**14N Nuclear Quadrupole Resonance in hexamethylenetetramine (HMT)**

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**Abstract**

The 14N nuclear quadrupole resonance (NQR) in hexamethylenetetramine was observed using pulsed techniques on a home built superheterodyne spectrometer with a hybrid tee bridge configuration. High S/N was achieved with robust isolation techniques, high quality fast recovery amplifiers, and high Q resonant tank.

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### The quadrupole coupling constant and NQR transitions

The quadrupole coupling constant $C_q$ is defined as

$$C_q = \frac{e^2 Q V_{zz}}{h},$$

where $V_{zz} = e Q$ is the largest absolute eigenvalue of the diagonalized electric field gradient tensor, $e$ is the electron charge, $Q$ is the quadrupole moment and $h$ is Planck’s constant. We consider a nucleus of spin $S$ and define

$$A = \frac{e^2 V_{zz} Q}{4S(2S-1)}$$

The NQR frequencies can be expressed in terms of $A$

$$\nu_q = \frac{3|A|}{2h(2m+1)}$$

where $m$ is the lowest of the two levels $m$ and $m+1$ over which a transition has occurred. For integral spins there are $S$ unique transitions. For half integral spins there are $I-1/2$ unique transitions.

### NQR frequencies for half integral spins

NQR is observed in nuclei with $I = 3/2$, $I = 5/2$ and $I = 7/2$. For $I = 1/2$, there are no transitions. The $I = 5/2$ and $I = 7/2$ are perhaps more complicated, but in the case $I = 3/2$, there is a degeneracy that causes there to be one frequency of half the quadrupole coupling constant,

$$C_q = \frac{e V_{zz} Q}{2h}.$$  

For example, $^{35}$Cl has $I = 3/2$ so there is only 1 transition. Using $I = 3/2$ equation 3 above, we obtain

$$\nu_q = \frac{1}{2} \frac{e V_{zz} Q}{h} = \frac{1}{2} C_q$$

for axially symmetric field gradients. For non-axially symmetric gradients, we define the asymmetry parameter

$$\eta = \frac{V_{xx} - V_{yy}}{V_{zz}},$$

The axes are chosen so that $|V_{zz}| > |V_{yy}| > |V_{xx}|$ which ensures $0 \leq \eta \leq 1$. If there is axial symmetry and $V_{yy} = V_{xx}$, $V_{zz}$ is the only nonzero component in the diagonalized electric field gradient tensor, forcing $\eta = 0$. When $\eta$ is nonzero, the single transition for $I = 3/2$ is given by

$$\nu_q = \frac{1}{2} \frac{e V_{zz} Q}{h} \left(1 + \frac{1}{3} \eta^2\right)^{1/2}$$

For $\eta = 0$ and $I = 5/2$ there are of course two lines for the $I - 1/2$ allowed transitions as $|\Delta m| = 1$

$$\nu_q^+ = \frac{3}{10} \frac{e V_{zz} Q}{h}$$

for $5/2 \rightarrow 3/2$ and

$$\nu_q^- = \frac{3}{20} \frac{e V_{zz} Q}{h}$$

for the $3/2 \rightarrow 1/2$ case.

### NQR frequencies for integer spins

We return to equation (2) and begin with $I = 1$ as is the case for nitrogen. Axial field gradients with $\eta = 0$ lead to a degeneracy and we find there is a single transition having frequency

$$\nu_q = \frac{3}{4} \frac{e V_{zz} Q}{h}$$

For $\eta > 0$ there are two transitions given by

$$\nu_q^\pm = \frac{3}{4} \frac{e V_{zz} Q}{h} (1 \pm \eta)$$
Experimental

Impedance matching in We wish to find expressions for both $C_1$ and $C_2$ in terms of $L$, $\omega$, and that satisfy the matching conditions $\text{Re}[Z] = 50\Omega$ and $\text{Im}[Z] = 0$.

The total impedance looking into matching network A is

$$Z = \frac{1}{j\omega C_1 + \frac{1}{r + jL\omega}} \text{ } - \frac{j}{C_2 \omega} \quad (12)$$

Because the second term in (12) is pure imaginary, the real part of the impedance must be equal to the real part of the first term only.

$$\text{Re}Z = \text{Re} \left( \frac{1}{r + jL\omega} \right) - \frac{j}{C_2 \omega} \quad (13)$$

This expression does not involve $C_2$ so $C_1$ must be a function of $\omega$. 