**SFI 5800: 3rd exam. Data de entrega: 29.11. 2021**

1. **Give term symbols and g-factors for the following species. Which of them are expected to be EPR active ? Which are NMR active ?**

**2H, H2, V2+, V3+, V4+, V5+, Mn7+, Ce3+, Ce4+, Pr3+, Eu2+, Er3+, NO, Yb3+, Lu3+. For the EPR active species indicate which interactions influence the spectra.**

1. **Chromium ions can occur in the following valence states: Cr2+, Cr3+, Cr4+, Cr5+, Cr6+. Develop a spectroscopic strategy on how to differentiate these valence states spectroscopically. Use a matrix, indicating the key experiment for differentiation. Describe the outcomes of these 10 different experiments.**
2. **a) Using the double group formalism, develop a sketch of the energy levels and irreducible representations for Cr3+ in an octahedral environment. Assume the spin-orbit coupling to be weaker than the ligand field splitting.**
3. **Predict the optical spectrum**
4. **Predict the EPR spectrum**
5. **Discuss the salient features of EPR and Mößbauer spectra of the following complexes:**
   1. **Fe3+ (high-spin) in an octahedral environment**
   2. **Fe3+(high-spin) in a tetrahedral environment**
   3. **Fe2+ (low-spin) in an octahedral environment**
   4. **Fe2+ (high-spin) in an octahedral environment**
6. **To measure the spin-lattice relaxation times the following two pulse sequences are being used: (a) apin-lattice relaxation times are measured by the inversion recovery sequence 180°-t-90° -acquire. (b) Spin-spin relaxation times are measured by the Hahn-spin echo method 90°-t-180-t-acquire. In both pulse sequences the time t is systematically incremented. Illustrate, using a vector model, how these sequences work describe how the values T1 and T2 are obtained from the data measured at variable t values.**
7. **Barium acetylide possesses the following chemical shift tensor components: 11= 320 ppm, 22= 320 ppm, 33 = 45 ppm with respect to a tetramethylsilane reference**
   1. **sketch the NMR spectrum measured on a powdered sample**
   2. **what chemical shift is measured if the triple bond of the molecule makes an angle of 45° relative to the magnetic field direction ?**
   3. **sketch the MAS-NMR spectrum at a fast spinning conditions**
8. **Predict the results of a Stern-Gerlach experiment excuted on the following species:**
9. **H atoms, (b) D atoms, (c) H2 molecules (d) Xe gas**