Found Chem (2018) 20:43–49
https://doi.org/10.1007/s10698-017-9295-2

An allegory on molecular periodicity

Ray Hefferlin[1]

Published online: 13 September 2017

In the late 1860s, a Peruvian explorer learned of a mysterious village, never entered by outsiders, in the jungle of his country. The rumors placed it somewhere southeast of el Rio Marañón and northwest of el Rio Ucayan, more of less between the Allpahuayo-Mishana and the Pacaya-Samiria Reservas Naturales.

He came across a friend who was a Greek sociologist, and said "Come now, friend, wouldn't you like to join me in this expedition?" His friend said "Of course! It sounds like something really interesting".

The two gathered supplies, equipment, and pack animals; they consulted geographic maps to plot their approach to the area through the dangerous rain forest. Eventually, after surviving many dangers, they found the village.

They found that the little village was populated by 12 extremely diverse men and 12 equally diverse women.[1] The sociologist jotted down the major characteristic of each one of the 12 in his journal:

Religious Poor
Quiet
Tall
Rich [owns two cows]
Antisocial
Short [of height] Middle-class

[1] Each person, irrespective of gender, represents a different elemental atom.

Ray Hefferlin—Deceased

✉ Ray Hefferlin
hefferln@southern.edu

[1] Southern Adventist University Collegedale, Collegedale, TN 37315, USA

Atheist
Agnostic [indifferent to religion]
Medium [average height]
Social [extrovert]

"What do you make of this?" the sociologist asked. After a moment, the explorer said "Notice the 'Tall, Medium, and Short' triad! I remember something like that in chemistry. Why don't we try to see if the other people are in triads too?" The result was the same as Table 1 except that the two boxes connected with the heavy line were reversed in order. The sociologist was puzzled. "It's nice, but it's based on what you call major characteristics. Those are subjective chosen, isn't it so? Take your three heights, for instance. If you had chosen some other characteristics, such as their hobbies, that column could have turned out to be quite different." (Scerri 2009).

Some time later they found that the members of the village each have a number, rather like a passport number or a Social Security number in America.[2] When the members were put into the table *by number* the result was Table 1, which corrected a mistake (the Antisocial person had originally above the Self-effacing person) (Scerri 2009)![3] The enthusiasm engendered by this correction back home was palpable. Everyone recognized that all of the groups were triads in logical order. The sociologist said "Now we have something that will be one of the foundations, if not the foundation, of all of sociology!"[4]

One day the sociologist said to her explorer colleague "You seem bored. What's wrong?" "Right. I am bored. I think that I'll go up near Lake Titicaca to check out the floating villages …" and the next morning he was gone, leaving her all alone with the villagers.

Our sociologist was not bored; she knew that there was more to do in the community that they had found. She had noted that seven of the men had married[5] seven of the women. She had often marveled at how different mature individuals could form so close a relationship as exists in a happy marriage, and hoped to experience it herself. And yet "To what extend do the individuals who marry still retain their own individualities?" she wondered.[6]

These musings led her to think "Maybe, just maybe, if I can tease out the essence of these seven marriages then I might be able to predict what will happen in *future* romances! After all, there are 144 possible marriages (12 times 12 combinations of a man and a woman), of which just seven have occurred; that leaves 137 to predict!"

She collected the major characteristics of the married people. She then interviewed the couples at length, in their homes, to gauge whether their happiness was on the surface or deep down, assigning to each couple a compatibility coefficient (CC) from 3 (seemingly the happiest) down to 0. The zero applies to a couple where a man who was Antisocial. Her final chart is shown in Table 2.

Her next steps were to construct a formula containing the two ID numbers as the independent variables and the compatibility coefficient as the dependent variable. Then she used regression methods to see how well the formula reproduced the coefficients. The first

[2] Atomic number; this number uniquely identifies atoms whatever their other properties may be.

[3] So it was that the use of atomic numbers corrected erroneous placements based on atomic weights.

[4] The periodic table of the elements is considered one of the foundations of chemistry.

[5] Bonded with, as atoms in diatomic molecules.

[6] To what extend do atoms retain their identities in molecules [the central question of Atoms in Molecules theory (Bader 1991).

Table 1 The explorer's arrangement of the villagers' major personal characteristics

Rich	Religious	Tall	Social
Middle-class	Agnostic	Medium	Quiet
Poor	Atheist	Short	Antisocial

Clearly this is an analog of the periodic table of the elements

Table 2 The sociologist's table of independent variables (in columns two and three) and the dependent variable (column 4)

Couple ID numbers	Major characteristic of the woman	Major characteristic of the man	Compatibility coefficient
6 and 23[a]	Agnostic (2, 2)[b]	Short (3, 3)	2
2 and 14	Religious (1, 2)	Religious (1, 2)	1
9 and 24	Poor (3, 1)	Antisocial (3, 4)	0
5 and 13	Middle-class (2, 1)	Rich (1, 1)	3
4 and 20	Social (1, 4)	Quiet (3, 1)	3
6 and 16	Agnostic (2, 2)	Social (1, 4)	2
3 and 23	Tall (1, 3)	Short (3, 3)	2

[a] ID numbers 1 through 12 are for the women represented in Table 1 and ID numbers 13–23 are for the man similarly represented; the numbers go from upper left across rows to lower right

[b] The numbers in parentheses are the period number and the group number of the person's location in the periodic table

try, using the sums of the ID numbers failed miserably (it would seem that 2 + 14 should produce a higher compatibility coefficient than 4 + 20, but they did not).

Hours later, after many failures, she asked herself. "Why not use the two row numbers and also the two group numbers?" She constructed a formula which included them as independent variables, and began using various combinations of six rows of the seven rows[7] of Table 2. The predictions of CCs were reasonably good[8] and the predictions of the remaining, seventh-row, CCs were also reasonably good. She then predicted CCs for the 137 marriages which could take place in the future (Wohlers et al. 1998).

Then our very determined sociologist employed neural networks to the same data (see footnote 8). The computer (after many, many tries) built networks based on the inputs[9] known CCs, and predicted CCs for all possible choices of six rows of data and in each choice the one remaining row of test data. The test cases indicated that the networks were reasonably good. Thus, she was able again to predict the CCs for the 137 marriages which could take place in the future (Hefferlin et al. 2003; Davis and Hefferlin 2006).

[7] She did it on purpose, using only six of the seven rows to get parameters that yielded good predictions of the compatibility coefficients, and then using the parameters on the seventh row. This procedure is called "save out one," meaning save out one case for an determination of precision.

[8] the resulting predictions, compared with those of the regression methods, made it possible to determine the precision of the method (the random errors).

[9] Another name for independent variables.

The predicted CCs for the 137 unknown marriage outcomes calculated using the least squares and neural network methods differed in some cases—and many of them differed by more than the sums of their error measures.

This embarrassing situation gave birth to an idea "Why not keep only those neural-network predictions that agree, within their error measures, with least-squares predictions for the same couples?" This clever idea resulted in a smaller number (44) of combined CC predictions, but they had somewhat smaller error measures (Hefferlin 2010, http://viXra.org/abs/1208.0026.

The sociologist, her work seemingly done, returned to her university in Athens. She presented lectures and wrote articles about the research, but there was little interest. The usual response was "Who cares?" or "It's cute, but we are busy with societies having huge numbers of inhabitants."[10] However, as years passed, a few colleagues expressed interest in the work and five of them even asked her to lead them in a visit to the village. One was a mathematician from the Netherlands and, oddly enough, the other four were all chemists with various specialties (one from China, one from Guatemala, and two from Russia).

Great was the excitement when they learned that after the sociologist's departure from the village there had been five marriages, two of them among the couples for which she had the best predictions of CCs. In the first instance, two of the inhabitants, who had been seen smiling shyly at each other some time, asked the village head man to marry them. The bride was Poor and the groom Rich. There was another marriage, this one between a Tall woman and a Middle-class man. The sociologist made friends with the couples and sized up their states of mind. She found the CCs to be 1 ± 0.7 and a very romantic 3 ± 0.2, in that order. She checked them against her CC predictions (2 ± 0.4 and 2 ± 0.8) and announced the results to the visiting group; "In the first case, the actual and predicted CCs are clearly in agreement; the error bars overlap. In the second case, I can call it a marginally successful prediction because the error bars just meet!"

The mathematician from the Netherlands had become lost on the trail. Fortunately he successfully found their track again and came into the village just as the sun was setting one evening. There was a quarter moon, but it would not have been of much help under the rain forest canopy. He said "I've so glad to have found you! I was very afraid of not finding you, not so much because of dying but because I wouldn't want to miss learning about your work!"

As he learned what the sociologist had done, an idea formed in his head. "You employ four independent variables for your calculations. This really means that your CC data are scattered in a four-dimensional space: the axes are your independent variables—two period numbers and two group numbers!" The sociologist and the other visitors seemed unimpressed, so he explained. "These four numbers suggest that you have a space with variables w, x, y, and z for the village men (Hefferlin 2008) and a similar space for the village women! The period numbers go from one to three, and the group numbers go from one to four, so you have 12 village ladies scattered in a hypercube with 144 locations and 12 village men likewise distributed in their hypercube!" He wandered off to sit on a rock, and began trying to sketch two hypercubes with the sparse populations of each hypercube connected to those in the other hypercube. He was never seen again and it was speculated that he had disappeared into four-space.

Another of the visitors was a very intuitive chemist from China. He said "This hypercube idea is visually challenging but what does it contribute? I propose a completely different procedure. Let's add the period numbers and let them serve as the period number of a new periodic table for the married folks, and add the group numbers to serve as the group number for it. Look, I have plotted the nine data we have and the plot seems to have

[10] Large biological molecules.

promise![11] Furthermore, this periodic table is flat, so that it can be published and displayed conveniently" (Kong and Wu 2012).

One chemist from Russia brought out what he had been thinking: "why not use group theory?[12] First find a group that results in a multiplet conforming to Table 1 for men; then bootstrap the group into space D (2). This will produce multiplets that partition married couples!" (Zhuvikin and Hefferlin 1983). Everyone was impressed but wanted to know if he had any predictions. "Nyet … no, I'm sorry. My colleague in America says that attempts to use least squares on unknown data result in oscillations (Zhuvikin and Hefferlin 1994); and he says that neural networks aren't working very well on these multiplets."[13]

Another of the chemists, also from Guatemala, explained that he had created, from first principles, what Table 1 would look like if the village were to exist in two dimensions (no up and down) (Asturias and Aragon 1985). "Tall, Medium, and Short are characteristics that simply …". At that moment, a very real three-dimensional jaguar roared quite near the camp. The visitors huddled in terror while the villagers calmly threw more wood on the smoldering fire. After the confusion

Several other schemes for investigating the villagers' marriage possibilities (Hefferlin and Burdick 1994; Hefferlin 2006) were discussed in exhaustive detail, especially that of the other chemist from Russia. He had proposed a hyperperiodic system which includes Table 1; the marriages (past and future); and also classifications of families composed of three or more villagers (Babaev and Hefferlin 1996)!

The visiting scientists concluded that their visit had been mutually stimulating. They also hoped that their new friends in the village will find the predictive work of some use in their future marriage plans.

On the last evening of the visit, the villagers feasted the visitors and played haunting music with the Andean zampoña (sikus), mandolina, quena flauta, charango, and wanqara. The moon was full. The villagers and scholars were sitting congenially around the glowing embers of a campfire, talking about their cooperation in such a strange intellectual and social journey.

A young villager, the Religious one, rose with dignity. She swept back her luxurious black hair and reverently recited the following verses in Quechua (http://www.poemas-del-alma.com/alturas-de-macchu.htm, http://www.neruda.uchile.cl/obra/obracantogeneral5.htmld):

> And here comes the guardian of the universal table and Andean symbols of the Amautas[14] arranged from Moses to Meldeleev, in their infinite rows and columns.

[11] This work does allow estimates of vast numbers of spectroscopic constants.

[12] There is a group theory in sociology, and quite another used for the mathematical analysis of symmetries.

[13] In the first attempts to fit data to diatomic-molecular multiplets derived from group theory on molecules, such a skewed surface did frustrate prediction settled down, our Guatemalan chemist continued "As I was saying before the rude interruption—Tall, Medium, and Short obviously are characteristics that simply couldn't exist in two dimensions! I will start over with nine flat men and nine flat women, and the five remaining marriages, and predict what happens if any other combinations of villagers marry.".

[14] Sages, teachers.

Intuitively, from prophet to prophet from Janet[15] to Baca Mendoza[16] and their tables of the law,[17] with the key, simple and wonderful. of an inaccessible cosmos finally understood by human nature" proud, egotistic, individualistic.

And God, timeless geometer, Where were You?
Being lit from plasma or phlogiston?
Weaving unknown orbitals, atom after atom?
In the burning bush of the Sinai[18] or in the golden sun of the Incas?

Therefore, by the ascent from the earth He[19] has climbed through the inhuman thicket of lost jungles up to you, Macchu Picchu.
The high city of stone steps, a final home whose earth is no longer[20] concealed by forest canopy.

She sat gracefully, and there was a silence, as various ones contemplated the juxtaposition of the laws of Moses and Mendeleev, the weaving of atomic orbitals, the allusions to God, and especially the gloomy depictions of natural man's mind.

The Quiet man, who had been gathering courage to speak in the unfamiliar language of the visitors, finally broke the silence. "Why no you honable … honorable visitors … go home … use … use your big talk … on
… what you call them? … molecules?"

References

Asturias, F.J., Aragon, S.R.: The hydrogenic atom and the periodic table of the elements in two spatial dimensions. Am. J. Phys. **53**, 893–899 (1985)

Babaev, E.V., Hefferlin, R.: The concepts of periodicity and hyper-periodicity: from atoms to molecules. In: Rouvray, D.H., Kirby, E.C. (eds.) Concepts in Chemistry, pp. 41–100. Research Studies Press Limited, Taunton, Somerset (1996)

Bader, R.F.W.: A quantum theory of molecular structure and its applications. Chem. Rev. **91**, 893–928 (1991)

Davis, W.B., Hefferlin, R.: An atlas of forecasted molecular data 2: vibration frequencies of main-group and transition-metal neutral gas-phase diatomic molecules in the ground state. J. Chem. Inf. Model. **2006**(46), 820–825 (2006)

Hefferlin, R.: Kronecker-product periodic systems of small gas-phase molecules and the search for order in atomic ensembles of any phase. Comb. Chem. High Through. Screen **11**, 690–706 (2008)

Hefferlin, R.: Vibration frequencies using least squares and neural networks for 50 new s and p electron diatomics. J. Quant. Spectr. Radiat. Transf. **111**, 71–77 (2010). doi:10.1016/j.jqsrt.2009.08.004

Hefferlin, R., Burdick, G.W.: Periodic systems of molecules: physical and chemical. Russ. J. Gen. Chem. **64**, 1659–1674 (1994)

Hefferlin, R.: Internuclear separations using least squares and neural networks for 46 new *s* and *p* Electron Diatomics. http://viXra.org/abs/1208.0026

[15] Dr. Charles Janet is recognized in many French books as the author of the left-step periodic table of the elements (2009).

[16] Dr. Baca Mendoza is highly respected in Peru for his version of the periodic table of the elements (Mendoza 1953).

[17] Presumably the Ten Commandments and the periodic table of the elements.

[18] The Bible claims that God spoke to Moses from a burning bush.

[19] It is not clear to whom "He" refers; the capitalization is supplied.

[20] "no longer" may refer to the clearing of the jungle after Machu Picchu was found by an American explorer, after centuries of neglect, in 1904.

Hefferlin, R.: Periodic systems of molecules. Presuppositions, problems, and prospects. In *Philosophy of chemistry*; Baird, D.; Scerri, E.; McIntyre, L., Eds.; Springer: Dordrecht, pp. 221–243. Fig. **7** of the chapter is in error and the correct figure will be sent upon request (2006)

Hefferlin, R., Davis, W.B., Ileto, J.: An atlas of forecasted molecular data 1: internuclear separations of main-group and transition- metal neutral gas-phase diatomic molecules in the ground state. J. Chem. Inf. Comp. Sci. **2003**(43), 622–628 (2003)

Kong, F.-A., Wu, W.Q.: Wu, Periodic tables of diatomic and triatomic molecules. Sci. China Chem. **55**, 618–625 (2012). doi:10.1007/s11426-012-4495-z

Mendoza, O.B.: Genetic Laws of the Chemical Elements. A New Periodic System, Presented at the Fourth Peruvian Congress of Chemistry, Lima. National University of Cusco, Cusco (1953)

Scerri, E.R.: Discusses the uniqueness of atomic identification based on atomic numbers in, "The Dual Sense of the Term "Element," Attempts to Derive the Maderlung Rule, and the Optimal Form of the Periodic Table, If Any. Int. J. Quant. Chem. **109**, 959–971 (2009)

Stewart, P.J.: Charles Janet, Unrecognized Genius of the Periodic System, Foundations of Chemistry, Springer, 2009. Published online 10 January, 2009. 10.1007/s10698-008-9062-5

The third verse is the first two sentences of part VI of Alturas de Macchu Picchu, by Chilean poet Pablo Neruda. http://www.poemas-del-alma.com/alturas-de-macchu.htm. Accessed 20 Nov 2010. http://www.neruda.uchile.cl/obra/obracantogeneral5.htmld. Accessed 21 Nov 2012. The first two verses are from the pen of Julio Guitérrez Samanez, Universidad Nacional de San Antonio Abad del Cusco, Department Académico de Quimica. The combination is named by Julio Guitérrez "The Apocrypha of Pablo Naruda." The loose translation into English is by Ray Hefferlin with corrections by Julio Guitérrez

Wohlers, J., Laing, W.B., Hefferlin, R., Davis, W.B.: Least- squares and Neural-network Forecasting from Critical Data: diatomic Molecular re and Triatomic) Ha and IP, in Carbo-Dorca, R. and P. G. Mezey, Advances in Molecular Similarity, JAI Press, Stamford, CT **1998**, 265–287 (1998)

Zhuvikin, G.V., Hefferlin, R.: Symmetry principles for periodic systems of molecules. In: Joint report #1 of the physics Departments of Southern College, Collegedale, TN, USA and St. Petersburg University, St. Petersburg, Russia, Sept. 11 (1994)

Zhuvikin, G.V., Hefferlin, R.: Periodicheskaya Sistema Dvukhatomnykh Molekul: teoretiko-gruppovoi Podkhod. Vestnik Leningradskovo Universiteta **16**, 10–16 (1983)