Hydrocarbon Mononitriles

Table 1: ^{14}N χ_{zz} (MHz) in Hydrocarbon Mononitriles. (See Tables 2 - 6 below.) χ_{zz} marked with an asterisk are excluded from average.

Alkanes	χ_{zz} (MHz)	Alkynes	χ_{zz} (MHz)
Acetonitrile [a]	-4.22473(80)	Cyanoacetylene [a]	-4.31924(1)
Propionitrile	-4.219(19)	Methylcyanoacetylene	-4.0(2) *
t-Propyl cyanide	-4.194(44)	Methylcyanodiacetylene	-4.25(3)
g-Propyl cyanide	-4.30(29) *	3-Butynenitrile	-4.274(44)
Isopropyl cyanide	-4.209	5-Hexynenitrile, aa	-4.10(73) *
1-Butyl cyanide, aa	-4.198(19)	5-Hexynenitrile, ag	-4.233(16)
1-Butyl cyanide, ag	-4.179(40)	5-Hexynenitrile, ga	-4.195(20)
1-Butyl cyanide, gg	-4.205(16)		
tert-Butyl cyanide	-4.2143(9)	Average	-4.254
Cyclopropyl cyanide	-4.153(60)		
Cyclobutyl cyanide	-4.203(41)	Aryls	
Cyclohexyl cyanide, ax	-4.200(156) *	Benzonitrile [a]	-4.23738(36)
Cyclohexyl cyanide, eq	-4.215(18)	Benzyl cyanide	-4.225(96)
		o-Tolunitrile	-4.219(12)
Average	-4.201	m-Tolunitrile	-4.2188(23)
		p-Tolunitrile	-4.212(1)
Alkenes		9-Cyanoanthracene	-4.191(4)
Acrylonitrile [a]	-4.290(1)		
Methacrylonitrile	-4.266(14)	Average	-4.217
c-Crotonitrile	-4.256(64)		
t-Crotonitrile	-4.244(33)	Alkene-Alkyne	
		Vinylcyanoacetylene	-4.22(4)
Average	-4.264	Vinylcyanodiacetylene	-4.2(1) *
		(E)-pent-2-en-4-ynenitrile	-4.29(3)
		(Z)-pent-2-en-4-ynenitrile	-4.318(38)
Cyanide anion	-4.238(32)	Average	-4.276

[a] Methylation appears to effect a slight decrease in the magnitude of χ_{zz}.

With few exceptions, the χ_{zz} shown above all lie within the range -4.25(7) MHz.

Table 2: ^{14}N NQCC tensors (MHz) in Alkanes and Cycloalkanes Mononitriles. (References are given below.)

Methyl	χ_{zz}	-4.22473(80)			
Ethyl	χ_{aa}	-3.3572(18)	t-1-Propyl	χ_{aa}	-3.405(45)
	χ_{bb}	1.2982(39)		χ_{bb}	1.341(50)
	χ_{cc}	2.0590(39)		χ_{cc}	2.064(39)
	$\lvert\chi_{ab}\rvert$	2.180(28)^a		$\lvert\chi_{ab}\rvert$	2.090(32)^a
	χ_{xx}	2.160(19)		χ_{xx}	2.130(48)
	χ_{yy}	2.0590(39)		χ_{yy}	2.064(39)
	χ_{zz}	-4.219(19)		χ_{zz}	-4.194(44)
	η	0.0239(47)		η	–0.015(15)
g-1-Propyl	χ_{aa}	-1.6825(27)	2-Propyl	χ_{aa}	-3.93838(23)
	χ_{bb}	-0.2490(27)		χ_{bb}	2.11117(30)
	χ_{cc}	1.9315(26)		χ_{cc}	1.82721(24)
	$\lvert\chi_{ab}\rvert$	3.12(30)^b		$\lvert\chi_{ac}\rvert$	1.278^c
	$\lvert\chi_{ac}\rvert$	0.70(17)		χ_{xx}	
	$\lvert\chi_{bc}\rvert$	0.560(28)^a		χ_{yy}	
	χ_{xx}	2.24(29)		χ_{zz}	-4.209
	χ_{yy}	2.06(4)		η	0.003
	χ_{zz}	-4.30(29)			
	η	-0.041(7)			
Cyclopropyl	χ_{aa}	-3.45976(82)	1-Butyl	χ_{aa}	-2.726(2)
	χ_{bb}	1.74564(90)	*anti-anti*	χ_{bb}	0.674(2)
	χ_{cc}	1.71412(90)		χ_{cc}	2.050(3)
	$\lvert\chi_{ac}\rvert$	2.017(98)^a		$\lvert\chi_{ab}\rvert$	2.678(22)^a
	χ_{xx}	2.407(60)		χ_{xx}	2.146(19)
	χ_{yy}	1.74564(90)		χ_{yy}	2.050(3)
	χ_{zz}	-4.153(60)		χ_{zz}	-4.198(19)
	η	-0.159(15)		η	0.0229(5)

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1-Butyl *anti-gauche*	χ_{aa}	-3.645(3)	1-Butyl *gauche-gauche*	χ_{aa}	-0.042(2)
	χ_{bb}	1.988(3)		χ_{bb}	-1.935(2)
	χ_{cc}	1.657(4)		χ_{cc}	1.977(3)
	$\lvert\chi_{ab}\rvert$	0.867(72)[a,b]		$\lvert\chi_{ab}\rvert$	2.968(16)[a,b]
	$\lvert\chi_{ac}\rvert$	1.522(72)[a]		$\lvert\chi_{ac}\rvert$	0.512(16)[a]
	$\lvert\chi_{bc}\rvert$	0.194(72)[a]		$\lvert\chi_{bc}\rvert$	0.607(16)[a]
	χ_{xx}	2.134(61)		χ_{xx}	2.162(18)
	χ_{yy}	2.045(61)		χ_{yy}	2.043(16)
	χ_{zz}	-4.179(40)		χ_{zz}	-4.205(16)
	η	-0.021(21)		η	-0.0285(56)
tert-Butyl	χ_{zz}	-4.2143(9)			
Cyclobutyl	χ_{aa}	-3.663(5)	Cyclohexyl, ax	χ_{aa}	-1.0741(23)
	χ_{bb}	2.086(6)		χ_{bb}	2.1336(17)
	χ_{cc}	1.577(6)		χ_{cc}	-1.0595(8)
	$\lvert\chi_{ac}\rvert$	1.767(72)[a]		$\lvert\chi_{ac}\rvert$	3.133(156)[a]
	χ_{xx}	2.117(41)		χ_{xx}	2.066(156)
	χ_{yy}	2.086(6)		χ_{yy}	2.1336(17)
	χ_{zz}	-4.203(41)		χ_{zz}	-4.200(156)
	η	-0.0074(98)		η	0.016(37)
Cyclohexyl, eq	χ_{aa}	-3.8565(22)			
	χ_{bb}	2.1069(152)			
	χ_{cc}	1.7495(126)			
	$\lvert\chi_{ac}\rvert$	1.462(38)[a]			
	χ_{xx}	2.108(21)			
	χ_{yy}	2.107(15)			
	χ_{zz}	-4.215(18)			
	η	-0.0002(62)			

[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 algebraic sign of the product $\chi_{ab}\chi_{ac}\chi_{bc}$ is negative.

[c] Scaled *ab initio* value. See H.S.P.Muller, A.Coutens, A.Walters, J.-U.Grabow, and S.Schlemmer, J. Mol. Spectrosc. 267,100(2011).

Table 3: ^{14}N NQCC tensors (MHz) in Alkene Mononitriles. (References are given below.)

Acrylonitrile	χ_{aa}	-3.78907(40)	Methacrylonitrile	χ_{aa}	-4.2327(88)
	χ_{bb}	1.68606(43)		χ_{bb}	2.169(17)
	χ_{cc}	2.10301(49)		χ_{cc}	2.063(17)
	$\lvert\chi_{ab}\rvert$	1.730(2)[a]		$\lvert\chi_{ab}\rvert$	0.465(72)[a]
	χ_{xx}	2.187(1)		χ_{xx}	2.203(20)
	χ_{yy}	2.10301(49)		χ_{yy}	2.063(17)
	χ_{zz}	-4.290(1)		χ_{zz}	-4.266(14)
	η	-0.0196(3)		η	-0.0327(61)
c-Crotonitrile	χ_{aa}	-1.8958(49)	t-Crotonitrile	χ_{aa}	-3.7192(70)
	χ_{bb}	-0.1055(65)		χ_{bb}	1.7729(92)
	χ_{cc}	2.0013(65)		χ_{cc}	1.9463(92)
	$\lvert\chi_{ab}\rvert$	3.130(66)[a]		$\lvert\chi_{ab}\rvert$	1.777(60)[a]
	χ_{xx}	2.255(64)		χ_{xx}	2.298(34)
	χ_{yy}	2.0013(65)		χ_{yy}	1.9463(92)
	χ_{zz}	-4.256(64)		χ_{zz}	-4.244(33)
	η	-0.060(15)		η	-0.0828(82)

[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

Table 4: ^{14}N NQCC tensors (MHz) in Alkyne Mononitriles. (References are given below.)

Cyanoacetylene	χ_{zz}	-4.31924(1)			
Methylcyanoacetylene	χ_{zz}	-4.0(2)	Methyldicyanoacetylene	χ_{zz}	-4.25(3)
3-Butynenitrile	χ_{aa}	-2.2558(22)	5-Hexynenitrile, aa	χ_{aa}	-2.18(9)
	χ_{bb}	0.2102(29)		χ_{bb}	0.59(5)
	χ_{cc}	2.0456(29)		χ_{cc}	1.59(10)
	$\lvert\chi_{ab}\rvert$	3.008(48)[a]		$\lvert\chi_{ab}\rvert$	0.465(72)[a]
	χ_{xx}	2.228(44)		χ_{xx}	2.51(73)
	χ_{yy}	2.0456(29)		χ_{yy}	1.59(10)
	χ_{zz}	-4.274(44)		χ_{zz}	-4.10(73)
	η	-0.0427(104)		η	-0.22(18)
5-Hexynenitrile, ag	χ_{aa}	0.502(5)	5-Hexynenitrile, ga	χ_{aa}	-3.5920(15)
	χ_{bb}	-2.493(3)		χ_{bb}	2.0222(15)
	χ_{cc}	1.991(6)		χ_{cc}	1.5698(21)
	$\lvert\chi_{ab}\rvert$	2.782(18)[a,b]		$\lvert\chi_{ab}\rvert$	0.554(34)[a,b]
	$\lvert\chi_{ac}\rvert$	0.392(18)[a]		$\lvert\chi_{ac}\rvert$	1.764(34)[a]
	$\lvert\chi_{bc}\rvert$	0.577(18)[a]		$\lvert\chi_{bc}\rvert$	0.231(34)[a]
	χ_{xx}	2.179(18)		χ_{xx}	2.157(34)
	χ_{yy}	2.054(13)		χ_{yy}	2.038(34)
	χ_{zz}	-4.233(16)		χ_{zz}	-4.195(20)
	η	-0.0295(53)		η	-0.028(11)

[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 algebraic sign of the product $\chi_{ab}\chi_{ac}\chi_{bc}$ is negative.

Table 5: ^{14}N NQCC tensors (MHz) in Aryl Mononitriles. (References are given below.)

Benzonitrile	χ_{aa}	-4.23738(36)	Benzyl cyanide	χ_{aa}	-1.313(2)
	χ_{bb}	2.2886(11)		χ_{bb}	-0.657(3)
	χ_{cc}	1.9488(11)		χ_{cc}	1.970(4)
	$\lvert\chi_{ab}\rvert$	—		$\lvert\chi_{ab}\rvert$	3.223(96)[a]
	χ_{xx}	2.2886(11)		χ_{xx}	2.255(96)
	χ_{yy}	1.9488(11)		χ_{yy}	1.970(4)
	χ_{zz}	-4.23738(36)		χ_{zz}	-4.225(96)
	η	-0.084		η	–0.067(23)
o-Tolunitrile	χ_{aa}	-4.094(2)	m-Tolunitrile	χ_{aa}	-3.6263(8)
	χ_{bb}	2.143(3)		χ_{bb}	1.6837(10)
	χ_{cc}	1.951(3)		χ_{cc}	1.9426(10)
	$\lvert\chi_{ab}\rvert$	0.892(44)[b]		$\lvert\chi_{ab}\rvert$	1.8700(27)
	χ_{xx}	2.268(12)		χ_{xx}	2.2761(25)
	χ_{yy}	1.951(3)		χ_{yy}	1.9426(10)
	χ_{zz}	-4.219(12)		χ_{zz}	-4.2188(23)
	η	-0.0752(30)		η	-0.079
p-Tolunitrile	χ_{aa}		9-Cyanoanthracene	χ_{aa}	2.299(3)
	χ_{bb}			χ_{bb}	-4.191(4)
	χ_{cc}			χ_{cc}	1.893(4)
	$\lvert\chi_{ac}\rvert$			$\lvert\chi_{ab}\rvert$	—
	χ_{xx}	2.310(3)[c]		χ_{xx}	2.299(3)
	χ_{yy}	1.902(3)		χ_{yy}	1.893(4)
	χ_{zz}	-4.212(1)		χ_{zz}	-4.191(4)
	η			η	-0.0969

[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] *Ab initio* value. Diagonalization with the experimental value of 0.8(5) MHz gives χ_{zz} = -4.195(124) MHz.

[c] Unpublished, cited in N.Hansen, H.Mäder, and T.Bruhn, Mol. Phys. 97,587(1999).

Table 6: ^{14}N NQCC tensors (MHz) in Alkene-Alkyne Mononitriles. (References are given below.)

Vinylcyanoacetylene	χ_{aa}	-4.12(2)	Vinyldicyanoacetylene	χ_{aa}	-4.2(1)
	χ_{bb}	1.97(3)		χ_{bb}	2.1(2)
	χ_{cc}	2.15(4)		χ_{cc}	2.1(2)
	$\lvert\chi_{ab}\rvert$	0.787(120)[a]		$\lvert\chi_{ab}\rvert$	0.55(2)[a]
	χ_{xx}	2.07(4)		χ_{xx}	2.1(2)
	χ_{yy}	2.15(4)		χ_{yy}	2.1(2)
	χ_{zz}	-4.22(4)		χ_{zz}	-4.2(1)
	η	0.019(14)		η	0.0
(E)-pent-2-en-4-ynenitrile	χ_{aa}	-3.90(2)	(Z)-pent-2-en-4-ynenitrile	χ_{aa}	0.248(2)
	χ_{bb}	1.82(3)		χ_{bb}	-2.424(2)
	χ_{cc}	2.08(4)		χ_{cc}	2.176(2)
	$\lvert\chi_{ab}\rvert$	1.543(38)[a]		$\lvert\chi_{ab}\rvert$	2.941(42)[a]
	χ_{xx}	2.21(3)		χ_{xx}	2.142(38)
	χ_{yy}	2.08(4)		χ_{yy}	2.176(2)
	χ_{zz}	-4.29(3)		χ_{zz}	-4.318(38)
	η	-0.030(12)		η	-0.0078(89)

[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

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