Shedding light on an interstellar gas: Researchers derive theoretical spectrum of H2-CO

June 15 2012, by Bob Yirka

(Phys.org) -- One of the more frustrating problems in studying space and the universe is the fact that it's made up of mostly hydrogen molecules that in the cold confines of space, are impossible to see. Perhaps even more frustrating is that researchers have known for some time that if they could get a handle on H2-CO molecules, they could very well get a better idea of how hydrogen molecules are organized because they come about when the two elementary molecules interact. Unfortunately, because the spin or rotation existent in such molecules is greater than the vibration produced by its components, the spectral images produced have been very nearly impossible to decipher. Now however, a team of researchers has figured out a way to interpret such images using sophisticated computer calculations and have written a paper describing their results and have had it published in the journal *Science*.

H2-CO molecules come about when hydrogen molecules (H2) and carbon monoxide molecules (CO) interact; past researchers have found that their interaction is weak, with the resulting molecule acting more like a duel molecule than a separate new one. Once the two molecules combine they wind up with one of two kinds of spin around the two nuclei: aligned in the same direction, known as an "ortho" state, or not, known as a "para" state. The new molecule also has an internal vibration of course. In this new research, the team studied H2-CO molecules in their "ortho" state because more of them are generally seen in space.

What intrigues space researchers though is evidence that H2-CO molecules come about in space when the two elementary molecules meet, which by inference would lead scientists to the H2 that they actually want to study.

Sadly, trying to decipher the spectral signature of H2-CO has been stymied by the fact that such molecules have the peculiar property of having their vibrations overrun their spin, which is what researchers look for when studying imagery from space. Because of this, researchers have not been able to use H2-CO to study just H2. Now however, it appears that work by a team of researchers using sophisticated calculations on a computer to find the precise quantum mechanical alterations that each atom in the new molecule has undergone, has resulted in findings that match the properties of H2-CO, thereby giving researchers a better picture of how vibration and spin work within the molecules, which, by extension, should give researchers studying the far reaches of space a much better idea of what to look for.

More information: Theory Untangles the High-Resolution Infrared Spectrum of the ortho-H2-CO van der Waals Complex, *Science* 1 June 2012: Vol. 336 no. 6085 pp. 1147-1150. DOI: 10.1126/science.1221000

ABSTRACT
Rovibrational spectroscopy of molecules boasts extremely high precision, but its usefulness relies on the assignment of spectral features to corresponding quantum mechanical transitions. In the case of ortho-H2-CO, a weakly bound complex abundant in the interstellar medium (although not yet observed there), the rather complex spectrum has been unexplained for more than a decade. We assigned this spectrum by comparison with a purely ab initio calculation. For most lines, agreement to within 0.01 centimeter^{-1} between experiment and theory was achieved. Our results show that the applicability of rovibrational spectroscopy can be extended with the assistance of high-accuracy

quantum mechanical computations.