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Nuclear Magnetic Resonance and Humanistic Mathematics: A Farewell

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One important tool in various chemical disciplines is nuclear magnetic resonance spectroscopy, commonly referred to as NMR. Because protons are positively charged, their spinning motion creates a magnetic field. When exposed to an external magnetic field, the proton can either align with (α)or against (β) the field. Exposing a proton to the right strength of magnetic field will cause it to flip from one orientation to the other, a condition called resonance. By exposing a molecule to a range of magnetic fields, the strength of field needed to achieve resonance of each NMR-active nucleus in the molecule can be seen as a peak on a spectrum (Figure 1). Nuclei with even numbers of both protons and neutrons are NMR-inactive; they do not appear on spectra. Also, chemically equivalent nuclei, such as the four hydrogens in methane, CH_4, will resonate at the same field strength and thus appear as one peak. Chemists commonly look at the resonance of hydrogen, ^1H. Figure 1 shows the NMR spectrum of 1,1-dichloroethane.

I was introduced to NMR in my sophomore organic chemistry course. Professor Phil Myhre explained the basics, in somewhat more detail than I have presented them here, then went on to talk about how you can use an NMR spectrum to figure out what an unknown molecule looks like.

One important aspect of NMR spectrum interpretation is coupling. In an organic (carbon-based) molecule, hydrogen atoms that are one carbon-carbon bond away can "see" one another. In the spectrum, this corresponds to a single peak for one hydrogen (or several chemically equivalent hydrogens) being split into many peaks. How many? The number of neighbors plus one, for the hydrogen could see its neighbors in, for the case of three, $\alpha\,\alpha\,\alpha$, $\alpha\,\alpha\,\beta$, $\alpha\,\beta\,\beta$, $\beta\,\beta\,\beta$. What are the intensities of these peaks? There's only one way to get each $\alpha\,\alpha\,\alpha$ and $\beta\,\beta\,\beta$, but three ways to get each $\alpha\,\alpha\,\beta$ ($\beta\,\alpha\,\alpha$, $\alpha\,\beta\,\alpha$) and $\alpha\,\beta\,\beta$ ($\beta\,\beta\,\alpha$, $\beta\,\alpha\,\beta$). Thus, in this case you get a quartet with peak intensities of 1:3:3:1. This can be seen in Figure 1; the hydrogen attached to the carbon with the two Cl atoms sees three ^1H neighbors and so appears as a 1:3:3:1 quartet around 330 Hz. The three hydrogens are chemically equivalent and see one ^1H neighbor, so they appear as a 1:1 doublet around 120 Hz.

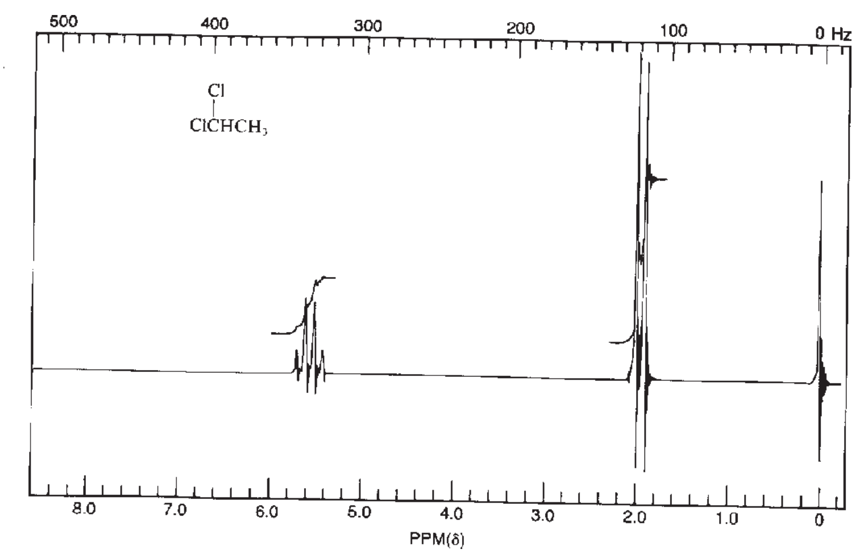

Figure 1
^1H NMR spectrum of 1,1-dichloroethane

Think about other splitting possiblities. To get a triplet a nucleus would see two neighbors. These neighbors could be in four different combinations: $\alpha\,\alpha$, $\alpha\,\beta$, $\beta\,\alpha$, and $\beta\,\beta$. Since $\alpha\,\beta$ and $\beta\,\alpha$ are the same, this works out to splitting with peak intensities of 1:2:1.

Seeing a pattern? Put everything together and you find Pascal's Triangle (Figure 2). The elegant pattern that gave me the binomial coefficients in algebra class also tells me ideal peak intensities in chemical spectra.

And so it was, sitting in chemistry class, looking at Pascal's Triangle on the overhead, that I really understood what humanistic mathematics is. It is finding the mathematics that is everywhere.

I have been the production manager of the HMNJ since March 1998 (Issue #17). I majored in chemistry and am now off to University of California, Santa Cruz to pursue a graduate degree in science writing. I leave the HMNJ in wonderful hands. Expect to see issues in your mailbox more frequently; Stephanie, Fess, Mary and Kathe are a great team, and I wish them well.

0	singlet (1)	1
1	doublet (2)	1 : 1
2	triplet (3)	1 : 2 : 1
3	quartet (4)	1 : 3 : 3 : 1
4	quintet (5)	1 : 4 : 6 : 4 : 1
5	sextet (6)	1 : 5 : 10 : 10 : 5 : 1
6	septet (7)	1 : 6 : 15 : 20 : 15 : 6 : 1

Figure 2
Pascal's Triangle.

"Stairway to Seven"

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May be sung to the tune of the 7 verse song "Stairway to Heaven" by Jimmy Page and Robert Plant.

There's a student who's sure if she rolls two fair dice,
The most likely sum is seven.
On the seventh day she knows many stores will be closed
'Cause lots of folks call it the day of rest.
Ooh, ooh, she's inquiring: "Where is there a seven?"

Well there's a seven on the wall, but she wants to be sure
'Cause you know uncrossed sevens can look like ones.
From seven notes in a scale, there's a songbird who sings—
It's the first sour note in the harmonic series.
Ooh, it's quite a number. Ooh, seven wonders.

There's a feeling I get from the seven continents
And shuffles needed to mix the cards:
Snow White's dwarves all could be a water polo team—
It's the limit of short-term mem'ry.
Ooh, it's quite a number. Ooh, telephone number.

It's the steps in ballet's art, it's the Big Dipper stars,
And it's how many times you can fold paper.
First polygon to elude the classical tools
And it's how many patterns for borders.

If a track meet takes a long time, don't be alarmed now—
It's just what's called a heptathlon.
Can you remember when the 7th month was September?
Then Caesar added August and July! And it makes me wonder...

Seven verses make this song maybe too long,
The piper fights for airplay!
First whole number whose reciprocal does use
Its maximum block of digits.

As we wind on down the road, with 7 chakras I am told,
And 7 colors of the rainbow make white light when they all show.
If you listen to this rhyme of this odd Mersenne prime,
May it make you want to find each number's special shine...
And she's buying a stairway to seventh heaven!