

2 Molecular spectrum (8 points)

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Consider the molecule NH consisting of a nitrogen and a hydrogen atom. Like atoms, molecules have quantized energetic states. For NH the energetic structure is depicted in figure 2.1. There are two electronic states, which are labeled with the Greek capitals Δ and Π . Each of these electronic configurations contains a series of rotational states, labeled by the quantum number J . In the Δ - and Π -states the lowest value occurring for J is 2 and 1, respectively. The energy of the rotational states are given by $B_J(J+1)$, where the factor B denotes the rotational constant of the electronic configuration. The value of B is inversely proportional to the moment of inertia of the molecule.

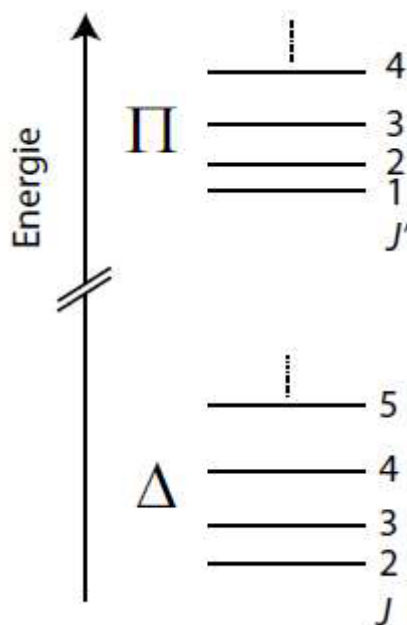


Figure 2.1: Schematic of the rotational states in the electronic Π - and Δ -states of NH.

In figure 2.2 (next page) the spectrum of the $(\Delta, J \rightarrow \Pi, J')$ transitions in NH is depicted (the unit cm^{-1} corresponds to the energy of a photon with wavelength 1 cm). Different rotational transitions are visible, labeled by the letters P, Q and R. The P-, Q- and R-lines are the transitions with $\Delta J = -1, 0$ and $+1$ respectively. Each line in the spectrum is further marked with the value of J in the Δ -state.

Question 1: Deduce from the R-lines in the spectrum whether the rotational constant B_{Π} of the Π -state is larger or smaller than the rotational constant B_{Δ} of the Δ -state.

Question 2: Give an estimation of the ratio B_{Π}/B_{Δ} based on figure 2.2.

Question 3: In which ways will the spectrum change if the H-atom in NH is replaced by a D-atom (deuterium)? In particular, elaborate on the relative positions of the lines in the spectrum. Assume that the equilibrium distance between the nuclei is the same for NH and ND.

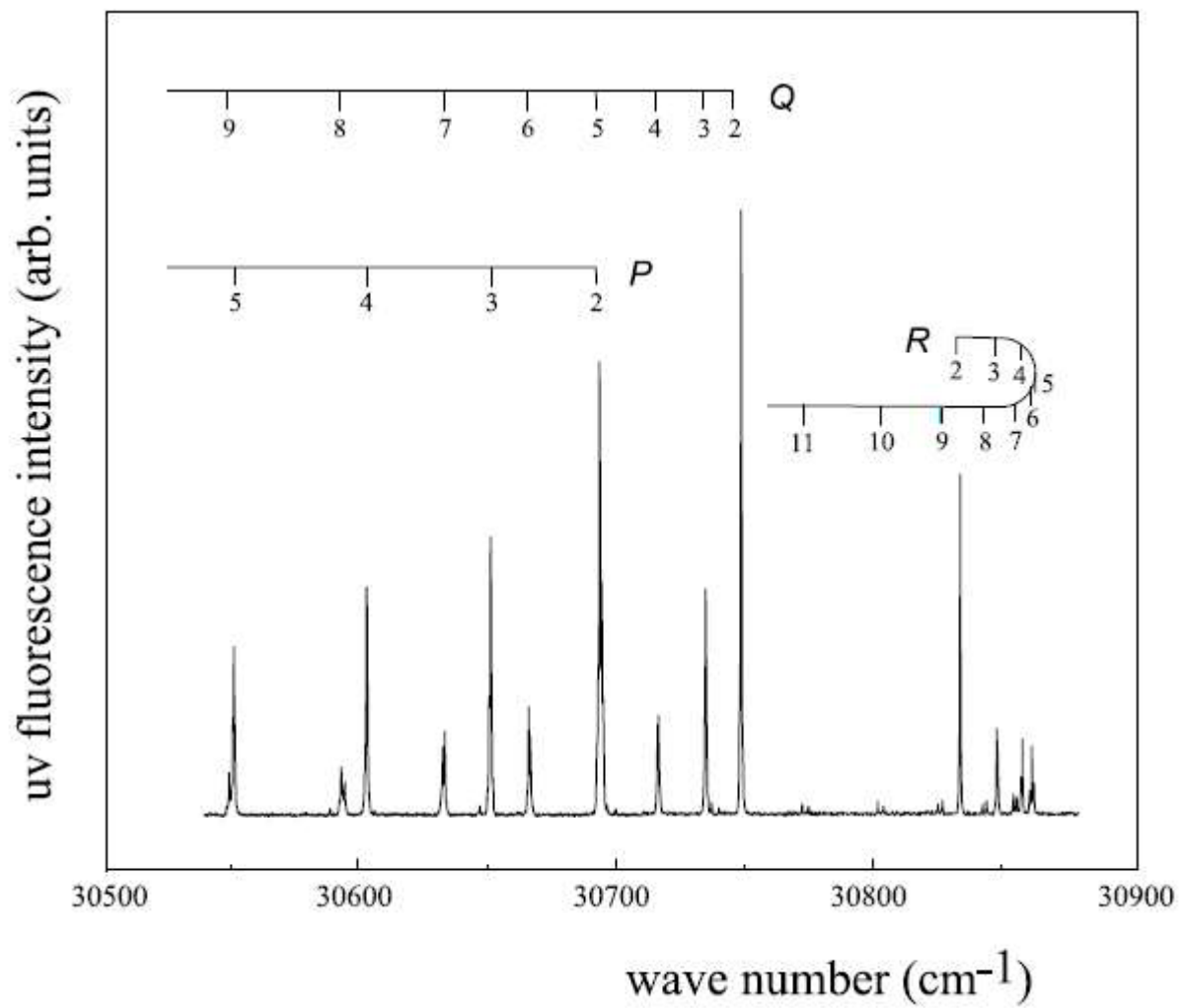


Figure 2.2: Spectrum of the $(\Delta, J \rightarrow \Pi, J')$ -transitions of NH.