

[Exercise]

- Using the symmetry of the radical deduce the number of equivalent groups.
- Counts the number of experimental lines; calculate the number of theoretical lines (Eq. (9)); write down both values and observe the difference.
- Measure (with the mouse) the heights of the three first lines of the spectrum. From these heights deduce if the smaller splitting arises from the two atoms of N or from the four equivalent H of the ring, since both would give a quintet but with different relation of intensities.
- Measure the distance between the lines 2 and 3. This distance is the same than that between the lines 1 and 2.
- Seek the lines that form the first quintet and from the line 4, with the distance 1-2 find the 2<sup>nd</sup> quintet. Write down the lines that form the first and the second quintet of the spectrum.
- The distance among the central lines of the previous quintets (lines 3 and 10) is the second hyperfine splitting (it can also be measured among the lines 1-4).
- With the distance among the lines 3-10, find the following multiplet (triplet or quintet?); Write down the lines of that multiplet.
- Measure the length of the experimental spectrum and apply the Eq. (8) to calculate the third hyperfine splitting.
- From the center of the spectrum (line 35), write down the lines that are generated when the third splitting is applied.
- Measure the heights of all the lines to determine the order (multiplicity) of the hyperfine splitting.
- In the form of results that you print with the simulator, number the nuclei of the radical and assign the hyperfine splittings to each nucleus showing the positions that are equivalent.

**Table for the interpretation of 1,4-dihydro pyrazine cation radical [a028].**

L (spectrum) = ..... mT.  $N_{theoretical}$  : .....  $N_{experimental}$  : .....

| Multiplet                                    | Lines                | Lines intensities |  |
|--|----------------------|-------------------|--|
| 1 <sup>st</sup> quintet<br>(distance 2-3)    | 1, 2, 3, ..... ..... | Pixels            |  |
|  |                      | Normalized        |  |
|  |                      | Theoretical       |  |
| 2 <sup>nd</sup> quintet<br>(distance 2-3)    | 4, ..... .....       | Pixels            |  |
|  |                      | Normalized        |  |
|  |                      | Theoretical       |  |
| 2 <sup>nd</sup> multiplet<br>(distance 3-10) | 3, 10, ..... .....   | Pixels            |  |
|  |                      | Normalized        |  |
|  |                      | Theoretical       |  |
| 3 <sup>th</sup> multiplet                    | ..... .....          | Pixels            |  |
|  |                      | Normalized        |  |
|  |                      | Theoretical       |  |