Trapping and excitation of the simplest molecule: Precise measurement matches theoretical predictions

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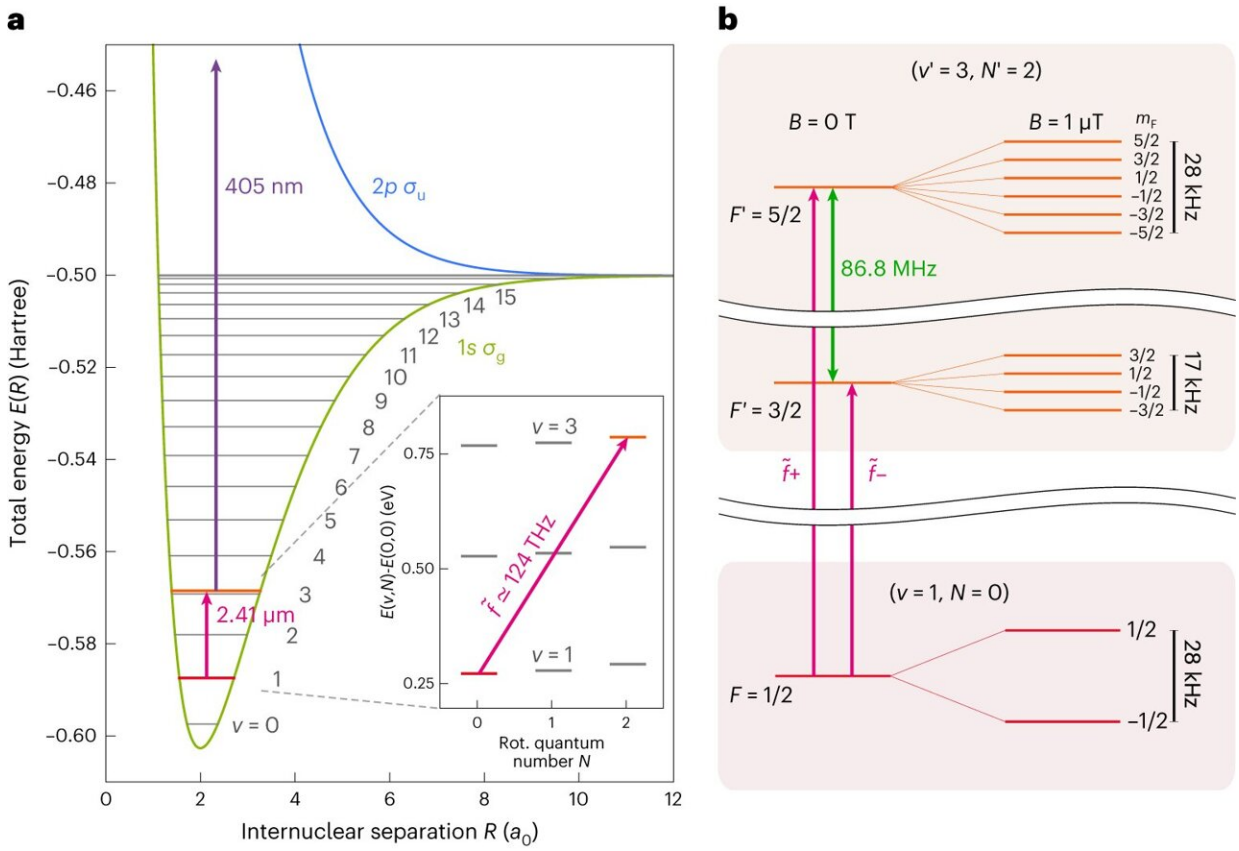

Energy levels of H_2^+ and transitions relevant to this work. **a**, H_2^+ molecular energy as a function of proton separation R in units of the Bohr radius a_0 for the two energetically lowest electronic states $1s\ \sigma_g$ and $2p\ \sigma_u$. The inset shows the first three rotational (Rot.) levels of the vibrational states. b, Hyperfine and Zeeman structure of the two rovibrational levels pertinent to the present study. Credit: *Nature Physics* (2024). DOI: 10.1038/s41567-023-02320-z

The simplest possible molecule H_2^+ was one of the very first molecules to form in the cosmos. This makes it significant for astrophysics, but also an important object of research for fundamental physics. However, it is difficult to study in experiments.

A team of physicists from Heinrich Heine University Düsseldorf (HHU) has now succeeded in measuring the vibrations of the molecule with a laser for the first time. The result matches the theoretical prediction very closely, according to a study published in *Nature Physics*.

H_2^+ was one of the first molecules to form after the Big Bang. It consists of the most fundamental components that were formed very early on in the universe: two hydrogen nuclei (the protons) and one electron. The electron binds the two protons together to form the molecule. In the interplay of particle movements and forces, the two protons vibrate and rotate.

Despite its relative simplicity, H_2^+ has remained relatively unexplored to date. Due to the charge and mass symmetry of the two atomic nuclei, the molecule absorbs and emits almost no visible and infrared radiation. Accordingly, it is almost impossible to observe it with telescopes, meaning that it is extremely difficult for astronomers to find H_2^+ in the universe and study it.

The different vibrational and rotational states of the molecule correspond to specific excitation energies. When a molecule transitions between two such states, it absorbs or emits a characteristic amount of energy, a photon. This is a quantum of electromagnetic radiation with a specific frequency. Previous laboratory experiments have mostly measured these quanta of H_2^+ indirectly and none of them have used lasers.

Postdoc Dr. Soroosh Alighanbari, doctoral student Magnus Schenkel and Professor Stephan Schiller Ph.D. from the Institute for Experimental Physics at HHU have now taken the first direct look at how the H_2^+ molecule can be made to rotate and vibrate using laser light.

Schenkel developed a unique laser system that proved effective in exciting a transition between two vibrational states. The laser system is particularly complex because it requires monochromatic laser radiation, i.e., having a very specific frequency, in the infrared spectrum at a wavelength of 2.4 micrometers, and high power.

The aim of the physicists in Düsseldorf was to measure the frequency of the required radiation quanta as precisely as possible and they achieved an unprecedented level of accuracy in their experiments. Their measurements, which they describe in detail in *Nature Physics*, revealed a frequency value that matched the theoretical predictions. The key aspect here was that the physicists confined the molecules to be examined in a trap in which a further laser cooled them to a temperature close to absolute zero.

Comparing the precise measurement of the rotational and vibrational energies of H_2^+ with their theoretical calculation also has a more fundamental area of application: It enables testing of the fundamental laws of physics that govern the interaction between particles, since these laws form the basis for the theoretical calculation of the energies.

In addition, the energies of H_2^+ depend on fundamental constants of physics such as the proton-electron mass ratio. Careful measurement of the energies therefore allows the determination of the physical constants. Schiller and his team have now succeeded in achieving this using laser spectroscopy. The mass ratio was determined with a relative uncertainty of 3×10^{-8}. That is not as accurate as with alternative methods, but this measurement is just the first step.

In the future, the physicists are aiming to improve their measurement results further. Dr. Alighanbari, one of the authors of the study, states, "We tested the potential of our approach with a 'cousin' of H_2^+—the molecule HD^+—which allowed us to proceed much more quickly."

In HD^+, a proton is replaced by a deuteron, which makes the molecule more accessible in spectroscopic terms. Alighanbari says, "We can actually make even more precise measurements using our apparatus, motivating us to try again with H_2^+ in the near future."

The possibility of performing ultra-precise spectroscopy of vibrational transitions in H_2^+ also opens up the more far-reaching perspective of exploring new frontiers in physics.

Schiller states, "Our current result is the very first step towards a precise comparison of the behavior of matter and antimatter: We would use spectroscopy of H_2^+ and its antimatter counterpart to seek extremely small differences that may exist in their vibration energies. Such measurements may be significant for our understanding of why our universe is full of matter, yet barely contains any antimatter."

Why is spectroscopy of H_2^+ so difficult? The difference between HD^+ and H_2^+ is that HD^+ has an electric dipole moment, which H_2^+ lacks. That is why the team made use of the molecule's electric quadrupole moment. However, their transition rate is substantially lower compared with electric dipole moments. The physicists solved this issue by using a high-performance laser.

More information: M. R. Schenkel et al, Laser spectroscopy of a rovibrational transition in the molecular hydrogen ion H_2^+, *Nature Physics* (2024). DOI: 10.1038/s41567-023-02320-z

Provided by Heinrich-Heine University Duesseldorf