Week 11: NMR, EPR, post-HF

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Diskusjonsoppgaver

- Explain in your own words how NMR spectroscopy works.
- Explain in your own words how EPR spectroscopy works.
- **Q17.3** Why is it useful to define the chemical shift relative to a reference compound as follows?

$$\delta = \frac{\nu - \nu_{\text{ref}}}{\nu_{\text{ref}}} \cdot 10^6$$

- Explain why two magnetic fields, a static field and a radio-frequency field, are needed to carry out NMR experiments. Why must the two field directions be perpendicular?
- Hartree-Fock skalerer ca. som $O(M^4)$ i antall basisfunksjoner M. En beregning for et vannmolekyl tar ett sekund. Hvor lang tid tar det for 3 vannmolekyler når man bruker samme basis?
- Møller–Plesset perturbasjonsteori er ikke variasjonell. Fortell hva det betyr og hva du kan si om kvaliteten til energien man får.

Regneoppgaver gjort av meg

- **P17.22** Calculate the gain in proton spin polarization at room temperature for each increase in external magnetic field of 1.0 T. *Hint: You may use a Taylor expansion of the polarization as defined in Equation (17.9) with the assumption that the argument of the tanh function is very small.*
- **P17.9** Predict the number of chemically shifted ^{1}H peaks and the multiplet splitting of each peak that you would observe for 1,1,1,2-tetrachloroethane. Justify your answer.
- **Exercise 13.12** Predict the hyperfine structure of the EPR spectrum of a radical with 2 ^{14}N nuclei and 1 proton. The hyperfine coupling constants are a $= \alpha =$ 1.61 mT for 14 N and $\alpha =$ 0.35 mT for the protons.

Regneoppgaver for dere (1)

- **P17.3** The nuclear spin operators can be represented as 2×2 matrices, and α and β can be represented as column vectors in the form

$$\alpha = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{and} \quad \beta = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

Given that

$$\hat{I}_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \hat{I}_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \text{and} \quad \hat{I}_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

and

$$\hat{I}^2 = \frac{3\hbar^2}{4}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

show that

$$\hat{I}^2\alpha = \frac{3\hbar^2}{4}\alpha, \quad \hat{I}^2\beta = \frac{3\hbar^2}{4}\beta, \quad \hat{I}_z\alpha = \frac{\hbar}{2}\alpha \quad \text{and} \quad \hat{I}_z\beta = -\frac{\hbar}{2}\beta$$

Regneoppgaver for dere (2)

- **P17.11** Predict the number of chemically shifted ^{1}H peaks and the multiplet splitting of each peak that you would observe for nitroethane. Justify your answer.
- **P17.13** Predict the number of chemically shifted ^{1}H peaks and the multiplet splitting of each peak that you would observe for 1,1,2-trichloroethane. Justify your answer.
- **Exercise 13.13** The EPR spectrum of a radical with a single magnetic nucleus is split into four lines of equal intensity. What is the spin of the magnetic nucleus?
- CCSD(T)-metoden, en Post-Hartree-Fock-metode, skalerer som $O(M^7)$ i antall basisfunksjoner. Anta at en beregning på en datamaskin tar 10 sekunder for et vannmolekyl. Hvor lang tid tar det for to vannmolekyler (i samme basis)?
- Eksamensoppgavene fra tidligere år