

Multiple Quantum NMR of Coupled Spin- 1/2 Solids

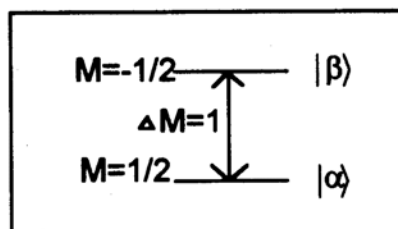
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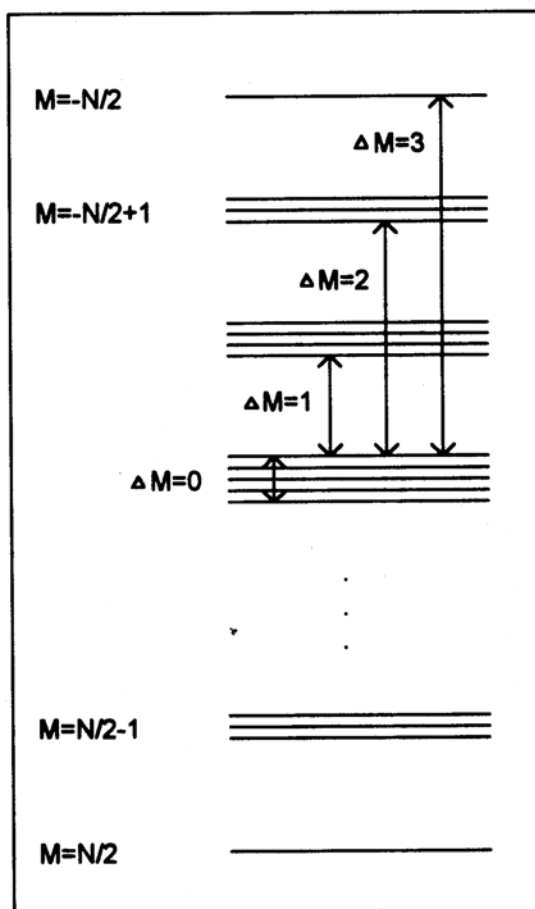
Ba, Yong; Veeman, Wiebren S., Experimental detection of multiple-quantum coherence transfer in coupled spin solids by multi-dimensional NMR experiments. *Solid State Nucl. Magn. Reson.* 2(3), 131 (1993).

Ba, Yong; Veeman, Wiebren S., On multiple quantum NMR of coupled spins in solids. *Isr. J. Chem.* 32(2-3), 173 (1992).

Multiple-quantum (MQ) transitions

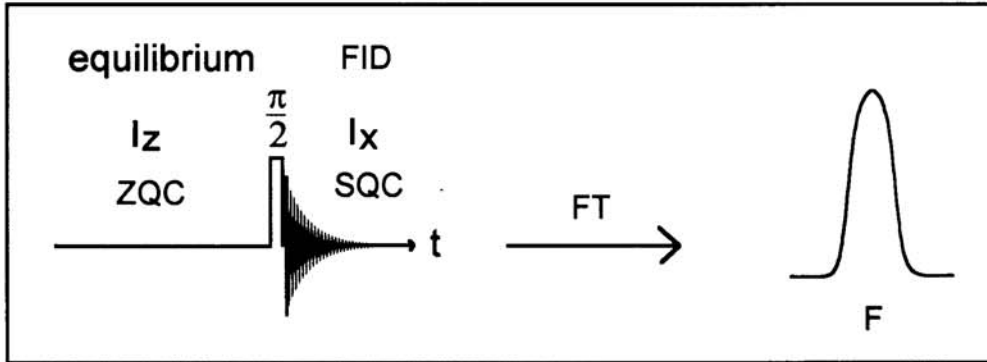


Energy levels for a single spin-1/2 system and single-quantum transition

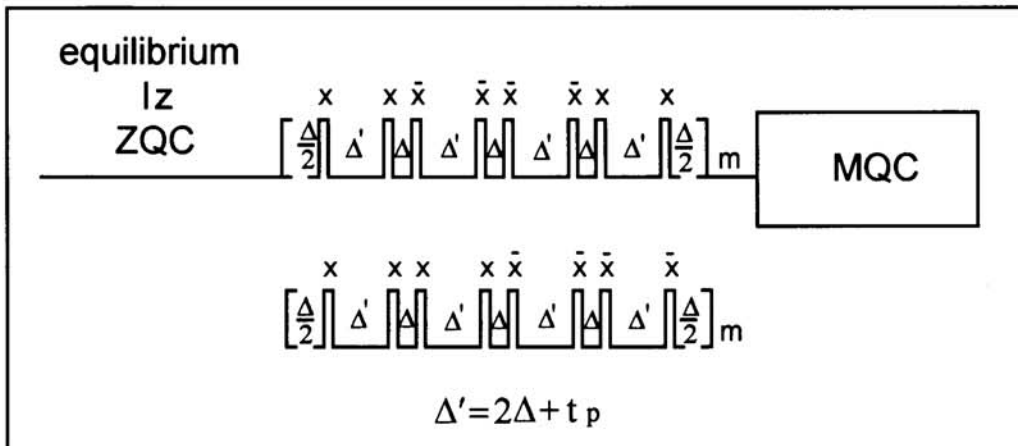


Energy Levels for an N coupled spin-1/2 system and multiple quantum transitions

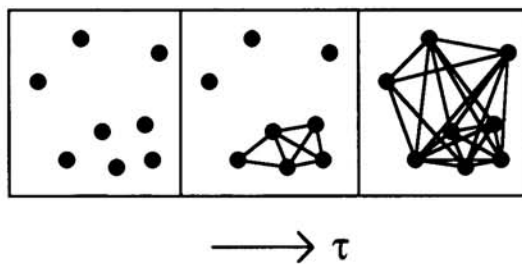
MQ Coherence



Excitation of single-quantum coherence and its NMR spectrum

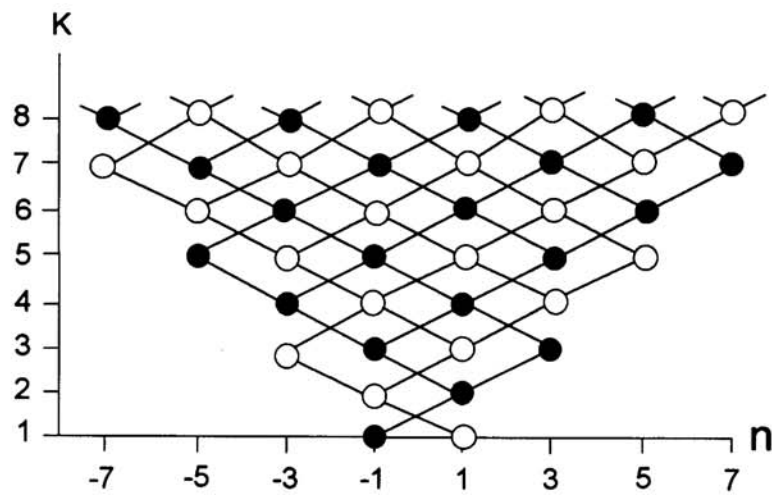
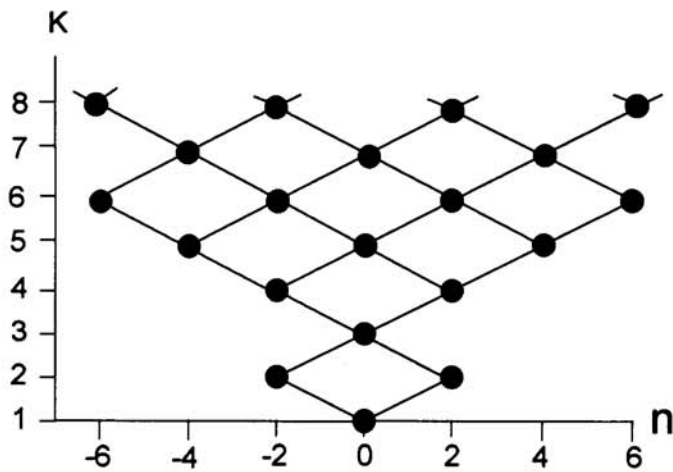
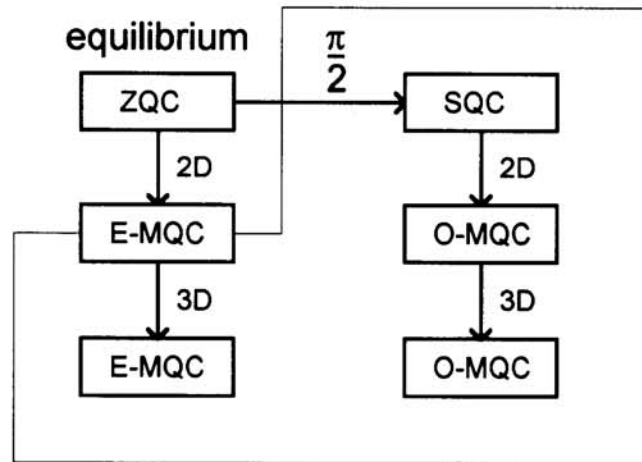


Excitation of MQ coherences of coupled spin-1/2 nuclei



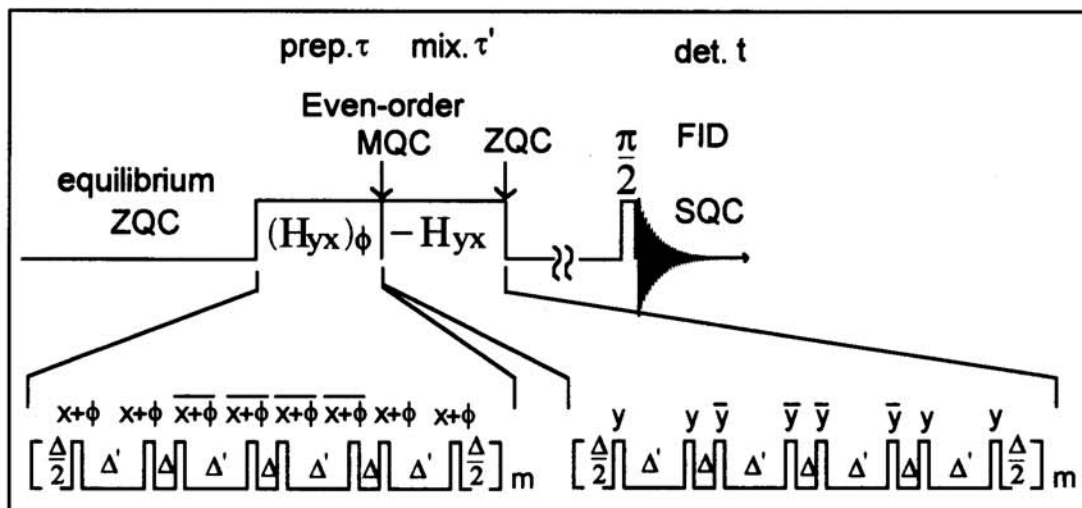
Development of MQ coherences among spins

Selection rules



Pathways of the development of MQ coherences
 K-coupled spin number n-coherence order

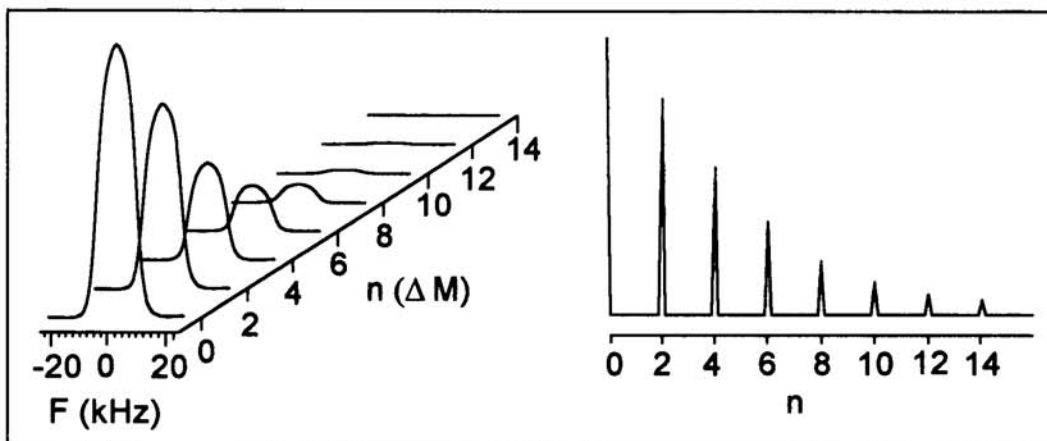
MQ Experiment and MQ spectra



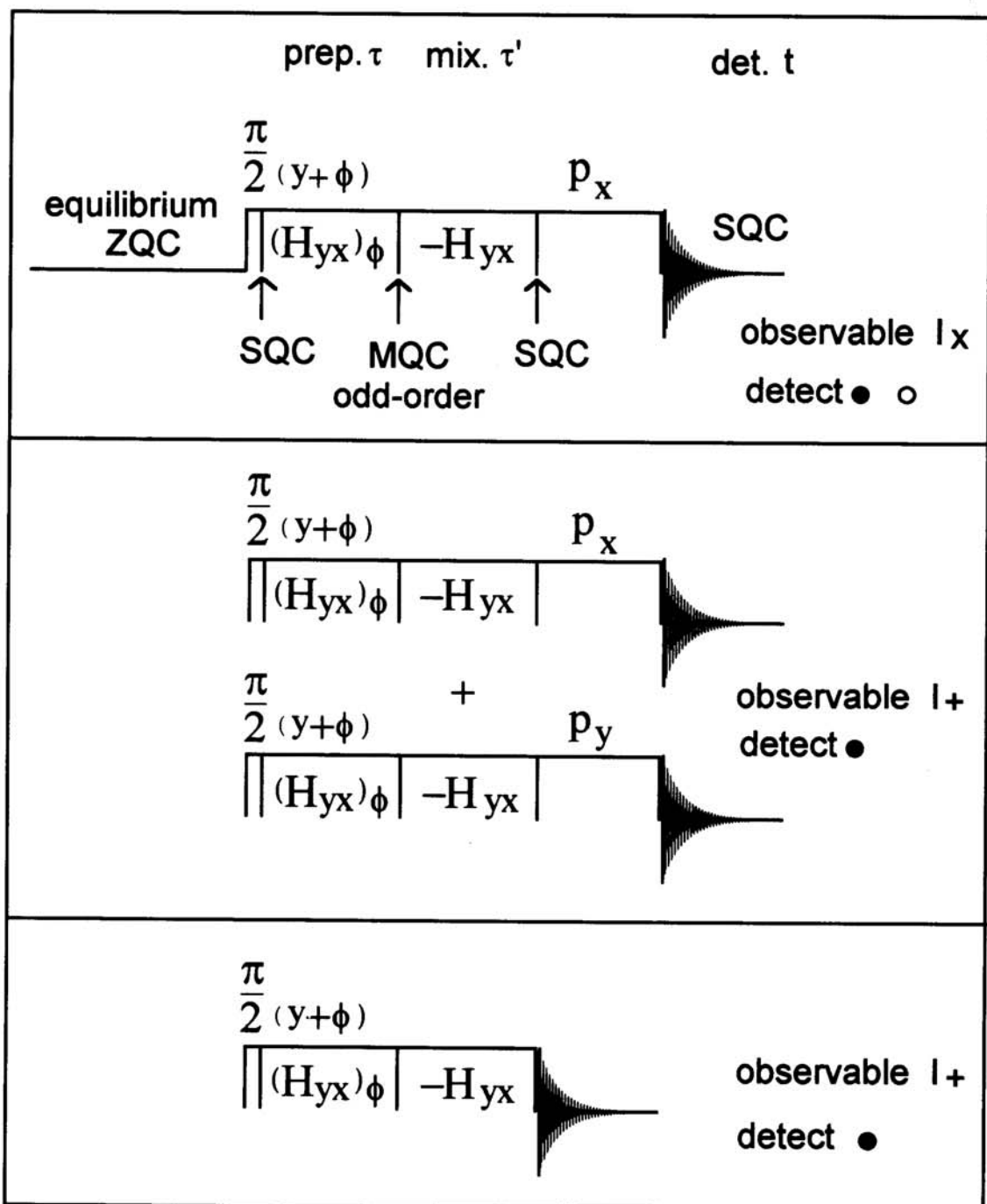
2D MQ NMR experiment of coupled spin-1/2 nuclei in solids

$$S_{zz}(\tau, \phi, t) = \sum_1 |b_1^n(\tau)|^2 \exp(in_1\phi) \sum_{i,j} Z_{ij} \exp(-i\omega_{ij}t)$$

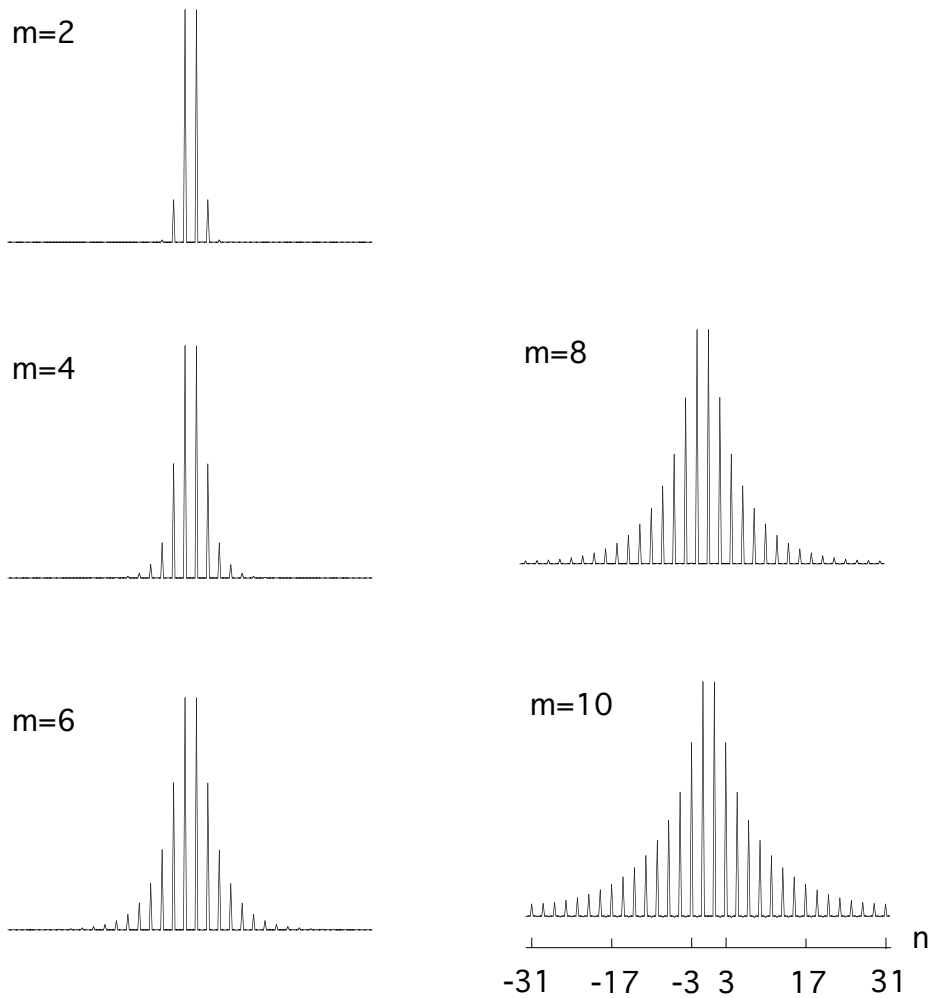
$$\phi, t \xleftrightarrow{2D \text{ FT}} n, \omega$$



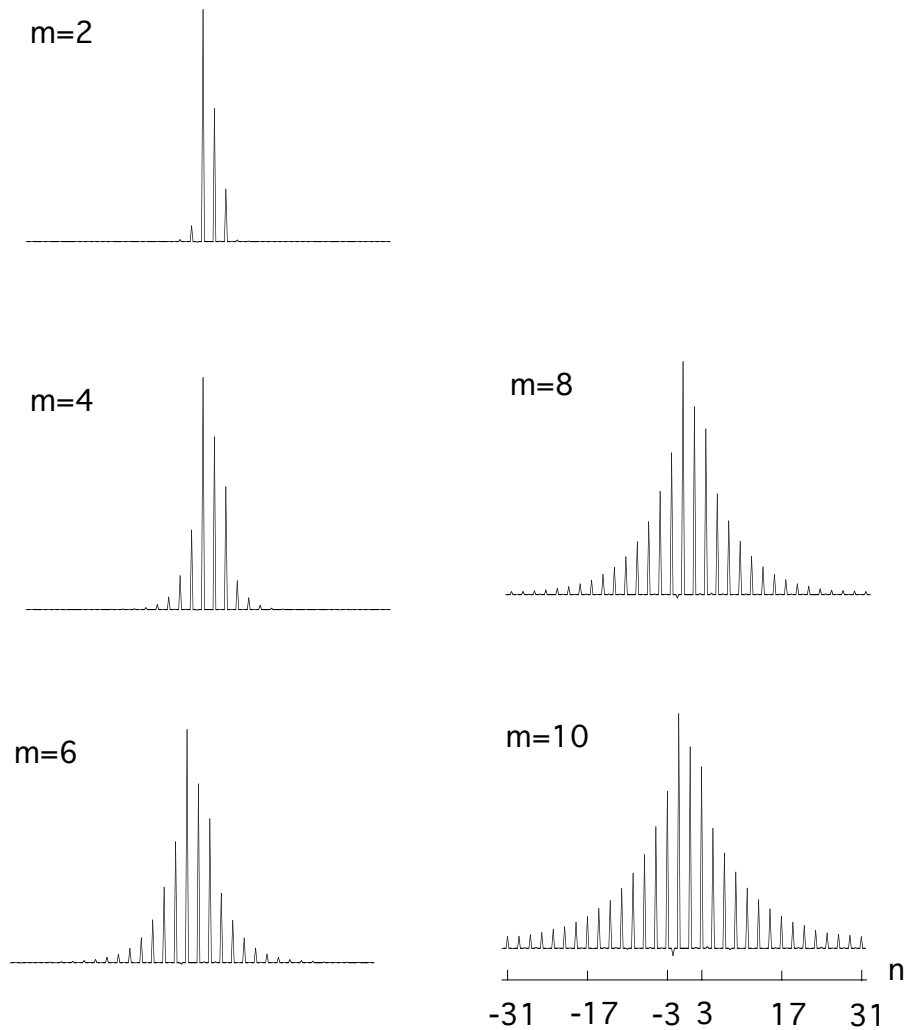
Proton MQ spectra of adamantane solid



Pulse sequences for detecting odd-order MQ coherences

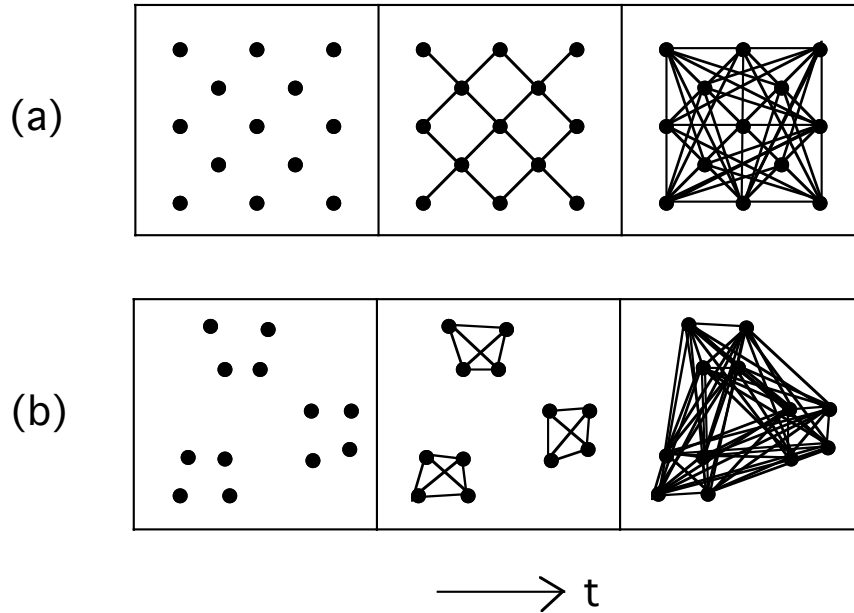


Odd-order multiple-quantum coherences of adamantane. The spin system is excited from I_x and the observable is also I_x . The excitation cycle m is indicated in the figure. One cycle lasts $60 \mu\text{s}$.



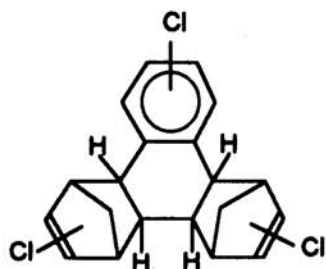
Odd-order multiple-quantum coherences of adamantane. The spin system is excited from $|x\rangle$ and the observable is I_+ . The excitation cycle m is indicated with the spectra. One cycle lasts $60 \mu\text{s}$.

MQ Spin Counting

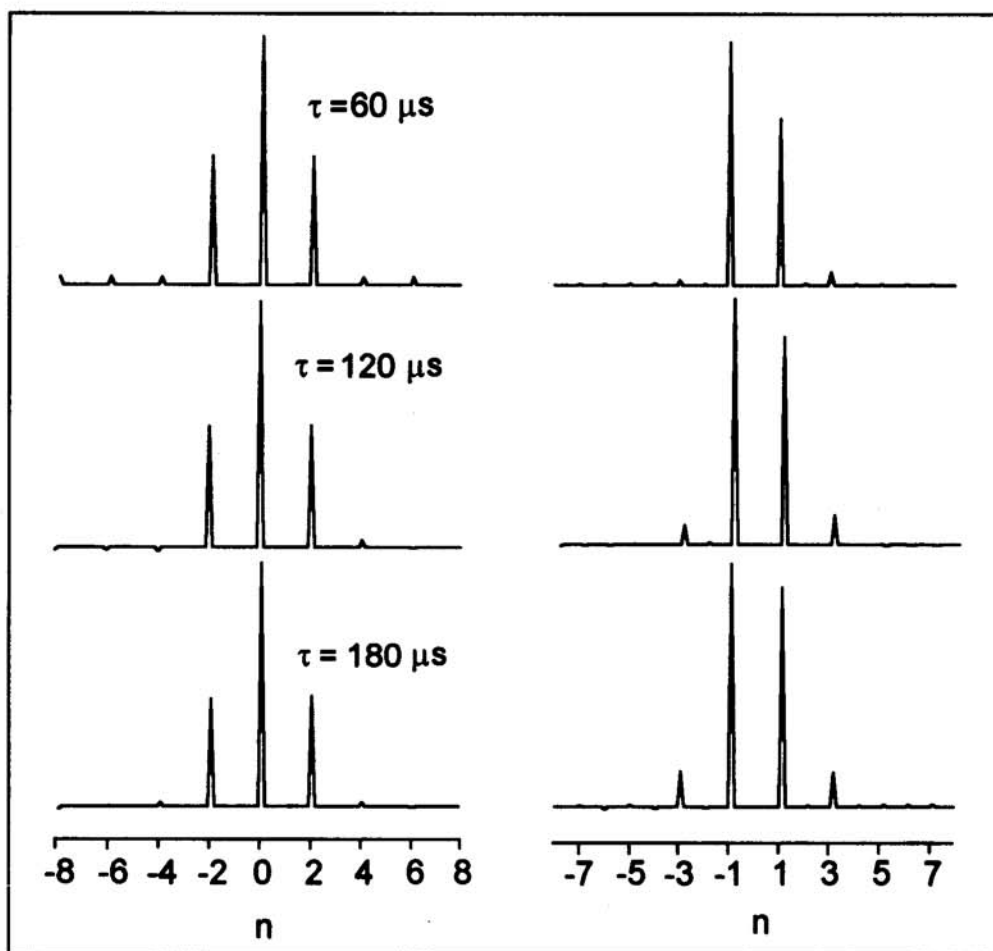


Schematic description of the development of MQ correlation among coupled spins in solids with excitation time t . (a) Uniformly distributed spins, which exhibit a monotonical development of multiple-spin correlations. (b) Clustered material. With short excitation time, the number of correlated spins will be limited to the number of atoms within the cluster, whereas with longer excitation time intercluster correlations develop.

Spin counting



1,2,3,4-tetrachloronaphthalene-
bis(hexachlorocyclopentadiene)-
adduct



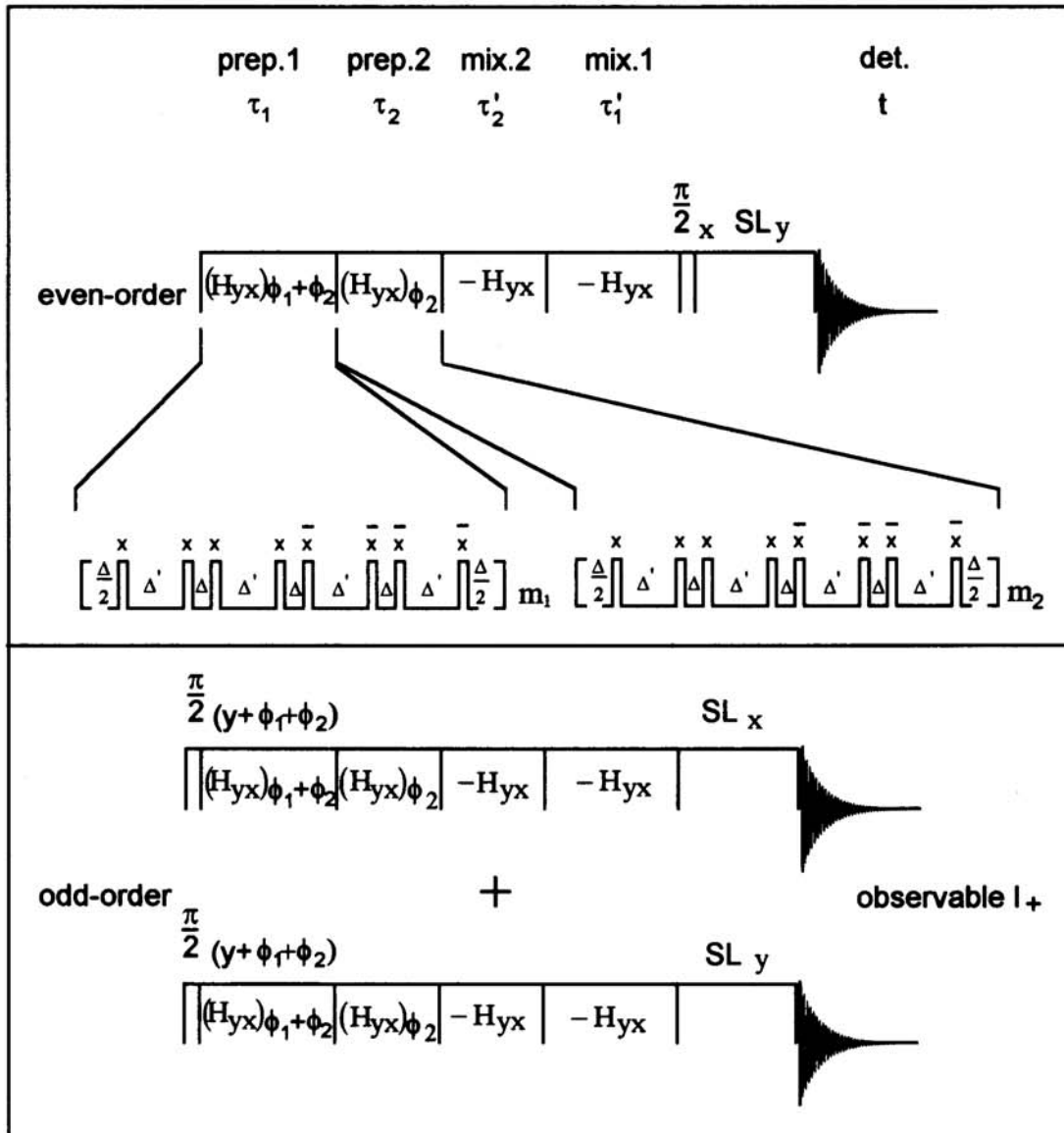
Even-order MQ coherences

Odd-order MQ coherences

Three-dimensional MQ Experiment

- To directly monitor the coherence transfer between various multi-spin multiple-quantum modes, three- or higher-dimensional experiments need to be employed.

3D MQ experiments

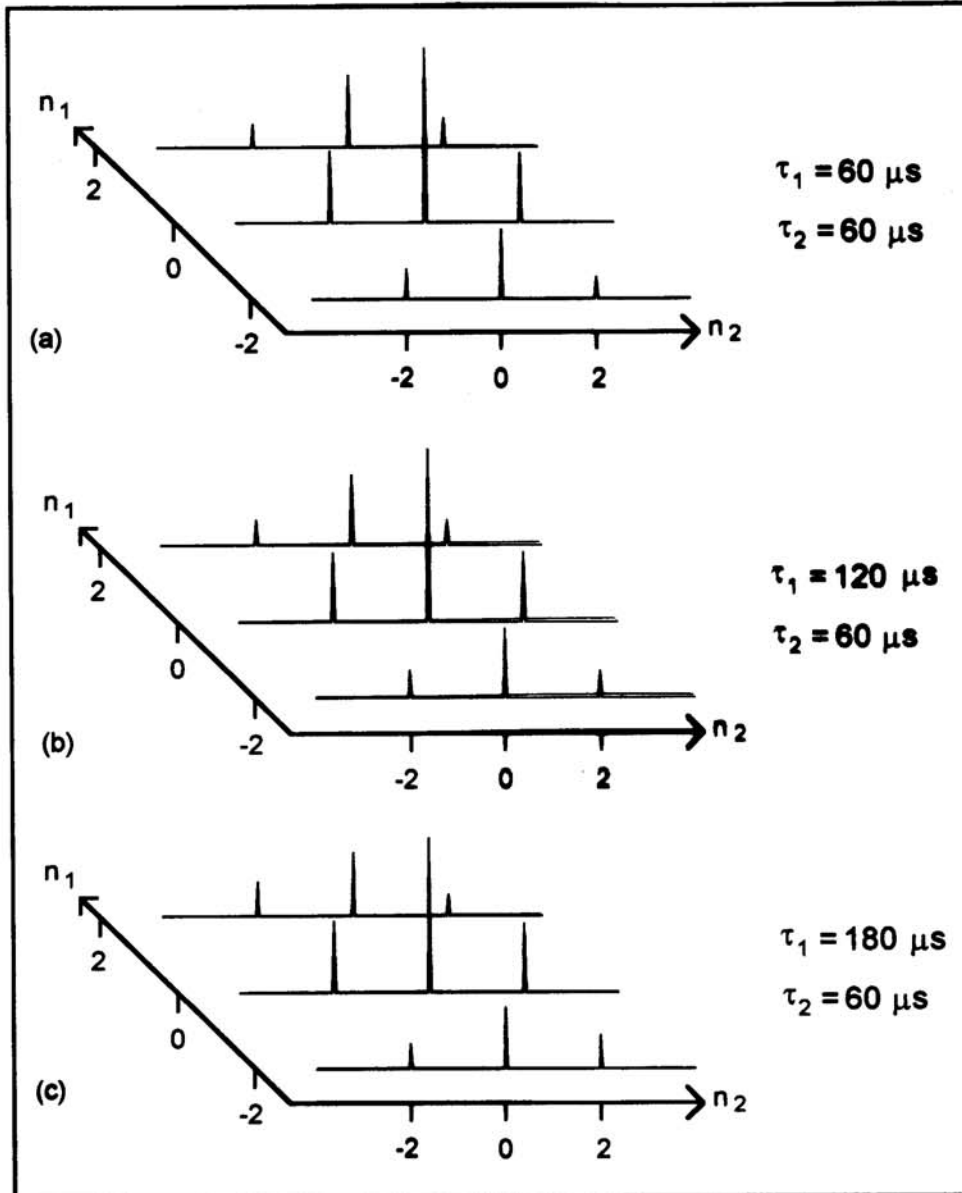
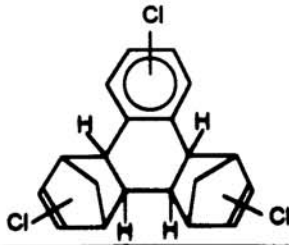


Detection of MQ coherences developed from MQ coherences

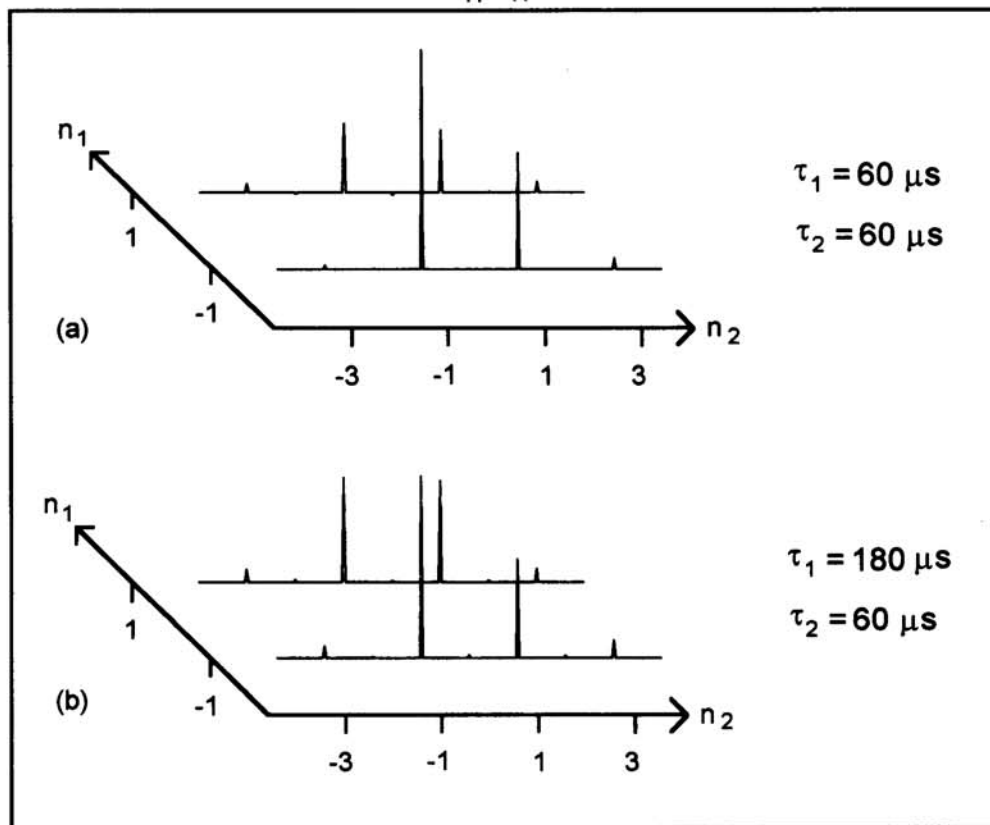
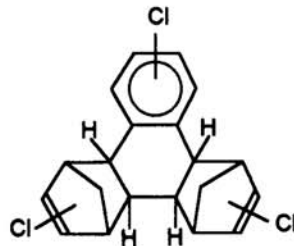
$$S(\tau_1, \tau_2, \phi_1, \phi_2, t) = \sum_l \sum_k |b_{l,k}(\tau_1, \tau_2)|^2 \exp(in_1^l \phi_1) \exp(in_2^k \phi_2) \sum_{i,j} Z_{ij} \exp(-i\omega_{ij}t)$$

$$\phi_1, \phi_2, t \xleftrightarrow{3D FT} n_1, n_2, \omega$$

3D MQ spectra



Even-order MQ coherences \rightarrow Even-order MQ coherences



Odd-order MQ coherences \rightarrow Odd-order MQ coherences