**Espectroscopia Física 2021, Prova 2**

1. **For the HBr molecule calculate the rotational constant B and predict quantitatively the vibrational-rotational spectra at 100 K and 1000 K**

**paying attention to the peak intensities**

1. **Predict the vibrational-rotational absorption spectra and the rotational Raman spectra of a) H2 and b) HD at 300 K.**
2. **Consider two Ni2+ ion complexes in a square-planar and a tetrahedral (4-coordinated) environment. Based on the relevant Tanabe-Sugano diagrams, discuss the spectroscopic properties of these complexes, using group-theoretical arguments.**
3. **Starting from the electron configuration in the extremely strong external field limit, and without considering Jahn-Teller effects, make an assessment of the relative stabilities of octahedral versus tetrahedral complexes for the first row transition metals series d1-d9. Identify the dn systems with the highest and the lowest preference of the octahedral environments.**
4. **a) using group theory, develop the irreducible represenations of a Fe2+ ion in a cubic eight-coordinated environment in the weak external field limit. The electronic states of the free ion are 5D, 3H, 3P, 3F, 3G and 1I.**
5. **predict the spectroscopic transitions for the weak field case.**
6. **Six-coordinated transition metal ions with electron configuration dn (4 ≤ n ≤ 7) can occur both in the high-spin and in the low-spin states. Discuss the spectroscopic differences between the high-spin and the low-spin states as observed in:**
7. **the infrared absorption spectrum of a d6 ion with coordination number six,**
8. **the UV-VIS- absorption spectrum of a d8 ion with coordination number six.**
9. **Predict the number of peaks observed for the following open-shell species**

**a)**



1. **A tetrahedral Na43+ ion in a diamagnetic matrix**
2. **An MnF64- ion in a single crystal**
3. **An MnO42- ion in a single crystal**
4. **For which of the above species do you expect no g-anisotropy ?**