Fluorinated and Methylated Acetonitriles

Table 1: ^{14}N NQCC tensors (MHz) in increasingly fluorinated acetonitriles. (References are given below.)

$CH_3C{\equiv}N$	χ_{zz}	-4.22473(80)
$CH_2FC{\equiv}N$	χ_{aa}	-3.7039(26)
	χ_{bb}	1.8918(26)
	χ_{cc}	1.8122(37)
	$\lvert\chi_{ab}\rvert$	2.119
	χ_{xx}	2.604
	χ_{yy}	1.812
	χ_{zz}	-4.416
	η	
$CHF_2C{\equiv}N$	χ_{aa}	-4.3899(33)
	χ_{bb}	2.4017(39)
	χ_{cc}	1.9883(39)
	$\lvert\chi_{ac}\rvert$	1.247(56)[a]
	χ_{xx}	2.223(21)
	χ_{yy}	2.4017(39)
	χ_{zz}	-4.625(21)
	η	0.0385(46)
$CF_3C{\equiv}N$	χ_{zz}	-4.666(4)

[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/ClFAcetonitriles.pdf.

Going from $CH_3C{\equiv}N$ to $CH_2FC{\equiv}N$ to $CHF_2C{\equiv}N$ to $CF_3C{\equiv}N$,

changes in $|\chi_{zz}|$ are +4.5 %, +4.7 %, and +0.9 %.

Table 2: ^{14}N NQCC tensors (MHz) in increasingly methylated acetonitriles. (References are given below.)

$CH_3C{\equiv}N$	χ_{zz}	-4.22473(80)
$CH_3CH_2C{\equiv}N$	χ_{aa}	-3.3572(18)
	χ_{bb}	1.2982(39)
	χ_{cc}	2.0590(39)
	$\lvert\chi_{ab}\rvert$	2.180(28)[a]
	χ_{xx}	2.160(19)
	χ_{yy}	2.0590(39)
	χ_{zz}	-4.219(19)
	η	0.0239(47)
$(CH_3)_2CHC{\equiv}N$	χ_{aa}	-3.93838(23)
	χ_{bb}	2.11117(30)
	χ_{cc}	1.82721(24)
	$\lvert\chi_{ac}\rvert$	1.278[b]
	χ_{xx}	
	χ_{yy}	
	χ_{zz}	-4.209
	η	0.003
$(CH_3)_3CC{\equiv}N$	χ_{zz}	-4.2143(9)

[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/CH3CH2CN.html.

[b] 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).

References

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