

Pressing the simplest element to exotic quantum states

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The hydrogens—hydrogen and its isotopes—are the simplest and most abundant of the elements in the universe. Conceptually hydrogen, with a single proton and electron is the simplest atomic system in the periodic



table of the elements, yet has exceptionally complex behavior due to its light mass and interactions with other hydrogen atoms.

As a neutral electron spin-polarized gas, it does not form a liquid in the $T \rightarrow 0$ K limit; unpolarized it readily forms stable molecules that solidify at ~14 K. When pressurized to millions of bars it is predicted to dissociate to an atomic metal, predicted to have exotic properties such as high-temperature superconductivity, metastability, and a liquid state at megabar pressures in the low temperature limit. Understanding these quantum effects and establishing the phase diagram of the various isotopes of molecular hydrogen has been an intriguing scientific challenge for decades. Harvard physicists have taken yet another step toward a more complete understanding of the hydrogens.

In the latest issue of *Physical Review Letters*, Professor Isaac Silvera and research scholars, Dr. Ranga Dias and Dr. Ori Noked study hydrogen deuteride and report the discovery of two novel quantum phase transitions that significantly depart from the behavior of pure hydrogen or deuterium and provide a clear demonstration of how the dissociation process may proceed.





Phase diagram of hydrogen deuteride

Recent theories have predicted that at megabar pressures the solid hydrogen transforms to a structure with graphene-like planes and as a precursor to the metallic phase the molecules can dissociate and the nucleons recombine. Unfortunately if this process occurs for hydrogen or deuterium the final state is again hydrogen or deuterium so there is no evidence of the process.

The Harvard researchers have squeezed HD to very high pressures using



a diamond anvil cell and studied the infrared spectrum of the sample to 3.4 megabars, which is the highest pressure to which this molecule has ever been compressed (the pressure at the center of planet Earth is about 3.6 megabars).

The HD sample was stable with behavior similar to that of H2 or D2 to 2 megabars. At this pressure the HD sample underwent a transition to a new phase named HD-IV*. In this phase the new process takes place to form H2 and D2 (2HD \leftrightarrow H2 D2); the newly formed molecules are identified by their IR spectra. The nucleon exchange is due to a process in which the HD molecules dissociate followed by rapid recombination, called DISREC.

This reveals the processes that were predicted to take place in the pure species. At still higher pressures and low temperatures, HD-IV* transforms to still another new phase, named HD-PRE.

In contrast to pure isotopic systems, H2 and D2, the new pressure/temperature <u>phase</u> lines are almost vertical and appear to intersect the T=0 K axis. DISREC confirms a phenomenon that has only been observed in theoretical simulations and cannot be observed in either H2 or D2. None of the newly observed phases are metallic.

Low density HD is also of special astronomical interest with the recent detection of HD in interstellar clouds. Deuterium is believed to have been created primordially in the Big Bang nucleo-synthesis. Determination of the deuterium abundance, relative to hydrogen in the atmospheres of planetary systems and nebulae provides important cosmological constraints on planetary and stellar formation.

More information: "Hydrogen Deuteride: New Phases and unexpected behavior when pressed to 3.4 million atmospheres," *PRL* 116, 145501 (2016).



Provided by Harvard University

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