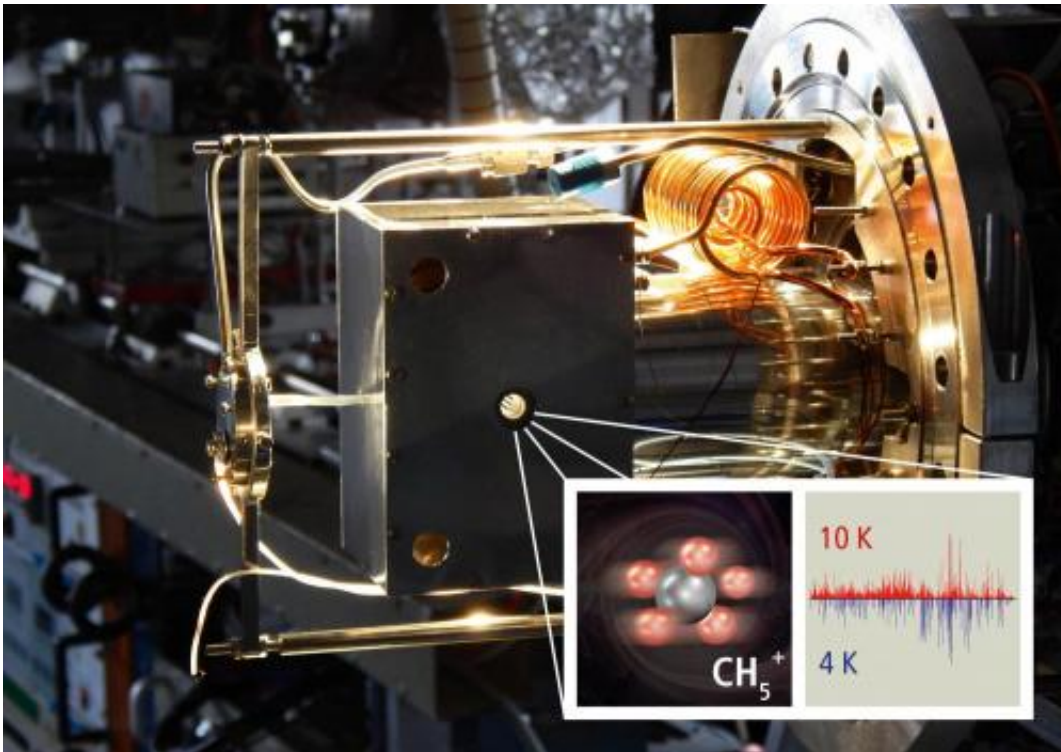


# The taming of the shrew: Scientists decipher the spectrum of CH<sub>5</sub><sup>+</sup> for the first time

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The CH<sub>5</sub><sup>+</sup> molecular ions were investigated in an ion trap setup such as this. The trap itself is the illuminated cylindrical cavity in the middle of the photo, in which some trap electrodes can be seen. In this trap, several thousand CH<sub>5</sub><sup>+</sup> ions were stored, cooled, and investigated by a laser. The obtained high-resolution spectra are shown in the inset, as well as a sketch of the CH<sub>5</sub><sup>+</sup> molecule in motion. Credit: Debora Schiffer/Oskar Asvany, University of Cologne

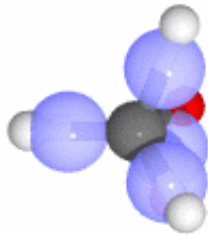
For the first time ever, a team of scientist from the University of Cologne headed by Professor Stephan Schlemmer succeeded in understanding the spectrum of the highly fluxional molecule  $\text{CH}_5^+$ . This insight, gained in collaboration with a Japanese colleague, was made possible by the extreme cooling of this enigmatic molecule and a highly accurate measurement of its vibrational transitions. The results will be presented on March 20, 2015 in *Science* magazine.

$\text{CH}_5^+$ , formed by adding a proton ( $\text{H}^+$ ) to the well-known methane ( $\text{CH}_4$ ) molecule, is the prototype of fluxional molecules. In contrast to common molecules, which are depicted as a rigid structure consisting of balls (atoms) and sticks (chemical bonds), the five [hydrogen nuclei](#) in  $\text{CH}_5^+$  can move quite freely around the [carbon nucleus](#). It is thus constantly in motion, even at an extremely low temperature. Bonds are broken and reformed all the time, and therefore the simple model of balls and sticks does not apply. There has thus been a long debate whether  $\text{CH}_5^+$  has a structure at all.

This extraordinary fluxional behavior is reflected in the spectra of  $\text{CH}_5^+$ . Usually such spectra are recorded in the lab to characterize and identify molecules. With the help of suitable [theoretical models](#), the vibrational spectra can yield information about bond strengths and molecular structure. For  $\text{CH}_5^+$ , however, the hitherto known spectra have been so chaotic that not a single of the many hundred vibrational transitions could be understood or assigned. This has been considered one of the last mysteries of molecular physics.

By developing and applying new ion trap experiments, physicists from the University of Cologne have now succeeded in storing a pure sample of  $\text{CH}_5^+$  ions and cooling it down to a temperature close to absolute zero. With the help of a so-called frequency comb, the vibrational transitions could be measured with high accuracy, leading to a reconstruction of the lowest energy levels. This very technical approach

was necessary due to the complete lack of theoretical models for this exceptional molecule. The results are thus based only on the experimental data and the fundamental principle of quantum mechanics, according to which the observed vibrational transitions are based on a scheme of discrete energy levels.



This animation illustrates the extreme fluxionality of the  $\text{CH}_5^+$  molecule. The black ball in the middle is the carbon nucleus, and the red and white balls are hydrogen nuclei. The blue clouds symbolize the binding electron pairs. Credit: Dominik Marx, Ruhr-Universität Bochum

Surprisingly, the results are in accordance with the simple notion that the five hydrogen nuclei can move quite freely around the central carbon nucleus, with their distance to it being more or less fixed. Whether this simple picture is valid will have to be tested in further investigations. In any case, the highly accurate data will challenge future theoretical models to interpret the discovered [energy levels](#). The entire class of fluxional molecules will profit from these developments.

**More information:** Taming  $\text{CH}_5^+$ , the "enfant terrible" of chemical structures, *Science*, [www.sciencemag.org/lookup/doi/...](http://www.sciencemag.org/lookup/doi/...)

[1126/science.aaa6935](https://phys.org/news/2015-03-shrew-scientists-decipher-spectrum-ch5.html)

Provided by University of Cologne

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