Roentgenium generation

Taye Demissie relates unununium's unusually smooth route to roentgenium, and how predicting its properties relies on relativistic calculations.

The heaviest elements of the periodic table do not occur naturally, they are created in nuclear fusion reactions that are either carefully carried out in a few laboratories around the world or take place in thermonuclear reactions — einsteinium and fermium, for example, were first found in the radioactive debris of weapon tests before being made in high-flux neutron reactors. Among these superheavy-element-hunting laboratories is the GSI Helmholtz Centre for Heavy Ion Research (GSI) near Darmstadt, Germany, where element 111 was first synthesized in December 1994[1]. Officially, it went for a decade by its temporary name 'unununium' (for 1-1-1-ium), according to the naming system of the International Union of Pure and Applied Chemistry (IUPAC). In reality, along with the other superheavy elements, it was more commonly referred to by its atomic number.

The GSI team led by Sigurd Hofmann bombarded a target of ^{209}Bi with a beam of ^{64}Ni nuclei and successfully detected three ^{272}111 nuclei. Another element-hunting team at the Joint Institute for Nuclear Research in Dubna, Russia, had previously attempted to generate the element in 1986 — using the same reaction — but no data supporting the formation of 111 had been gathered. In 2002, the GSI team observed the detection of another three ^{272}111 nuclei[2]. Taken together, the six decay chains, among which three proceeded through the known nuclei ^{260}Db and ^{256}Lr, represented strong enough evidence for the IUPAC and IUPAP (International Union of Pure and Applied Physics) Joint Working Party (JWP) to attribute the priority of discovery of element 111 to the GSI team. Independent confirmation came from researchers at the RIKEN linear accelerator facility in Japan, who reported fourteen decay chains of the ^{272}111 isotope[3].

In contrast to the intense debate that some of the other superheavy elements were the subject of (so intense that the period was referred to as the 'transfermium wars'), the recognition and naming process was straightforward for element 111. Keeping with tradition, the discoverers proposed a name and symbol that were swiftly accepted, and in 2004 unununium became roentgenium[4] in honour of the German physicist Wilhelm Röntgen, who discovered the X-rays (the first X-ray image, of his wife's hand, is pictured). Just over a century before that, this finding had already earned Röntgen the first ever Nobel Prize in Physics in 1901.

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Roentgenium is extremely radioactive. All of its isotopes are very unstable, with half-lives ranging from a mere few minutes to milliseconds, and decay by α-emission or spontaneous fission. In the unlikely event that roentgenium could be observed, it is predicted to look silvery and be even denser than osmium, the densest known element (with densities of 28.7 versus 22.6 g cm^{-3}, respectively).

Artificial, extremely unstable transactinides do not lend themselves well to experimental chemistry. Scientists, undeterred, have developed sophisticated specialized technology for careful single-atom investigations, but it has not yet been possible to probe roentgenium. Element 111 has been explored instead using quantum-mechanical methods: the relativistic Dirac equation, instead of its non-relativistic Schrödinger counterpart, provides an exciting route to predict the chemical properties of the superheavies.

Towards the bottom of the periodic table, as nuclei become bigger and more highly charged, electrons approach relativistic speeds, making the atoms behave differently than what would otherwise be expected. Relativistic effects are known to be important already for understanding the electronic structure — and, in turn, the properties — of gold, roentgenium's above neighbour in group 11; they are crucial for superheavy elements.

The aqueous chemistry of Rg(I) was probed alongside that of the other group 11 ions: Au(I), Ag(I) and Cu(I). Using density functional theory, the formation of monoamine complexes from aquo ions was studied in the gas phase, and extrapolated to aqueous solutions[5]; Rg(I) was predicted to be a strong Lewis acid, even softer than Au(I). Its halide, cyanide and isocyanide species are among those investigated[6–8]. RgCN is predicted to feature a shorter bond than that of AuCN, with a covalent character that arises from the relativistic stabilization of the 7*s* orbital.

Although roentgenium has not yet been probed experimentally — and this may become possible if some of the less unstable isotopes can be generated directly — it is proving to be good playground for exploring relativistic effects. ❐

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