

ALL THE WAYS TO HAVE A BOND

The concept of a chemical bond, so essential to chemistry, and with a venerable history, has life, generating controversy and incredible interest. Even if (or maybe because) we can't reduce it to physics. Prof. Hoffmann will discuss some of the common experimental criteria for judging the presence and strength of a bond: length, energy, force constants, magnetism, energy splittings and other spectroscopic criteria. On the theoretical side, he will look at bond orders, population analyses, bond critical points, and electron localization functions. And will give a personal opinion on the utility of the various measures. His advice at the end is likely to be: Push the concept to its limits. Think about any bond in terms of all the various criteria, experimental and theoretical, that we have discussed. Accept that (at the limits) a bond will be a bond by some criteria, maybe not others. Instead of wringing your hands about how terrible it is that this concept cannot be unambiguously defined, have fun with the fuzzy richness of the idea. Try to understand what motivates other people to say there is a bond there or isn't. Always think about what change (chemical perturbation) you can do to probe your ideas.

RETURNING, REMEMBERING, FORGIVING

Roald Hoffmann tells his story, and that of his town, in this account of survival, of the complexity of Ukrainian-Jewish relations, and his return to where he was born in 1937 in a happy Jewish family in Złoczów, Poland, now Zolochiv, Ukraine. Soon the war descended, and the story turns into one of survival (of few, 200 out of 4,000 in Zolochiv) in those terrible times. The personal goodness, amidst much evil, of a Ukrainian family, played an essential role in that survival. After some years of postwar wandering, the story leads to America. The struggle to establish memorials in Zolochiv and surroundings will be told, as well as the role in the war of the Ukrainian Greek Catholic church. The story is a personal one, embedded in the geography and history of the people cohabiting that contested piece of the earth. And ultimately it is a story of the choices for good or evil that people must make in the worst of times.

Simulation vs Understanding: A Tension, and not just in our Profession

Understanding, simulating, knowing, explaining are all ideas that have a common sense feel to them, but are not so simple to define or implement. Certainly, computers, their power and speed have transformed chemistry, and especially theory in chemistry. We can calculate almost anything, simulate/predict most observables (chemical reactivity is tough). But do we understand what we calculate exceedingly well (think of the dipole moment of a water molecule, or its IR spectrum, for instance)? Does the computer understand these? Does the person(s) who wrote the software understand these observables?

In this lecture Prof. Hoffmann will move from the words, and philosophical ideas around them to the practical way in which simulation and quantum chemistry interact with experiment today. He will look in some depth at the example of searching for unknown extended structures; say something about the techniques of quantum chemistry, recent debates on where DFT is heading; and give another example of the difference in studies of metal hydrides under pressure. Then he will discuss simulation with a vengeance – the Harvard Clean Energy project and machine learning. The tension between simulation and understanding is there, of course, not only in chemistry – he will give examples of from economics, commerce, “big data” and machines that beat us at games. No solutions at the end, just a recognition of the problem and a plea to stay human.