



## Imines

Table 1:  $^{14}\text{N}$   $\chi_{zz}$  (MHz) in Imines. (References are given below.)

Methanimine	$\text{CH}_2=\text{NH}$	-4.4576(57)
Difluoromethanimine	$\text{CF}_2=\text{NH}$	-3.184(139)
Perfluoromethanimine	$\text{CF}_2=\text{NF}$	-4.738(104)
d-N-methylmethanimine	$\text{CD}_2=\text{NCD}_3$	-4.91(19)
trans-Ethanimine	t- $(\text{CH}_3)\text{C}(\text{H})=\text{NH}$	-4.273(11)
cis-Ethanimine	c- $(\text{CH}_3)\text{C}(\text{H})=\text{NH}$	-4.099(14)
trans-syn-Propenimine	t-s- $(\text{CH}_2)=\text{C}(\text{H})\text{C}(\text{H})=\text{NH}$	-4.311(13)
trans-anti-Propenimine	t-a- $(\text{CH}_2)=\text{C}(\text{H})\text{C}(\text{H})=\text{NH}$	-4.134(17)
Ketenimine	$\text{CH}_2=\text{C}=\text{NH}$	-2.866(182)
Hexafluoroacetone imine	$(\text{CF}_3)_2\text{C}=\text{NH}$	-4.672(16)

Table 2:  $^{14}\text{N}$  NQCC tensors (MHz).

	$\text{CH}_2=\text{NH}$	$\text{CF}_2=\text{NH}$	$\text{CF}_2=\text{NF}$	$\text{CD}_2=\text{NCD}_3$
$\chi_{aa}$	-0.9148(12)	0.968(5)	4.645(5)	1.28(37)
$\chi_{bb}$	-2.6665(6)	-2.482(5)	-3.178(14)	-4.87(19)
$\chi_{cc}$	3.5813(6)	1.514(3)	-1.467(14)	3.59(18)
$ \chi_{ab} $	2.519(6) <sup>a</sup>	1.707(198) <sup>b</sup>	3.826(148) <sup>c</sup>	0.509(98) <sup>d</sup>
$\chi_{xx}$	0.8763(57)	1.670(139)	6.205(104)	1.32(37)
$\chi_{yy}$	3.5813(6)	1.514(3)	-1.467(14)	3.59(18)
$\chi_{zz}$	<b>-4.4576(57)</b>	<b>-3.184(139)</b>	<b>-4.738(104)</b>	<b>-4.91(19)</b>
$\eta$	0.6068(15)	-0.049(44)	-1.619(42)	0.46(8)

<sup>a</sup> *Ab initio* value. The estimated uncertainty is  $2\times$  the root mean square difference between calculated and experimental diagonal components. See <http://nqcc.wcbailey.net/CH2NH.html>

<sup>b</sup> *Ab initio* value. The estimated uncertainty is  $2\times$  the root mean square difference between calculated and experimental diagonal components. See <http://nqcc.wcbailey.net/CF2NH.html>

<sup>c</sup> *Ab initio* value. The estimated uncertainty is  $2\times$  the root mean square difference between calculated and experimental diagonal components. See <http://nqcc.wcbailey.net/CF2NF.html>

<sup>d</sup> *Ab initio* value. The estimated uncertainty is  $2\times$  the root mean square difference between calculated and experimental diagonal components. See <http://nqcc.wcbailey.net/CH3NCH2.html>

Table 3:  $^{14}\text{N}$  NQCC tensors (MHz).

	t-Ethanimine	c-Ethanimine	Propenimine trans-syn	Propenimine trans-anti
$\chi_{aa}$	-3.6066(13)	0.9980(22)	-2.9938(22)	0.7414(11)
$\chi_{bb}$	0.5488(33)	-4.0524(22)	-0.1636(54)	-3.8461(11)
$\chi_{cc}$	3.0578(33)	3.0544(31)	3.1574(54)	3.1047(16)
$ \chi_{ab} $	1.792(16) <sup>a</sup>	0.489(72) <sup>b</sup>	2.337(16) <sup>c</sup>	1.185(38) <sup>d</sup>
$\chi_{xx}$	1.215(11)	1.045(14)	1.153(14)	1.029(17)
$\chi_{yy}$	3.0578(33)	3.0544(31)	3.1574(54)	3.1047(16)
$\chi_{zz}$	<b>-4.273(11)</b>	<b>-4.099(14)</b>	<b>-4.311(14)</b>	<b>-4.134(17)</b>
$\eta$	0.4313(29)	0.4902(38)	0.4649(38)	0.5020(48)

<sup>a</sup> *Ab initio* value. The estimated uncertainty is  $2\times$  the root mean square difference between calculated and experimental diagonal components. See <http://nqcc.wcbailey.net/tEthanimine.html>

<sup>b</sup> *Ab initio* value. The estimated uncertainty is  $2\times$  the root mean square difference between calculated and experimental diagonal components. See <http://nqcc.wcbailey.net/cEthanimine.html>

<sup>c</sup> *Ab initio* value. The estimated uncertainty is  $2\times$  the root mean square difference between calculated and experimental diagonal components. See <http://nqcc.wcbailey.net/TSPropenimine.html>

<sup>d</sup> *Ab initio* value. The estimated uncertainty is  $2\times$  the root mean square difference between calculated and experimental diagonal components. See <http://nqcc.wcbailey.net/TAPropenimine.html>

Table 4:  $^{14}\text{N}$  NQCC tensors (MHz).

	Ketenimine	Hexafluoroacetone imine
$\chi_{aa}$	0.030(46)	-3.050(17)
$\chi_{bb}$	1.523(40)	-1.008(22)
$\chi_{cc}$	-1.553(61)	4.058(14)
$\chi_{ab}$	—	2.431(10) <sup>b</sup>
$\chi_{ac}$	1.950(190) <sup>a</sup>	-0.238(10) <sup>b</sup>
$\chi_{bc}$	—	0.074(10) <sup>b</sup>
$\chi_{xx}$	1.343(180)	0.606(18)
$\chi_{yy}$	1.523(40)	4.066(14)
$\chi_{zz}$	<b>-2.866(182)</b>	<b>-4.672(16)</b>
$\eta$	0.063(64)	0.7405(56)

<sup>a</sup> *Ab initio* value. The estimated uncertainty is  $2\times$  the root mean square difference between calculated and experimental diagonal components. See <http://nqcc.wcbailey.net/H2CCNH.html>

<sup>b</sup> *Ab initio* value. The estimated uncertainty is  $2\times$  the root mean square difference between calculated and experimental diagonal components. See <http://nqcc.wcbailey.net/CF32CNH.html>

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