Nuclear Quadrupole Coupling Constants

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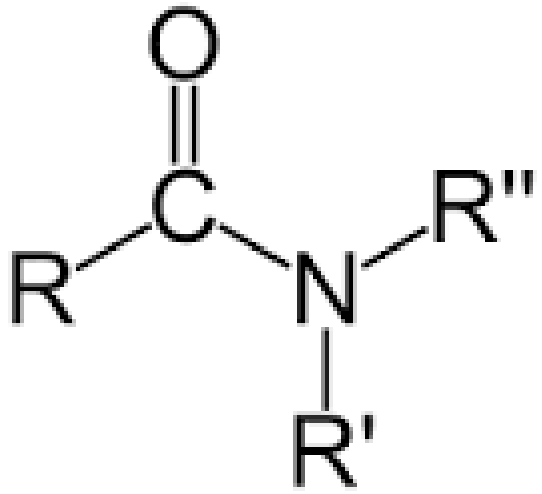

Amides

Table 1: ^{14}N χ_{zz} (= χ_{cc}) (MHz) in C_s Amides. (References are given below.)

Formamide	$HC(=O)NH_2$	–3.8510(11)
N-Methylformamide	$HC(=O)N(H)CH_3$	–4.0358(28)
N,N-Dimethylformamide	$HC(=O)N(CH_3)_2$	–4.364(2)
N-Vinylformamide, *trans*	$HC(=O)NH(CH=CH_2)$	–3.6416(11)
N-Vinylformamide, *cis*	$HC(=O)NH(CH=CH_2)$	–3.6396(20)
N-*tert*-Butylformamide *syn*	$HC(=O)N(H)C(CH_3)_3$	–3.7797(18)
N-*tert*-Butylformamide *anti*	$HC(=O)N(H)C(CH_3)_3$	–3.922(12)
Diformamide	$[HC(=O)]_2NH$	–3.41(7)
Acetamide	$(CH_3)C(=O)NH_2$	–3.9458(22)
N-Vinylacetamide, *trans*	$(CH_3)C(=O)NH(CH=CH_2)$	–3.7728(35)
N-*tert*-Butylacetamide	$(CH_3)C(=O)N(H)C(CH_3)_3$	–3.920(10)
N-Methylacetamide	$(CH_3)C(=O)N(H)CH_3$	–4.1410(9)
N-Acetylglycine	$(CH_3)C(=O)N(H)CH_2C(=O)OH$	–4.184(12)
N,N-Dimethylacetamide	$(CH_3)C(=O)N(CH_3)_2$	–4.6461(16)
Propionamide	$(CH_3CH_2)C(=O)NH_2$	–3.9762(48)
N-Methylpropionamide	$(CH_3CH_2)C(=O)N(H)CH_3$	–4.168(19)
N,N-Dimethylpropionamide	$(CH_3CH_2)C(=O)N(CH_3)_2$	–4.6765(34)
Propiolamide	$(HC\equiv C)C(=O)NH_2$	–3.82(8)
Acrylamide	$(CH_2=CH)C(=O)NH_2$	–4.60(30)
2-Fluoroacetamide	$(CH_2F)C(=O)NH_2$	–3.7008(27)
Cyanoformamide	$(C\equiv N)C(=O)NH_2$	–3.79(7)
Formanilide [a]	$HC(=O)N(H)C_6H_5$	–3.671(22)
Acetanilide [b]	$(CH_3)C(=O)N(H)C_6H_5$	–3.8189(38)
Paracetamol [c]	$(CH_3)C(=O)N(H)C_6H_4OH$	–3.8276(44)

[a] N-Phenylformamide [b] N-Phenylacetamide [c] N-(4-Hydroxyphenyl)acetamide

Table 2: ^{14}N NQCC tensors (MHz) in C_1 Amides. (References are given below.)

	N,N-Methylethyl Formamide	N,N-Diethylacetamide Conformer I	N,N-Diethylacetamide Conformer II
χ_{aa}	1.665(4)	1.06868(58)	1.49797(61)
χ_{bb}	2.132(5)	2.00481(50)	2.37712(63)
χ_{cc}	-3.797(4)	-3.07349(50)	-3.87508(63)
χ_{ab}	0.079(62)[a]	-0.119(50)[b]	-0.233(90)[b]
χ_{ac}	-1.389(62)[a]	2.675(50)[b]	-1.720(90)[b]
χ_{bc}	-0.778(62)[a]	0.121(50)[b]	-0.396(90)[b]
χ_{xx}	1.829(58)	2.001(14)	1.972(65)
χ_{yy}	2.387(59)	2.388(41)	2.435(45)
χ_{zz}	-4.216(31)	-4.389(40)	-4.408(50)
η	0.132(20)	0.0881(99)	0.105(18)

[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/MeEtNCHO.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/NNDEA.html

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	N-Ethylformamide	N-Ethylacetamide	N-Methyldiacetamide
χ_{aa}	1.3794(13)	1.7508(32)	1.7360(7)
χ_{bb}	0.8171(20)	1.8333(45)	2.0388(7)
χ_{cc}	-2.1965(20)	-3.5841(45)	-3.7748(7)
χ_{ab}	-0.735(54)[a]	0.1686[b]	0.030(34)[c]
χ_{ac}	-1.536(54)[a]	-1.651(71)	0.121(34)[c]
χ_{bc}	-2.318(54)[a]	0.595(59)	-0.155(34)[c]
χ_{xx}	1.882(46)	1.898(12)	1.7364(62)
χ_{yy}	2.110(58)	2.220(37)	2.0453(63)
χ_{zz}	-3.993(51)	-4.118(39)	-3.7816(25)
η	0.057(18)	0.0784(96)	0.0817(23)

	N-Acetylethanolamine[d]	N,N-Diethylpropionamide	
		Conformer OPM	Conformer OMM
χ_{aa}	1.55(3)	1.97018(79)	1.79861(93)
χ_{bb}	1.54(5)	1.1524(8)	2.4354(9)
χ_{cc}	-3.09(5)	-3.1225(8)	-4.2340(9)
χ_{ab}	0.362(112)[e]	-0.244(40)[f]	-0.057(56)[f]
χ_{ac}	-1.834(112)[e]	0.544(40)[f]	-1.062(56)[f]
χ_{bc}	1.068(112)[e]	2.262(40)[f]	-0.336(56)[f]
χ_{xx}	1.77(6)	2.025(8)	1.980(18)
χ_{yy}	2.19(8)	2.430(31)	2.452(6)
χ_{zz}	-3.96(9)	-4.455(31)	-4.432(19)
η	0.105(25)	0.0909(72)	0.106(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/NEFA.html

[b] *Ab initio* value derived by R.Kannengießer, et al. (Reference given below.)

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

[d] N-(2-Hydroxyethyl)acetamide

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

[f] *Ab initio* value. *ibid.* See http://nqcc.wcbailey.net/DEPA.html

Table 3: ^{14}N χ_{zz} (MHz) in Formamides, Acetamides, and Propionamides.

Formamide	$HC(=O)NH_2$	–3.8510(11)
Diformamide	$[HC(=O)]_2NH$	–3.41(7)
N-Vinylformamide, *cis*	$HC(=O)NH(CH=CH_2)$	–3.6396(20)
N-Vinylformamide, *trans*	$HC(=O)NH(CH=CH_2)$	–3.6416(11)
N-Phenylformamiide	$HC(=O)N(H)C_6H_5$	–3.671(22)
N-*tert*-Butylformamide *syn*	$HC(=O)N(H)C(CH_3)_3$	–3.7797(18)
N-*tert*-Butylformamide *anti*	$HC(=O)N(H)C(CH_3)_3$	–3.922(12)
N-Ethylformamide	$HC(=O)N(H)CH_2CH_3$	–3.993(51)
N-Methylformamide	$HC(=O)N(H)CH_3$	–4.0358(28)
N,N-Methylethylformamide	$HC(=O)N(CH_3)(CH_2CH_3)$	–4.216(31)
N,N-Dimethylformamide	$HC(=O)N(CH_3)_2$	–4.364(2)
Acetamide	$(CH_3)C(=O)NH_2$	–3.9458(22)
N-*tert*-Butylacetamide	$(CH_3)C(=O)N(H)C(CH_3)_3$	–3.920(10)
N-Acetylethanolamine	$(CH_3)C(=O)N(H)CH_2CH_2OH$	–3.96(9)
N-Ethylacetamide	$(CH_3)C(=O)N(H)CH_2CH_3$	–4.118(39)
N-Methylacetamide	$(CH_3)C(=O)N(H)CH_3$	–4.1410(9)
N-Acetylglycine	$(CH_3)C(=O)N(H)CH_2C(=O)OH$	–4.184(12)
N,N-Diethylacetamide I	$(CH_3)C(=O)N(CH_2CH_3)_2$	–4.389(40)
N,N-Diethylacetamide II	$(CH_3)C(=O)N(CH_2CH_3)_2$	–4.408(50)
N,N-Dimethylacetamide	$(CH_3)C(=O)N(CH_3)_2$	–4.6461(16)
Propionamide	$(CH_3CH_2)C(=O)NH_2$	–3.9762(48)
N-Methylpropionamide	$(CH_3CH_2)C(=O)N(H)CH_3$	–4.168(19)
N,N-Diethylpropionamide OPM	$(CH_3CH_2)C(=O)N(CH_2CH_3)_2$	–4.455(31)
N,N-Diethylpropionamide OMM	$(CH_3CH_2)C(=O)N(CH_2CH_3)_2$	–4.432(19)
N,N-Dimethylpropionamide	$(CH_3CH_2)C(=O)N(CH_3)_2$	–4.6765(34)

Table 4: ^{14}N χ_{zz} (MHz) in Formamides and Acetamides.

	Formamide	Acetamide
	–3.8510(11)	–3.9458(22)
N-*tert*-Butyl-	–3.7797(18)	–3.920(10)
N-Ethyl-	–3.993(51)	–4.118(39)
N-Methyl-	–4.0358(28)	–4.1410(9)
N,N-Diethyl- I		–4.389(40)
N,N-Diethyl- II		–4.408(50)
N,N-Methylethyl-	–4.216(31)	
N,N-Dimethyl-	–4.364(2)	–4.6461(16)
N-Phenyl-	–3.671(22)	–3.8276(44)
N-Vinyl- *trans*	–3.6416(11)	–3.7728(35)
N-Vinyl- *cis*	–3.6396(20)	
Di- *cis-trans*	–3.41(7)	
N-Methyldi- *cis-trans*		–3.7816(25)

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N,N-Dimethylpropionamide	*ibid*