Chemists discover new type of molecular bond near white dwarf stars

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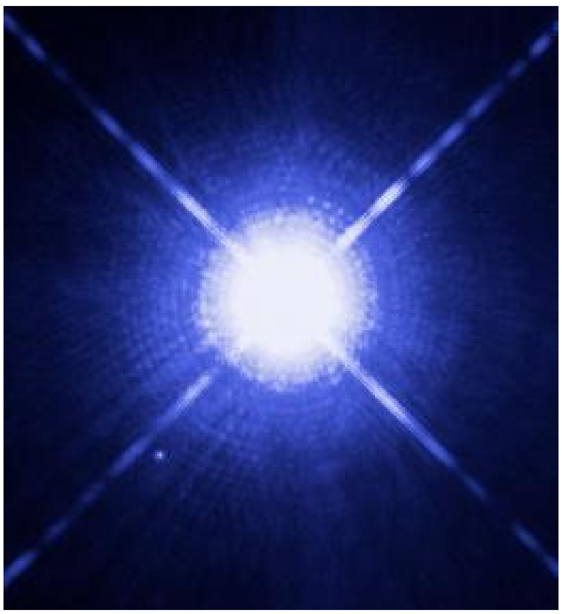

Image of Sirius A and Sirius B taken by the Hubble Space Telescope. Sirius B, which is a white dwarf, can be seen as a faint pinprick of light to the lower left of the much brighter Sirius A. Image: NASA, ESA

(Phys.org) -- Most any chemistry student when asked, will say that there are just two ways atoms bond to make molecules: covalent and ionic. In the former, atoms are bonded together by sharing electrons, in the latter it's due to the transfer of electrons from one atom to another leading to a Coulombic attraction between the ions. Now however, it appears there is a third kind of bond, though it doesn't exist here on Earth. E. I. Tellgren, Kai K. Lange, T. Helgaker and M. R. Hoffmann from the University of

Oslo, Norway and the University of North Dakota in the US have found that some molecules can form and hold together due to extremely high magnetic fields. As they write in their paper published in the journal *Science*, their calculations suggest that such molecules likely exist near white dwarf stars.

Because it's impossible, at least at this time, to create a magnetic field anywhere near as strong as that found near a white dwarf star, the researchers turned to quantum chemical simulations (full configuration-interaction) focusing on hydrogen atoms and the simple hydrogen molecule H_2. At extremely hot temperatures, such as would exist near a white dwarf, the covalent bond that normally holds the molecule together wouldn't survive and the molecule would come apart. But if there were a strong enough magnetic field (such as exists near a white dwarf) the spin states of the two atoms could align with the magnetic field (rather than exist as opposed) the molecule could bond and continue to stay that way. And that's exactly what the team's calculations showed, they're calling it - perpendicular paramagnetic bonding.

To further test their ideas, the team also ran helium through the simulations and found that they too could form perpendicular paramagnetic bonding of He_2 molecules, though they were less stable.

The researchers note that because of the different characteristics of hydrogen or helium molecules bonded together through magnetic forces near white dwarf stars, their spectrum should be different as well, which means that they should be detectable using telescopes tuned properly, assuming they exist in sufficient numbers.

And just because such a strong magnetic field cannot currently be created in the lab, it doesn't mean it can't ever happen. If it does become possible, not only would magnetically bonded molecules be observable, but they might also be controllable by adjusting the amount of magnetism, paving the way perhaps to a quantum memory computer.

More information: A Paramagnetic Bonding Mechanism for Diatomics in Strong Magnetic Fields, *Science* 20 July 2012: Vol. 337 no. 6092 pp. 327-331. DOI: 10.1126/science.1219703

ABSTRACT
Elementary chemistry distinguishes two kinds of strong bonds between atoms in molecules: the covalent bond, where bonding arises from valence electron pairs shared between neighboring atoms, and the ionic bond, where transfer of electrons from one atom to another leads to Coulombic attraction between the resulting ions. We present a third, distinct bonding mechanism: perpendicular paramagnetic bonding, generated by the stabilization of antibonding orbitals in their perpendicular orientation relative to an external magnetic field. In strong fields such as those present in the atmospheres of white dwarfs (on the order of 105 teslas) and other stellar objects, our calculations suggest that this mechanism underlies the strong bonding of H2 in the triplet state and of He2 in the singlet state, as well as their preferred perpendicular orientation in the external field.