Solving a subatomic shell game: Physicists decode hidden properties of the rare Earths

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Physicists at Michigan Technological University have filled in some longtime blank spaces on the periodic table, calculating electron affinities of the lanthanides, a series of 15 elements known as rare earths.

"Electron affinity" is the amount of energy required to detach an electron from an anion, or negative ion (an atom with an extra electron orbiting around its nucleus). Elements with low electron affinities (like iron) give up that extra electron easily. Elements with high electron affinities (like chlorine) do not.

"I remember learning about electron affinities in 10th grade chemistry," said Research Associate Steven O'Malley. "When I began working as a grad student in atomic physics, I was surprised to learn that many of them were still unknown."

Among them were the lanthanides, which are used in the production of lasers and sunglasses. In terms of their atomic structure, lanthanides are among the most complex elements on the periodic table, which is why no one had been able to calculate their electron affinities before.

Here's what makes them so tricky. Electrons orbit in shells around an atom's nucleus, something like the layers of an onion, but in stranger shapes. Within each shell are a number of subshells. A subshell is like an egg carton: it can hold from one to a certain number of electrons, but no more.

Typically, as you work your way down and across the periodic table to larger and larger atoms, the inner shells fill up with electrons, and then new shells and subshells are formed and fill up pretty neatly.

That's not what happens with the lanthanides. Before their so-called 4f subshell fills up, the additional electrons begin making new shells. Then, gradually, as you move across the periodic table to heavier atoms in the lanthanide series, that 4f subshell finally fills up with its maximum number of 14 electrons.

Why would this matter for electron affinity? A number of forces hold electrons in their orbits around the atom's nucleus. Two simple ones are electrons' attraction to protons in the nucleus and repulsion away from their fellow orbiting electrons, what physics professor Don Beck calls "the B.O. effect."

The forces exerted by a full shell on the electrons orbiting farther from the nucleus are pretty constant, which had made it relatively easy to calculate the electron affinities of most elements. But if there are vacancies in the shell—as there are in the lanthanides—the electrons in that shell can move around, playing musical chairs, as it were.

The forces an electron exerts from each spot in the shell are different. And, in addition to simple electrical factors, there are many complex variables to contend with at the subatomic level, including relativistic and many-body effects.

"It's a nightmare," says Beck. With several electrons bouncing around in those 14 slots, over 200 different arrangements of electrons of the 4f subshell are possible in some of the lanthanides.

In 1994, the Beck research group, supported by the National Science Foundation, began work on one of the simpler lanthanide atoms, cerium.

Then they started to approach the "nightmare" middle of the lanthanide row from both ends, one anion at a time. The most difficult was neodymium (Nd-) which took about six months.

In 2007, O'Malley and Beck began a final push to complete the remaining lanthanides (promethium through erbium) by

1. narrowing down which variables to include in the calculations; and
2. writing scripts and computer codes to automate much of the calculation.

Ultimately, they cut the overall work time by about 85 percent. In just 18 months, they found electron affinities for all the lanthanides, including electron affinities for high-energy, excited states of the anions. All in all, they discovered 118 lanthanide anion states, 63 of which were new.

What's next? The team's theoretical results have already been partially verified by experimentalists, but they are still working to better understand the lanthanides theoretically, to help identify just what is being measured experimentally.

In the meantime, they are turning their attention to the next row in the periodic table.

"We expect to have electron affinities for a portion of the actinides—actinum through plutonium—available sometime this summer," Beck said.

More information: For more in-depth information, visit www.phy.mtu.edu/~donald/ri.html#lea .

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