

Inner electrons behave differently in aromatic hydrocarbons

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In an international research collaboration between Tsinghua University in Beijing and Sorbonne University in Paris, scientists found that four hydrocarbon molecules, known for their internal ring structure, have a lower threshold for the release of excess energy than molecules without a similar ring structure, because one of their electrons decays from a higher to a lower energy level, a phenomenon called the Auger effect.

When an electron from one of the lower energy levels in an atom is knocked out of the atom by a collision with another electron, it creates a space into which one of the higher-energy electrons can fall, also releasing excess energy. This energy is released in an electron called an Auger electron—and produces an effect known as Auger decay. Now, Guoke Zhao from Tsinghua University in Beijing, China and colleagues at Sorbonne University in Paris, France have studied the Auger effect in four hydrocarbon molecules, including benzene, cyclohexane, and larger hydrocarbons. All of the molecules studied were aromatic, i.e., contained benzene rings with pi bonds, in which atoms that are next to each other share electrons. They found that molecules containing a benzene ring have a lower threshold for Auger decay. Applications include a treatment called Auger therapy, which is used to help cancer patients.

Auger decay often involves atoms being subjected to high-energy X-rays, and can be used to study the identity of atoms within a substance. But the Auger effect has yet to be thoroughly studied in certain molecules that are important in <u>everyday life</u>, particularly hydrocarbons.



In this study, the researchers studied the Auger spectra of molecules using computational models. They found that molecules with pi electrons have a lower threshold before Auger decay occurs than molecules without them. The authors hope their work will encourage further theoretical and experimental investigations in this direction.

More information: Guoke Zhao et al, Inner-valence Auger decay in hydrocarbon molecules, *The European Physical Journal D* (2019). DOI: 10.1140/epjd/e2019-90529-x

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