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Molecular Air Hockey: Understanding chemical reactions one collision at a time

Q: How do we work out the E/Z isomerism that a molecule shows?

A: There are loads of very good and accessible explanations of this available, so rather than start again from scratch, I'll just direct you to a couple of these on the internet: E-Z notation for geometric isomerism (chemguide.co.uk) and The E-Z system for naming alkenes - Chemistry LibreTexts

Q: How do you create an ultra-high vacuum?

A: First, you need a vacuum chamber which is completely sealed so that air molecules can't leak in. Usually, vacuum chambers and other vacuum components such as flanges ('end caps' or 'lids') and pumps are made mostly of stainless steel, with different components bolted together with either a metal or rubber seal between them. Once you have your sealed system you need to pump all the air out of it. Various types of pump are used for this, with the most common being turbomolecular pumps. These are essentially jet engines, designed to pull air through them very fast. This removes air from the chamber at very high speed, which is then pumped away at a slower speed by another type of pump called a rotary vane pump. Using this type of vacuum system we can easily get down to pressures of around 10^{-8} mbar (1/100,000,000,000 of atmospheric pressure), which is fine for our molecular scattering experiments. With a bit more effort (more careful choice of materials, 'baking' the vacuum system to remove any water or other molecules stuck to the surfaces, plus a few other tricks) it is possible to reach pressures significantly lower than this.

Q: Using the air hockey as a model, the more energy you put in, the more likely the bond breaks, so according to the air hockey table model could you say that if we constantly increase the kinetic energy can this cause the product bonds to break as well?

A: In a way, yes, but since the products don't exist until after the collision, perhaps a better way to think about it is that the products you form will depend on the collision energy. As we saw on the air hockey table, it is easier to form bonds in low-energy collisions, and if the collision energy is too high then the collision partners will often just bounce off each other without 'reacting'. We also found that high-energy collisions were very good at breaking our 'chemical bonds' (modelled by the magnetic attraction between the modified air-hockey pucks), leading to different products from those we saw in the low energy collisions. In a real molecular system, a very high energy collision tends to generate products with a lot of vibrational energy in the bonds. Unless the product molecules can lose this energy (usually through inelastic collisions with other molecules, which formed one of the other air-hockey demonstrations), this often causes the bonds in the product molecules to break, i.e. even though we might initially make one set of products, these are not stable and dissociate to form other (secondary) products.

Q: Does the shape of electron subshells affect reactions?

A: Yes. You are probably most familiar with the s, p, and d orbitals in an atom. When we move from considering atoms to considering molecules we have to think in terms of molecular orbitals rather than atomic orbitals, and because molecules come in many different shapes and sizes, we also have many different shapes and sizes of molecular orbitals. What happens in a chemical reaction is pretty much entirely determined by interactions between the electrons within these molecular orbitals, so the shapes of the orbitals play a huge role in determining the reactivity.

Q: What is the best part of physical chemistry?

A: Physical chemistry is concerned with understanding the 'physics' underlying chemical phenomena, as well as with measuring and quantifying a huge variety of quantities relevant to chemistry. It includes quantum mechanics of atoms and molecules, thermodynamics and statistical mechanics to understand energy flow in chemical systems, the study of chemical reaction rates and mechanisms, spectroscopy to understand molecular energy levels as well as to identify and quantify molecules and other chemical species, and much more. There is a very strong interplay between theory and experiment across virtually all of physical chemistry, with some researchers focusing entirely on theory, some on experiments, and some doing both. You're probably gathering from my answer so far that physical chemistry is a hugely diverse subject, and the 'best' part is going to be quite subjective and different for everyone. I think the best part for me is that there are a huge number of problems that can be solved using knowledge and methods from physical chemistry, so if you have the appropriate training you can go off in any direction that interests you. Within my research group, for example, alongside our work on molecular scattering we also apply mass spectrometry and machine learning methods to a variety of challenges in clinical medicine.