The unusual crystal structure of an accident

Accidental discoveries can be among the most fascinating ones in science. It was due to an accident (not to say: negligence) that Scotsman Alexander Fleming discovered in 1928 the antibacterial action of penicillin. Mitchell Feigenbaum, who was about to be fired from Los Alamos National Laboratory due to a lack of results, had been wearily pressing the enter button of his pc trying to find the solution to one equation, when he accidentally discovered a novel universal mathematical constant; today it is called the Feigenbaum constant, and used for the description of bifurcations and chaos. And thanks to a trivial mistake of Prof. Hideki Shirakawa’s student in the 1970’s a conducting form of polyacetylene (the prototype for all organic conducting polymers) was discovered. Later, a Nobel prize was granted for the discovery. The role of human error and coincidence in science cannot be overemphasised, and several books have been devoted to this topic. The room for mistakes in chemical synthesis is especially large, and when they occur can may have funny effects on the reaction product; many different novel chemical compounds can be formed even if only a few different types of atom are present in the reaction system.

Also by accident, an interesting discovery was made in the teams of Prof. Wojciech Grochala and Dr. Michał K. Cyrański at the University of Warsaw. The scientists had been analysing the chemical properties of a peroxydisulphate complex of silver(II) with pyrazine, a small organic molecule capable of binding to metal cations via its two nitrogen atoms (upper figure). The researchers were interested in whether they could modify the magnetic properties of this compound using various chemicals. While they did not fulfil their goal, the systematic investigations of Dr. Piotr J. Leszczyński resulted in new chemical complexes forming when the substrate reacted slowly with moisture. One of these had a very complex chemical formula, \([\text{Ag(II)}(\text{pyrazine})]_3(\text{HSO}_4)_2(\text{H}_2\text{O})_2\) (left). Its crystal structure, solved by Dr. Łukasz Dobrzycki, is amazing; it is an intergrowth of layers (just like a hamburger with slices of bread, meat and salad) containing pairs and triplets of Ag(I)(pyrazine) cations with counterions. Some of these counterions are ‘common’ hydrogen sulphate anions, \(\text{HSO}_4^-\), but some are very rare \(\text{H}(_2\text{SO}_4)_{2-3}\) anions containing so called symmetric hydrogen bonds. Thanks to its unusual structural features, the product of this accidental chemical reaction has proven more interesting than that originally targeted.

The communication “Thermal and chemical decomposition of di(pyrazine)silver(II) peroxydisulfate and unusual crystal structure of a Ag(I) by-product” will be published in Dalton Transactions, and featured on the issue’s front cover.