

Student name: _____ Date: _____ [tab-a021]

[Exercise]

- Load the simulator pressing the corresponding link.
- Verify the horizontal scale (in mT) and keeping in mind the previous explanations on the interpretation, measure the four hyperfine splittings.
- Fill the table of couplings on the simulator and reload the spectrum. If the interpretation is correct then the number of lines and the intensities should coincide with the experimental spectrum.
- Measure the length of the experimental spectrum (between the lines 1 and 48). Apply the Eq. (8) and if that length coincides with the experimental value then the interpretation is correct.
- Refine the hyperfine splitting values and/or the peak to peak linewidth (DHpp) by overlapping both spectra.
- When the simulation is correct, measure the heights of the lines 2, 6, 17 and 21 and write its value in the Table tab-a021.
- Print, in the simulator, the leaf of results with the spectra simulated and experimental without overlap and including the tree of splittings.
- Indicate on the tree of splittings the theoretical relative intensities of each multiplet originating by the three larger constants. An example of the assignment of intensities is presented in the interpretation of the radical [a018] (section 8.1.2), Fig. 17.
- Mark with an arrow the lines 2, 6, 17 and 21 and writes close to them its theoretical relative intensity.
- In the leaf of results number the nuclei with spin of the molecule and assigns, if it is possible, the hyperfine splittings originating in the protons. **Justify** the answer.
- Complete the Table of intensities (tab-a021).

Intensities Table 3. Benzyl neutral radical [a021].

	Line 2	Line 6	Line 17	Line 21
Pixels				
Normalized ^a				
Theoretical ^b				

^a Normalize the intensities so that the smallest one (line 2) will worth the unit.

^b Theoretical intensities normalized to line 2.

Spectrum length:

Using the Eq. (8) = mT;

Experimental = mT.