Consider the Electron

In loving imitation of David Foster Wallace's essay "Consider the Lobster"

Leif Sieben Moral philosophy is abound with highly intricate ethical decision problems, however, let us begin here with a very simple one: Go to your kitchen, turn on your stove, wait until it is fully heated and then proceed to put the full, open palm of your hand onto it. As the intelligent chemist that you are, you were unlikely to follow through with these commands[i]. Frankly, this sort of moral paradox is hardly worth its name. We can make this experiment slightly more interesting by not putting our own but rather our friend's hand onto the burning heat. Or if this does not do the trick, the hand of the professor of your least favourite subject might do just as well. Our hearty moral conundrum now reads: "Is it morally acceptable to burn someone's hand?" The answer is left as an exercise to the reader.

Evidently, all of this is rather trivial moral philosophy. We all know that putting your hand onto a hot stove plate is a terrible idea, and by extension it would not be right to force anyone else to do so either. That this appears so trivial to us is however rather unexpected. Granted, it would undoubtedly be *illegal* to burn someone's hand. But as a criterion in moral philosophy this does not fly, and many a law in the past was all but morally sound. Furthermore, we could certainly postulate that because we ourselves would not want to be burnt, we ought not to burn anyone else's hand either. If perhaps not logically waterproof, this general sentiment seems cogent advice in everyday life and has been advocated under the name of the "golden rule" or the "categorical imperative" by people as diverse as the authors of the bible, Immanuel Kant and the Buddha. "Do to others what you want them to do to you" (Mathew 7:12). But what if you were to encounter an entirely alien form of life, which is so fundamentally dissimilar to you that it might plausibly enjoy the feeling of heat?

Is It Immoral to Burn an Alien's Hand?

If we assume no prior knowledge about the alien, its perceptive organs or its neuronal architecture, we seem to be at a loss to find the righteous path of moral justice in this instance. But not so. It might be impossible to derive the morally correct path forward by means of theory alone, but as good chemists we know that where theory ends the experiment begins. We would have the answer to our question very quickly if we were to observe for example that whenever the alien touches the stove, it recoils its hand (or any other analogous bodily protrusion). We may assume that the alien does not express pain in any form, it does not hiss nor make a funny face while touching the stove; nor does it even have any memory of the encounter and it thus keeps on touching the stove. But every time it does so, it reliably withdraws its hand. A type of behaviour not observed when the stove is cold.

With this information at hand (pun intended), it would clearly appear *immoral* to force the alien's hand onto the hot stove plate. It is immoral because we would be acting against the apparent *preference* of the alien. We could induce this preference by the alien's reaction to the stove, i.e. its output to the input: the alien clearly prefers not having its hand burnt over the alternative incendiary option. The term "preference" is garnering increasing popularity among contemporary moral philosophy, and it is typically considered the basic condition that needs to be fulfilled for something to be of moral relevance. It is for example the implicit reason why we have not (so far) looked at the perspective of the stove top in this moral paradox of ours. If the stove has any preferences to speak of, we have (so far) not been able to determine any of them and even if existent, they would probably not be very meaningful to our decision. To play the lingo-bingo of the moral philosopher a little bit longer, systems that have some form of preference are at least considered to be moral *patients*, meaning that when acting upon them, we must consider the impact our decision has on them as potentially non-zero. They may or may not be moral *agents* in addition. We, in deciding to force the alien's hand onto the stove, are the moral agents in this case. The obedient, hopeless alien, on the other hand, is simply a moral patient. Doomed to suffer through our decision, but not having any agency itself over them.

Is Chemistry Fundamentally Immoral?

If we buy into this definition of preference and by extension of moral relevance, the number of moral patients that merit

[i] The author also wishes to explicitly make clear that no liability is assumed in any other case.

our consideration expands considerably beyond most people's scope of ethical interest. Our definition of a moral patient would certainly include any type of organism: any spineless nematode or dragonfly will express some form of preference. But let us note here that clearly not all preferences are relevant to all decisions and that even though many things can have preference, not all preferences are alike. We would certainly not let a person die of freezing in winter because making a fire could plausibly infringe on the moral preferences of the wood.

Indeed, *any* system that is capable of reproducibly expressing some form of output to a given form of input has some putative preference. Not all output can always be interpreted as a preference however: Flies tend to fly higher on days with low air pressure, clearly a reaction to a given input, but this does not convincingly imply that they have a clear preference for one state or the other. As admittedly vague and academic as these types of questions might seem, there are certain moral philosophers which claim exactly this. Information Integration Theory (IIT) posits that "consciousness corresponds to the capacity of the system to integrate information"[ii] and would therefore consider any of these systems as potentially morally relevant.

One needs not to accept these theories to appreciate them for countering some of our inherent biases as moral agents. Humans tend to prefer the local and immediate to the distant and indirect. Very few people would disagree with the statement that "all humans are created equal", but you rarely hear anyone in Switzerland advocate building cancer treatment facilities in Mississippi. Even though, foreign currency exchange rates could make such an investment much more cost-efficient. Humans also tend to attribute the most moral value to those things that seem most similar to ourselves. Not incidentally did the authors of the declaration of "human rights", all of which white men, extend these privileges exclusively to other white men. The definition has been in continuous reworking ever since. But just because the alien is not human does not necessarily mean it does not have moral value. A question that could plausibly become a rather acute one rather soon, with the emergence of an artificial intelligence that is highly capable of information integration and thus expressive of numerous

[ii] See also G. Tononi, 2004, *BMC Neurosc.*, 5, 42. https://bmcneurosci.biomedcentral.com/articles/10.1186/1471-2202-5-42

preferences, some of which potentially not aligned with ours.

Why Bother with the Electron?

Chemists are certainly not infallible moral judges in any case. Alfred Nobel discovered nitroglycerine, which would go on to have such devastating success in warfare that he saw himself forced to fund an obscure science prize with the fortune he earned from his invention so that the after-world would not (only) remember him as the "father of the dynamite". A cunning trick of marketing that worked out stunningly well, we can now safely say. Or Fritz Haber, who invented the Haber-Bosch process that produces the fertilizer our world is fed on but was also the first person to propose the usage of chlorine gas in the First World War. Interestingly, he only lent his name to one of his two inventions.

The theoretical chemist Roald Hoffman once defined chemistry as "the making and breaking of bonds"[iii]. But what is a bond if not some form of (admittedly ill-defined) electron density? If so, should we not consider the possibility that the electron too might *suffer* at our, the chemist's, hands. Even if the electron only has an infinitesimally small moral value – and it appears unlikely that many readers will be inclined to concede it any more than this – the sheer number of bonds in the Universe alone could give us cause for concern. A quick back-of-the-envelope calculation gives us an estimate of about $1.3 \cdot 10^{59}$ hydrogen bonds in the Universe, which make up a good 74 % of the elements in the interstellar medium and thus account for nearly all bonds found in space[iv].

If the making and breaking of bonds is itself an immoral action, this should not only be of concern to us as chemists, given we regularly partake in it in the laboratory, but because Earth is a place of unique density and diversity of bonds unrivalled by large swathes of the Universe. The distribution of chemical complexity is highly heterogeneous in the Cosmos, with some places being essentially devoid of any matter, others exclusively populated by monatomic gases.

[iii] The 2020 Dreyfus Lecture, 05.05.2022, Basel, personal transcript.

[iv] Modelling the Milky Way as a cylinder with a radius of $5 \cdot 10^4$ ly and a height of 10^3 ly, with one ly (lightyear) being $9.46 \cdot 10^{12}$ km. Surprisingly, it is very difficult to quantify how much molecular hydrogen there is in space. For simplicity, we assume that about 20 % hydrogen is in its molecular form, which is inaccurate but gives an estimate of the right order of magnitude, with an average density of $(0.1950 \pm 0.0033)\,\mathrm{cm}^{-3}$, see also P. Swaczyna et al 2020, *Astrophys. J.*, 903 48.

So-called dark clouds can indeed have some larger molecules with up to thirteen atoms[v], including such chemical mavericks as methanol or ethanol, but they are reasonably rare. There are about $1.3 \cdot 10^{50}$ atoms on Earth and it is a more than safe assumption that all of them form at least one bond[vi]. What is more, while the Universe is mostly a place devoid of anything interesting to the chemist (notwithstanding the occasional discovery of a C_{60} molecule shaped like a football), Earth is abound with strange and exceptionally rare molecular structures. In truth, any C−H, C−O and certainly S−O bond is the exception to the cosmological rule and indeed much rarer, and perhaps more stunning so, than we tend to give them credit for.

The Moral Philosophy of Total Synthesis and Other Related Subjects

Let us thus take the unbiased view and perform the same open-minded moral experiment for the electron that we have already done for our alien and the stove top: What is the preference of the electron? Clearly, if we are to position two electrons close to each other, one repels the other. By this simplistic experiment, it would certainly appear that electrons prefer nothing more than *not* to be in each other's immediate vicinity. What could be more cruel, then, than to force them into such chemical bondage, so to speak, as we chemists so regularly do?

Not so quick. In our toy-model of a bond, one electron was simply reacting to the presence of an electric potential induced by another negative point charge. The electron more plausibly just expressed its preference towards minimizing its potential. To put this into more chemical terms still, we can consider this analogous to a system minimizing its chemical potential and therefore trying to find the minimum in its Gibbs free energy[vii]. To state the obvious thing right away: Any bond exists in some local minimum of free energy. But this is a global value considering all combined energies of the bond. Let us restrict ourselves for the moment being however to the perspective of the electron and therefore neglect any other moral patients (such as the nuclei) that could be relevant to this system.

[v] Interestingly, thirteen seems to be the hard limit for chemical complexity beyond Earth. But exceptions apply!

[vi] Certainly if we include ionic bonds in crystal lattices or metallic bonds below the lithosphere. Essentially only free ions and noble gases form no bonds, both species only occur in the atmosphere, which has a comparatively low density of molecules already, and even there they are reasonably rare.

[vii] For further details, see the script to PC I: Thermodynamics.

But if we truly are to consider the electron, such broad values are of little use to us as it is quite conceivable that even though globally the formation of a bond minimizes the potential, the same might not be true of the electron itself. At the very least, we are still putting two negatively charged electrons next to each other. Let us therefore turn to the electronic structure of the simplest molecule: H_2. As we are only interested in the electron anyway, we will formulate the *electronic* Hamiltonian $\hat{H}_{el}$ (we could have just as well invoked the Born-Oppenheimer approximation) given by

$$\hat{H}_{el} = -\hat{h}_1 - \hat{h}_2 + V$$

where $\hat{h}_1 = \hat{h}_2 = \frac{1}{2}\nabla^2 + \frac{1}{|\mathbf{r}+\mathbf{R}_A|} + \frac{1}{|\mathbf{r}+\mathbf{R}_B|}$ with $\mathbf{r}$ referring to the position vector of either electron, where we have made use of the fact that both electrons are identical, and $\mathbf{R}$ referring to the position vector of either nucleus offset by a potential V. We now express the Hamiltonian in the two basis functions $|1s_A\rangle$ and $|1s_B\rangle$ and construct based on these the electronic wave function $|\Psi\rangle$ with some normalization factor c

$$|\Psi\rangle = c\left(|1s_A\rangle|1s_B\rangle + |1s_B\rangle|1s_A\rangle\right).$$

If we now express the Hamiltonian in this wave function $\langle\Psi|\hat{H}|\Psi\rangle$ we can distinguish four distinct contributions to the total energy

$$\begin{aligned} h_{1,2} &\equiv \langle 1s_A|\hat{h}_1|1s_A\rangle = \langle 1s_B|\hat{h}_1|1s_B\rangle \\ h_{A,B} &= \langle 1s_A|\hat{h}_1|1s_B\rangle = \langle 1s_B|\hat{h}_1|1s_A\rangle \\ K &= \langle 1s_A|\langle 1s_B|V|1s_B\rangle|1s_A\rangle \\ &= \langle 1s_B|\langle 1s_A|V|1s_A\rangle|1s_B\rangle \\ J &= \langle 1s_A|\langle 1s_B|V|1s_A\rangle|1s_B\rangle \\ &= \langle 1s_B|\langle 1s_A|V|1s_B\rangle|1s_A\rangle. \end{aligned}$$

Without solving any of these expressions explicitly, it is known that both terms that arise from the potential J, the Coulomb integral, as well as K, the exchange integral, are greater than zero. In other words, based on these terms alone, the bond would actually be energetically disfavoured. Furthermore, the resonance integral $\hat{h}_{A,B}$ is relatively small in our case[viii]. More relevant to our discussion however is the term $\hat{h}_{1,2}$, which corresponds to the average one electron energy. The surprising finding of this somewhat lengthy exercise is that it is only a slight overstatement to claim that the bond *exclusively* exists because of the energetic preference

[viii] For a good overview and further background concerning the nomenclature, see the script to OC IV: Physical Organic Chemistry.

of the electron. It appears indeed that we chemists have been absolved of our moral conundrum by the virtues of quantum mechanics.

A cogent critique of all of this is to point out that considering the bond as the primary question of moral concern in chemistry means missing the point. It is clear that most bonds in the Universe and even most bonds on Earth are *not* created nor destroyed by humans. Even though the argument that something is morally sound simply "because it has always been this way" is hardly convincing, this is not a point easily dismissed. Even worse, we have so far only considered half of the chemist's business: *making* bonds might be a good thing; *breaking* them however would seem much less appealing now. So long as we break these bonds in order to replace them with stronger (or at least more plentiful) bonds, however, we should be fine. If anything, our moral analysis could read as the philosophical imperative for the chemist to do total synthesis rather than elemental analysis.

Advice for the Moral Chemist

Yet this too might be our own biases speaking. If we were to truly take the long-view here, we know with certainty that the entropy of the Universe will be maximized by the second law of thermodynamics, in which no complex matter will exist, and all bond energies will have been converted to stray radiation permeating the ever-increasing nothingness of space[ix]. On that timescale, we are but a negligible, local dip in the relentless march towards maximal entropy. Of course, Earth is no exception to this rule. All the chemical complexity we experience does not violate the second law, it is simply that Earth as a system has its relatively low entropy compensated (mostly) by the continuous electromagnetic radiation of the sun. In the end, the bond too is only transient.

But perhaps in the end, thermodynamics, on the flip side, is our safest escape still: One possible maxim for the moral chemist could be to consider the ultimate preference of the Universe and by extension of all of its constituent elements, to be that of maximizing entropy. The second law of thermodynamics might plausibly serve as the "categorical imperative" of moral chemistry. Yet if we accept this, by our very own metric, we would be truly hopeless cases as chemists in terms of being moral inhabitants of the Cosmos. Not least, because we ourselves are ultimately nothing but a local density of electrons.

[ix] Again, the interested reader may be referred to the script to PC I: Thermodynamics.

There is certainly much left to expand this argument with, and many points of criticism could not be addressed here (only some of them due to constraints of space). Any such point will certainly be gladly taken up by the chemist, who wishes to do the right thing, but is unlikely to have ceased all laboratory practices based on some fuzzy ethics theory. At the very least, these vague speculations may serve as a useful reminder to us that none of our actions are ever devoid of moral implications and that, in any case, we ought to proceed with caution. If nothing else, our potential immorality as synthetic scientists should give us further cause to ensure that at least *what* we synthesize is in service of the highest moral goals.