



St. Petersburg State University
Center for Magnetic Resonance

NQR/NMR studies in zero-field at Center for Magnetic Resonance

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Tecmag Redstone

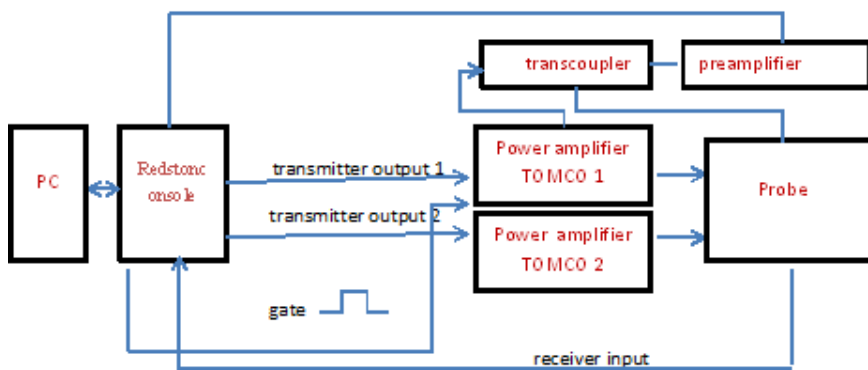


Spectrometer

Frequency range	0.5 MHz- 500 MHz
Pulse length range	10 ns – 43 s
Dwell time	300 ns – 21 ms
Temperature range	4 K- 400 K

Probe

Frequency range	27 - 120 MHz
Maximal input power	500 W
Goniometer resolution	0.1 °



Block diagrame

NMR spectroscopy : Magnetically ordered materials

Types of magnetic materials

According to magnetic polarization:

weak magnetism

diamagnetism

Induced magnetic dipoles directed reverse to the external magnetic field.

paramagnetism

Alignment of permanent magnetic dipoles in the direction of the external magnetic field.

strong magnetism

ferromagnetism

Spontaneous alignment of all permanent magnetic dipoles within a domain in the crystal lattice (only metals).

antiferromagnetism

Kompensation of all magnetic dipoles due to an antiparallel alignment.

ferrimagnetism

Spontaneous alignment of a part of the permanent magnetic dipoles within a domain in the crystal lattice (predominantly in one direction).

Some examples for investigation

Spinel (AM_2O_4 , $A = Mg^{2+}, Zn^{2+}, Mn^{2+}, Fe^{2+}, Ni^{2+}, Co^{2+}$
 $M = Al^{3+}, Mn^{3+}, Fe^{3+}, V^{3+}, Cr^{3+}$)

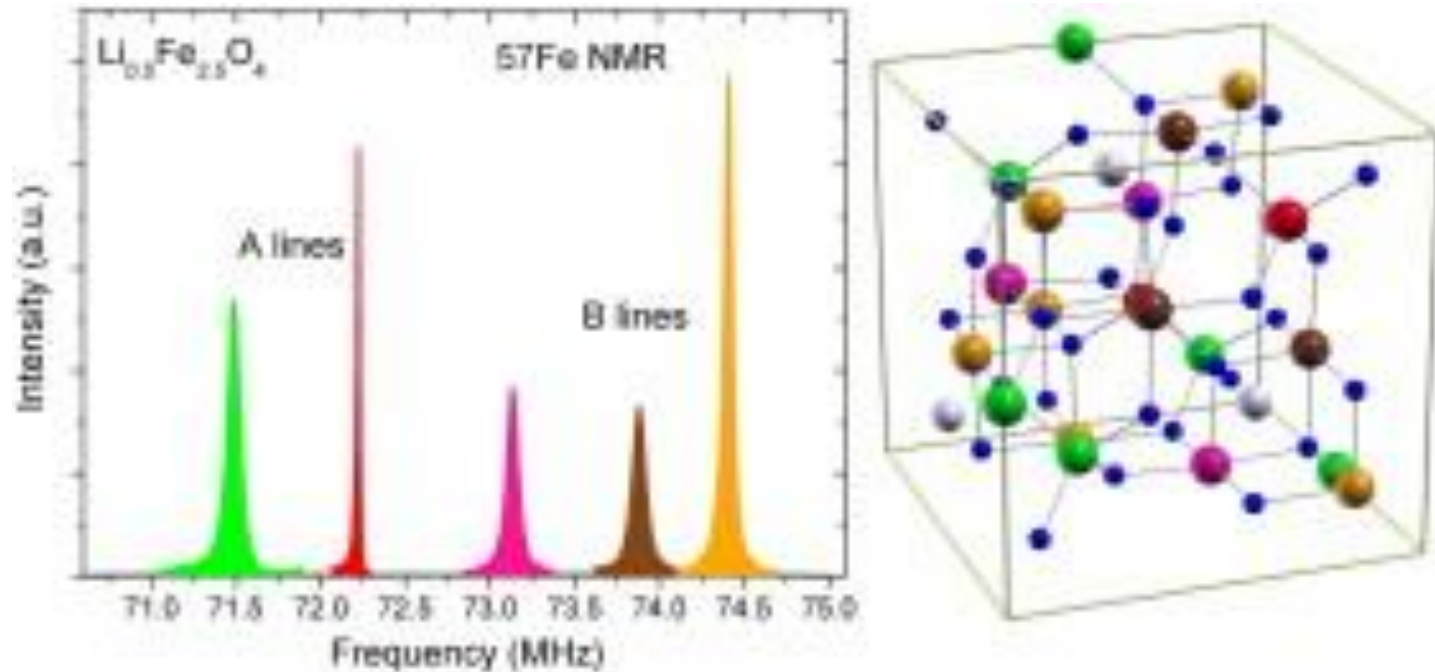
- Lithium ferrite $Fe_{2.5}Li_{0.5}O_4$
- Nickel ferrite $NiFe_2O_4$
- Magnesium ferrite $MgFe_2O_4$
- Manganese ferrite $MnFe_2O_4$
- Maghemite Fe_2O_3

Ferrite garnets YFe_5O_{12}

Ortoferrites ($RFeO_3$, $R = Y$ or Eu, Ho, Gd and etc.)

- **NMR provide both static and dynamic information**
- **Information about hyperfine interactions**
- **Structure of sublattice**
- **Local electronic structure**

NMR spectra of ^{57}Fe Lithium ferrite $\text{Fe}_{2.5}\text{Li}_{0.5}\text{O}_4$

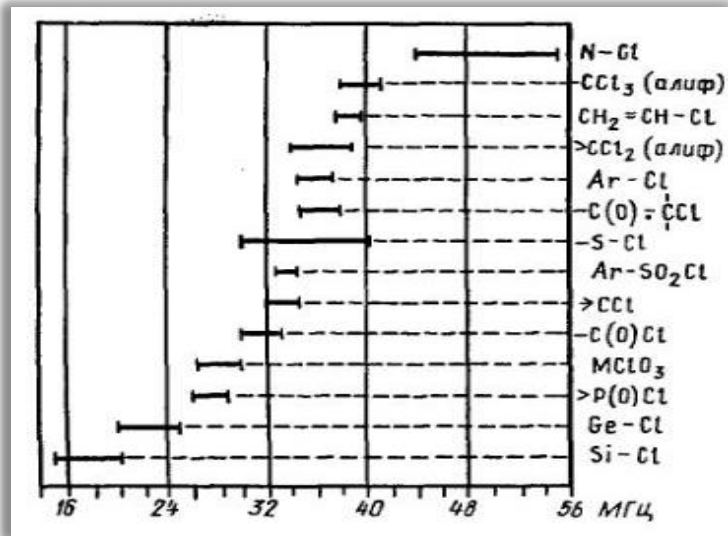


^{57}Fe spectra of lithium ferrite measured at 4.2 K

NQR Spectroscopy

Necessary conditions for the observation of NQR:

- The quadrupole moment of the nuclei $Q \neq 0$
- The gradient of the electric field at the location of the studied nuclei $\neq 0$



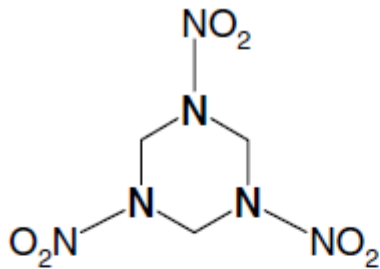
Frequency range for $^{35}\text{Cl} \sim 2 \dots 70$ MHz
 $^{75}\text{As} \sim 30 - 120$ MHz
 $\text{Bi} \sim 15 - 115$ MHz
 $^{121,123}\text{Sb} \sim 10 - 180$ MHz

The method allows one to obtain information about

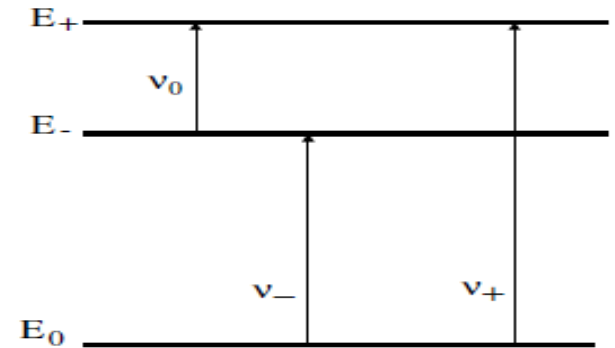
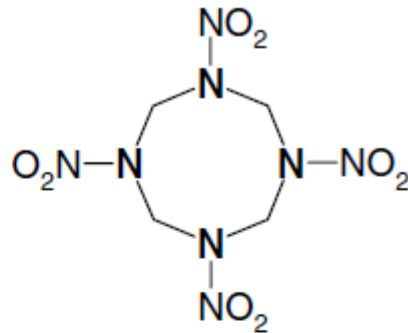
- local structure of the material
- the distribution of electron density in the proximity of the nucleus
- mobility of molecules and groups of atoms in a molecule
- phase transitions
- inter- and intramolecular interactions etc.

Examples of RDX and HMX explosives

HEXOGEN (RDX)

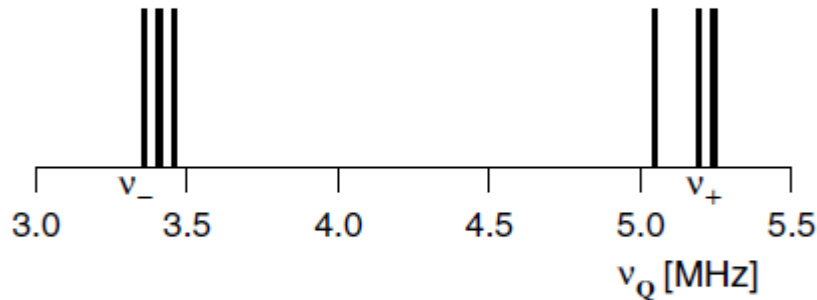


OCTOGEN (HMX)

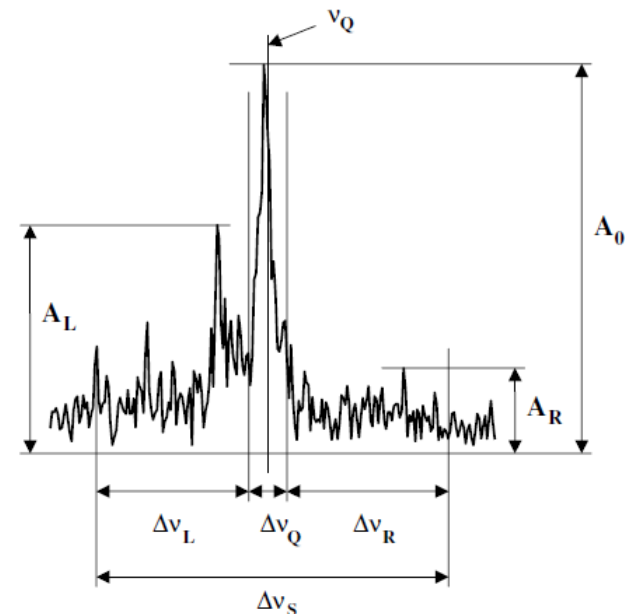
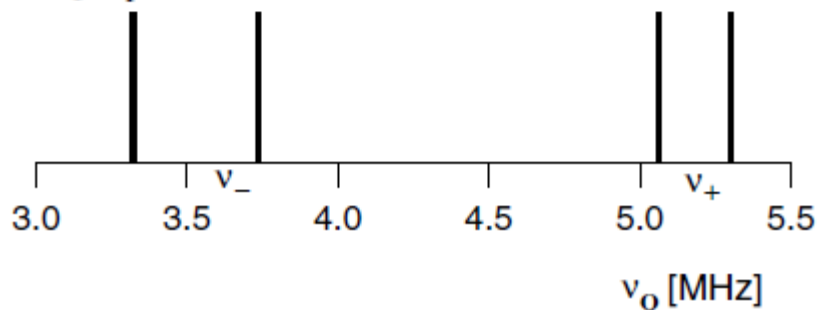


Quadrupole energy levels of an ^{14}N nucleus

^{14}N -NQR spectrum of RDX at 298 K



^{14}N -NQR spectrum of HMX at 298 K



Chemical formulas and ^{14}N -NQR spectra of RDX and HMX explosives at room temperature.

Thank you for your
attention