Amines

Table 1: ^{14}N NQCC tensors (MHz) in primary methyl and ethyl amine. (References are given below.)

	Methylamine	Ethylamine, anti
χ_{aa}	2.4136(12)	-1.65122(301)
χ_{bb}	1.8255(13)	-0.1473(34)
χ_{cc}	-4.2391(13)	1.7985(45)
$\lvert\chi_{ab}\rvert$	———	3.655(348)[b]
$\lvert\chi_{ac}\rvert$	1.794(140)[a]	———
χ_{xx}	2.866(66)	2.83(34)
χ_{yy}	1.8255(13)	1.7985(45)
χ_{zz}	-4.692(66)	-4.63(34)
η	-0.222(14)	-0.223(75)

[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/CH3NH2.html.

[b] *Ab initio* value. The estimated uncertainty is 2× the root mean square difference between calculated and experimental diagonal components. See http://nqcc.wcbailey.net/CH3CH2NH2.html.

Table 2: ^{14}N NQCC tensors (MHz) in secondary methyl, ethyl amines. (References are given below.)

	Dimethylamine	Diethylamine	Methylaminoethane
χ_{aa}	3.04(12)	2.67576(37)	2.82(9)
χ_{bb}	0.93(12)	0.83284	0.88(13)
χ_{cc}	-4.97(24)	-3.50860	-3.70(9)
$\lvert\chi_{ab}\rvert$	———	———	0.289(84)[a]
$\lvert\chi_{ac}\rvert$	———	———	0.523(84)[a]
$\lvert\chi_{bc}\rvert$	2.48(40)	2.9199(92)	2.960(84)[a]
χ_{xx}	2.01(50)	2.30050	2.33(12)
χ_{yy}	3.04(12)	2.67576	2.87(9)
χ_{zz}	-5.05(40)	-4.97626(31)	-5.20(10)
η	0.2	0.075	0.103(30)

[a] *Ab initio* value. The estimated uncertainty is 2× the root mean square difference between calculated and experimental diagonal components. The product $\chi_{ab}\chi_{ac}\chi_{bc}$ is negative. See http://nqcc.wcbailey.net/MeAminoEt.html

Table 3: ^{14}N χ_{zz} in methyl and ethyl amines (MHz).

Ammonia	–4.08984(70)
Monomethylamine	–4.692(66)
Dimethylamine	–5.05(40)
Trimethylamine	–5.5002(18)
Monoethylamine	–4.63(34)
Diethylamine	–4.97626(31)
Triethylamine	–5.2444(7)

References

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