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Rearrangements in the multiverse

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A brief and personal history of the binding interactions between Hans-Beat Bürgi and Roald Hoffmann is given, and a potential rearrangement of their molecules is considered.

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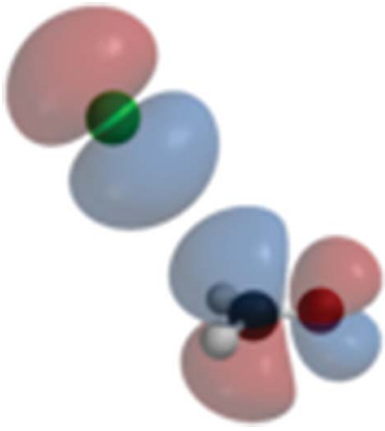
There is a parallel universe in which Hans-Beat Bürgi and I sort of trade places – he is at Cornell and I am in Switzerland.

I will eventually tell you why such a rearrangement, an alternative cosmos, is less improbable than you might think. But first about how Hans-Beat and I met. I spent the fall of 1971 at the ETH Zürich. At the time, the ETH was home to arguably the prime organic chemistry department in the world. People gravitated there quite naturally, so I came, as did Lionel Salem, an outstanding French theoretical chemist and friend. Space was at a premium in the old building of the ETH; Salem, I and a young *Oberassistent*, just back from a postdoc in the USA, Hans-Beat Bürgi, shared a not-too-large office. As you can imagine, we got to know each other very well. Can you guess who was the loudest, who the quietest, of the trio?

Later, the three of us continued in our own way to develop the ways that molecules transformed in the course of chemical reactions. We had different strengths, but I think it is fair to say that the strong coupling of molecular orbitals with the propensity of molecules to distort or react – measured by force constants of one or another kind, and by reaction paths – was a leitmotif in what we have done since.

The people we encounter in life shape our world – there is a resonant phrase in Hebrew, *avinu moreinu*, our fathers, our teachers, that summarizes the guidance we receive. In structural chemistry, Lipscomb, Dunitz and Bürgi were my teachers – not a bad cohort. They shared a love for real molecules. This student of theirs, a 'voracious consumer of crystal structures', still recalls with pleasure, 49 years after his first encounter with the work, the paper by Bürgi, Dunitz and Shefter in which they plot on one two-dimensional graph the essential features of the crystal structures of six quite diverse molecules containing an amine functionality interacting with a carbonyl group (Bürgi *et al.*, 1973). The rationale – the 'frontier-orbital guided' reaction path of a lone-pair interacting with a CO π^* – was not lost on the authors. Nor on any chemist who saw this paper. Static structure tracing a dynamic reaction path! One that made eminent theoretical sense! In a stunning piece of work, Hans-Beat Bürgi and his crew forged a link between crystallography and reactivity.



But back to the multiverse. One reason why I was in Zürich in 1971 (and met H.-B.) was that I was considering a couple of years earlier an offer of a professorship at ETHZ. I turned it down in the end, even as it was one of the two positions I

considered seriously in my life. And in the mid-seventies, Hans-Beat was looking for a job. He came to Cornell, wowed my colleagues, and we promptly offered him a position. Which he declined, with agony in his decision.

So . . . the parallel universe in which Hans-Beat and I trade countries, is not that outlandish, even as it remains in the realm of what might have been. What I am sure about is that we would have known and valued each other in both worlds. As we do now. And this is all that matters.

References

Bürgi, H. B., Dunitz, J. D. & Shefter, E. (1973). *J. Am. Chem. Soc.* **95**, 5065–5067.