χ_{cc}	33.319(17)	-268.68(1)	
	$\lvert\chi_{ab}\rvert$	57.4770(86)	431.50(3)	
	χ_{xx}	41.136(13)	-320.45(3)	
	χ_{yy}	33.319(17)	-268.68(1)	
	χ_{zz}	-74.455(13)	589.14(3)	
	η	-0.10499(29)	-0.08788(7)	

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		Cl	Br	I
1-Halo-1-Fluoroethylene	χ_{aa}	-72.92(4)	578.81(20)	
	χ_{bb}	38.63(3)	-302.31	
	χ_{cc}	34.30(4)	-276.50(11)	
	$\lvert\chi_{ab}\rvert$	6.30(102)[a]	54.3(15)	
	χ_{xx}	38.98(12)	-305.64(21)	
	χ_{yy}	34.30(4)	-276.50(11)	
	χ_{zz}	-73.27(12)	582.15(27)	
	η	0.0639(17)	-0.0700(4)	
1-Halo-2,2-Difluoroethylene	χ_{aa}	-54.8923(48)	453.959(20)	
	χ_{bb}	18.2356(57)	-160.648(11)	
	χ_{cc}	36.6567(56)	-283.311(11)	
	$\lvert\chi_{ab}\rvert$	47.02(13)	354.369(24)	
	χ_{xx}	41.24(10)	-322.400(14)	
	χ_{yy}	36.6567(56)	-283.311(11)	
	χ_{zz}	-77.89(10)	615.711(20)	
	η	-0.0588(13)		
Halotrifluoroethylene	χ_{aa}	-49.84817(83)		
	χ_{bb}	11.2341		
	χ_{cc}	38.6140		
	$\lvert\chi_{ab}\rvert$	49.489(34)		
	χ_{xx}	38.85(10)		
	χ_{yy}	38.614(3)		
	χ_{zz}	-77.46(10)		
	η			

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		Cl	Br	I
2-Halopropene	χ_{aa}	-68.072	534.5(61)	-1820.783(33)
	χ_{bb}	37.097	-286.5(48)	957.018(41)
	χ_{cc}	30.975	-248.0(41)	863.765(40)
	$\lvert\chi_{ab}\rvert$	9.72(98)[a]	60.(10)	147.5(10)
	χ_{xx}	37.99	-290.9(50)	964.83(11)
	χ_{yy}	30.97	-248.0(41)	863.765(40)
	χ_{zz}	-68.96	538.9(62)	-1828.59(11)
	η	-0.102	-0.0795(120)	-0.05527(7)
t-1-Halopropene	χ_{aa}	-60.3		
	χ_{bb}	28.7		
	χ_{cc}	31.6		
	$\lvert\chi_{ab}\rvert$	31.1(6)[a]		
	χ_{xx}	38.5		
	χ_{yy}	31.6		
	χ_{zz}	-70.1		
	η	-0.098		
c-1-Halopropene	χ_{aa}	-19.66		
	χ_{bb}	-11.39		
	χ_{cc}	31.05		
	$\lvert\chi_{ab}\rvert$	53.72(250)[a]		
	χ_{xx}	38.35		
	χ_{yy}	31.05		
	χ_{zz}	-69.40		
	η	-0.105		

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		Cl	Br	I
c-3-Halopropene	χ_{aa}	-18.19		
	χ_{bb}	-17.80		
	χ_{cc}	35.99		
	$\lvert\chi_{ab}\rvert$	54.37(112)[a]		
	χ_{xx}	36.37		
	χ_{yy}	35.99		
	χ_{zz}	-72.36		
	η	-0.0053		
g-3-Halopropene	χ_{aa}	-39.5(5)	349.4(13)	-1337.
	χ_{bb}	3.5(4)	-72.8(27)	387.
	χ_{cc}	36.1(6)	-276.6(10)	950.
	$\lvert\chi_{ab}\rvert$	50.38(76)[a,b]	363.(10)[c]	1081.[b]
	$\lvert\chi_{ac}\rvert$	2.75(76)[a]	13.92(138)[a]	98.(26)[a]
	$\lvert\chi_{bc}\rvert$	0.60(76)[a]	15.85(138)[a]	71.(26)[a]
	χ_{xx}	37.5(9)	-286.5(59)	899.
	χ_{yy}	35.4(9)	-272.1(35)	963.
	χ_{zz}	-72.8(8)	558.7(87)	-1863.
	η	-0.029(17)	-0.0256(123)	0.0343
1-Halo-2-Methylpropene	χ_{aa}	-52.591(1)		
	χ_{bb}	21.086(2)		
	χ_{cc}	31.505(1)		
	$\lvert\chi_{ab}\rvert$	39.037(99)		
	χ_{xx}	37.922(73)		
	χ_{yy}	31.505(2)		
	χ_{zz}	-69.427(72)		
	η	-0.092		

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		Cl	Br	I
c-1-Halo-2-Fluoropropene	χ_{aa}	-53.09(20)		
	χ_{bb}	19.45(5)		
	χ_{cc}	33.64(20)		
	$\lvert\chi_{ab}\rvert$	43.5(30)		
	χ_{xx}	39.84		
	χ_{yy}	33.64		
	χ_{zz}	-73.49		
	η	-0.0844		
g-3-Halo-3,3-Difluoropropene	χ_{aa}		477.5173(42)	
	χ_{bb}		-199.5456(56)	
	χ_{cc}		277.9717(37)	
	$\lvert\chi_{ab}\rvert$		254.96(12)[c]	
	$\lvert\chi_{ac}\rvert$		24.1(14)	
	$\lvert\chi_{bc}\rvert$		8.40(40)	
	χ_{xx}		284.833(94)	
	χ_{yy}		-278.73(13)	
	χ_{zz}		563.56(11)	
	η		-0.0108(3)	
Haloallene	χ_{aa}	-41.63(14)	377.11(94)	-1399.25(83)
	χ_{bb}	6.73	-97.16	428.34
	χ_{cc}	34.90	-279.95	970.91(64)
	$\lvert\chi_{ab}\rvert$	52.44(84)[a]	381.32(24)	1220.52(27)
	χ_{xx}	40.30	-306.07	1039.24(57)
	χ_{yy}	34.90	-279.95	970.91(64)
	χ_{zz}	-75.20	589.02	-2010.15(64)
	η	-0.0718	-0.04945	-0.03399(44)

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		Cl	Br	I
1-Halo-1-Fluoroallene	χ_{aa}	-37.74		
	χ_{bb}	1.18		
	χ_{cc}	36.56		
	$\lvert\chi_{ab}\rvert$	53.32(68)[a]		
	χ_{xx}	38.48		
	χ_{yy}	36.56		
	χ_{zz}	-75.04		
	η	-0.0256		
2-Halo-1,3-Butadiene	χ_{aa}	5.2(2)		
	χ_{bb}	-37.5(2)		
	χ_{cc}	32.3(3)		
	$\lvert\chi_{ab}\rvert$	51.0(7)[a]		
	χ_{xx}	39.1(7)		
	χ_{yy}	32.3(3)		
	χ_{zz}	-71.4(7)		
	η	-0.096(10)		
c-1-Halo-1,3-Butadiene	χ_{aa}	-2.62(28)		
	χ_{bb}	-27.85(14)		
	χ_{cc}	30.47(31)		
	$\lvert\chi_{ab}\rvert$	53.07(64)[a]		
	χ_{xx}	39.31(64)		
	χ_{yy}	30.47(31)		
	χ_{zz}	-69.78(64)		
	η	-0.127(10)		

[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 product $\chi_{ab}\chi_{ac}\chi_{bc}$ is negative.
[c] The product $\chi_{ab}\chi_{ac}\chi_{bc}$ is positive.

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