Submillimeter Spectroscopy – Water and Oxygen: Where are These Key Species in the Interstellar Medium?

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***Abstract*—Water and oxygen are two of the key species necessary for life. Water vapor and molecular oxygen are predicted to be abundant gas phase species in dense regions of the interstellar medium where formation of new stars and planetary systems is taking place. But observations to date have revealed that the abundances of H_2O and O_2 are much lower than expected, and suggest that a surprisingly large amount of atomic oxygen (OI) is present in molecular clouds. Resolving the disagreement between theory and observations will require better spectroscopic observations from new satellite and airborne facilities which fortunately will become available in the next few years. In this talk I briefly review the observations to date, the issues for theoretical models, and suggest what future observations will help resolve this "oxygen problem".**

I. BACKGROUND

Stars have formed throughout cosmic time and continue to form in dense regions of the Milky Way and other galaxies. The chemical composition of the interstellar medium is critical for the star formation process: one of the reasons is that molecular emission is the most efficient way for the gas in a cloud to radiate energy and thus enable it to contract en route to becoming a new star. Over a wide temperature range, a number of molecules can be far more efficient than atomic species in radiating energy that can escape from the cloud. The abundance of these key coolant species is thus critical for preventing the work done by gravity from heating the cloud and stabilizing it against further contraction.

Water and oxygen molecules have been predicted to be important coolants of interstellar clouds. In particular, water vapor, which has a complex energy level structure and many strong lines at millimeter through infrared wavelengths, is an efficient coolant[1], and it is critical for allowing gravitationally bound interstellar cloud cores to contract and form stars. The connection of these two species to life is well known. A consequence of their (fortunately) large local abundance is that the Earth's atmosphere is opaque at the frequencies of the transitions between the levels which are expected to have significant population in interstellar space. Two small satellite observatories, NASA's Submillimeter Wave Astronomy Satellite (**SWAS**) and the European **Odin** had water and oxygen as two of their key targets. Results from these two missions have indicated that in quiescent clouds, both of these species are at least two orders of magnitude less abundant than predicted by gas-phase chemical models for well-shielded regions (see e.g.[2,3,4,5]).

ESA's Infrared Space Observatory (**ISO**) satellite covered the wavelengths of the fine structure transitions of atomic oxygen (OI) at 145 μm and 63 μm, and the observations of these two spectral lines suggested (surprisingly) that most of the oxygen along the observed lines of sight through the Galaxy is gas phase OI [6,7,8]. However, a major limitation of the ISO data is that the spectral resolution, $R = \lambda/\delta\lambda \sim 6000$, although quite good for a Fabry-Perot system, corresponds to a velocity resolution of 50 km s^{-1}, which is insufficient to resolve the different regions that might contain atomic oxygen. There thus remains considerable uncertainty about exactly where along these lines of sight the observed atomic oxygen is located, and with what column density of hydrogen in atomic or molecular form it is to be compared. Other ISO observations of OI suggest that interpreting the OI lines is difficult due to confusion from foreground absorption[9]. The only way to improve this situation is to have much higher spectral and higher spatial resolution observations.

II. SUBMILLIMETER SPECTRA

A. Fine Structure Lines

In considering what might be the most important coolants of dense interstellar clouds, we have to consider what the abundant species are and what species have the greatest ability to radiate energy. The former consideration restricts us to the most common elements, C, N, and O, while the second limits us to atomic species that have well-placed fine structure lines and molecules that have numerous, strong transitions in the vicinity of the peak of the blackbody spectrum at temperature characteristic of the regions in question. Interstellar clouds have temperatures between ~ 10 K and ~100 K, although small regions close to embedded luminous sources or heated by shocks may be warmer. For neutral atomic species, the only energy states of significance are fine structure levels; those of CI and OI produce transitions at submillimeter and far infrared wavelengths. In Fig. 1 we show the fine structure levels and transitions of these two species. Both of the carbon lines are observable, albeit only in very good conditions, from high, dry terrestrial sites. The oxygen lines are totally blocked by the atmosphere.

B. Water Vapor

At dense cloud temperatures, the molecular energy levels of interest are those determined by the rotation of the molecule about its center of mass. Although the species in question do have vibrational levels, these are generally at considerably higher energies, starting at $\Delta E/k$ = 2300 K for H_2O. Water vapor is a simple triatomic molecule, but its three principal moments of inertia are unequal, making it an asymmetric top. Thus, its energy level structure is relatively complex. The spins of the two hydrogen atoms must, by symmetry, be either

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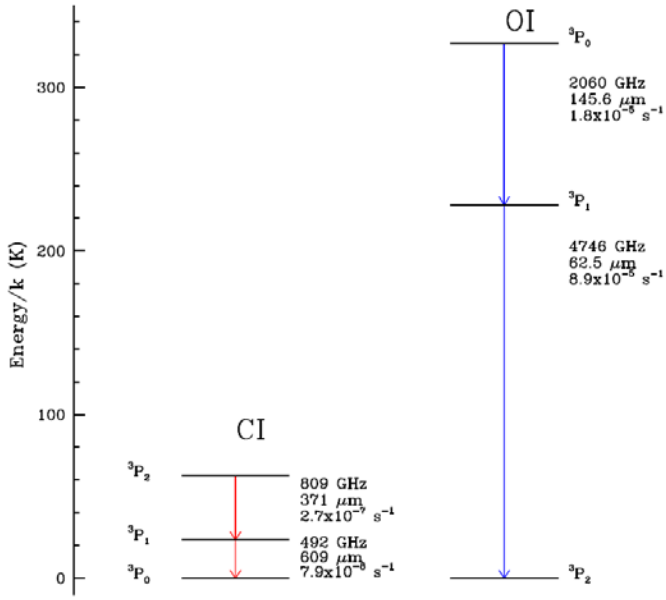

Fig. 1. Fine structure levels and transitions of neutral carbon and oxygen. The spontaneous decay rate is given below the wavelength of each transition.

parallel or antiparallel. The former situation results in ortho-H_2O, and the latter para-H_2O as shown in Fig. 2. The two species are not radiatively connected and although interconversion can occur when the water molecule is interacting with another body (dust grain or other molecule) ortho- and para- H_2O act as largely independent species.

The rotational transitions of water vapor are strong, since its permanent electric dipole moment is large (μ = 1.94 D). Lines at submillimeter wavelengths (ν ~ 500 to 3000 GHz) have very rapid spontaneous decay rates ~10^{-3} s^{-1} to 10^{-1} s^{-1}. The result is that (i) the collisional excitation rate will be much less than the spontaneous decay rate in all but the densest parts

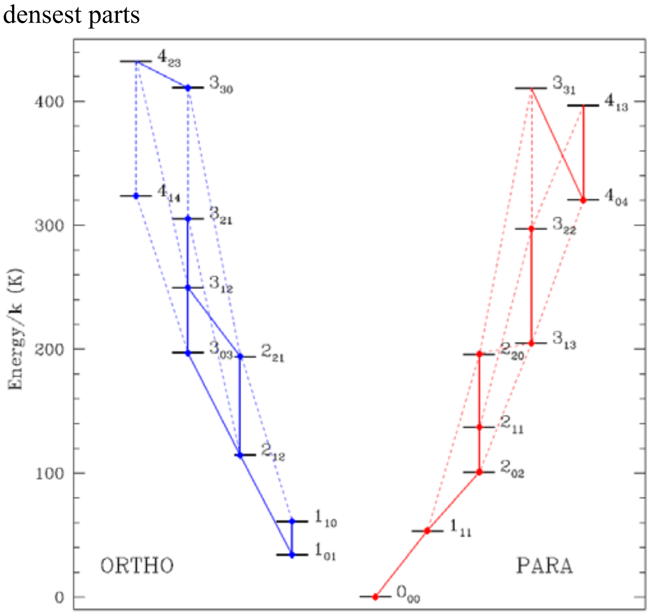

Fig. 2. Lower rotational energy levels and transitions of water vapor. The solid lines indicate the transitions that are in the frequency range of the Herschel HIFI instrument, and the dashed lines indicate other allowed transitions. The 1_{10}-1_{01} transition of ortho-H_2O at 557 GHz was observed by the SWAS and Odin Satellites. This transition, as well as many of the shorter-wavelength lines observed by ISO, will be observable with Herschel.

of the interstellar medium and thus the excitation will be highly subthermal, and (ii) moderate fractional abundances of water, $X(H_2O) = n(H_2O)/n(H_2)$, result in very optically thick lines in which the photon escape probability is low.

Analysis of the emission from interstellar water is thus complex, and the results depend on both the density of water vapor as well as of the H_2 responsible for the excitation. In regions where the density is known to be low, the emission is "effectively thin", meaning that every photon produced by spontaneous emission eventually escapes from the cloud, even if after repeated absorptions and reemission[10]. The intensity is proportional to the column density of water multiplied by the volume density of H_2, and if the latter is known, the water abundance can be deduced with some confidence. These results, which have been confirmed by more detailed radiative transfer models as well as by observations[10] of $H_2^{18}O$, indicate that the fractional abundance of water vapor in quiescent clouds is a factor 100 to 1000 below that expected for standard gas phase chemistry[2,5,10].

C. Molecular Oxygen

O_2 is a homonuclear molecule with no permanent electric dipole moment. Symmetry considerations restrict the rotational quantum number N to odd values. Two electron spins are parallel, yielding S = 1. The spin magnetic moment interacts with the molecular rotation, splitting each rotational level (total angular momentum J) into three as shown in Fig. 3.

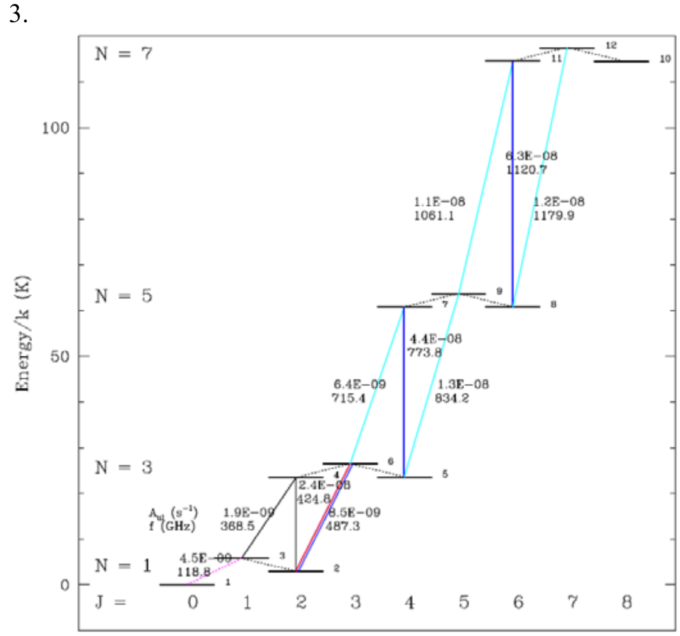

Fig. 3. Lower rotational levels and transitions of the O_2 molecule. The spontaneous decay rate A_{ul} is indicated with the frequency of each transition. The 118.8 GHz $\Delta N = 0$ transition was observed by Odin, and the 487.3 GHz line by SWAS. All other $\Delta N = 2$ transitions starting with the 487.3 GHz line will be observable with Herschel HIFI. The strongest lines should be those at 487.3, 773.8, and 1120.7 GHz.

The transitions between O_2 rotational levels are magnetic dipole transitions, which are relatively weak, as can be seen from the A-coefficients, which O_2 are more than 5 orders of

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magnitude smaller than those of water transitions having comparable frequencies. This makes the emission per oxygen molecule much weaker than the corresponding relation for water, but does have the virtue that transitions will be optically thin, and the level populations will be in local thermodynamic equilibrium (LTE), so that a detection of O_2 can readily be converted to a column density of the species, and a non-detection to an upper limit. Studies of various interstellar clouds by SWAS and Odin revealed O_2 fractional abundances ~ 2 orders of magnitude below the predictions of standard gas phase chemistry models[2-5]. Deep integrations on the ρ Ophiuchi cloud yielded a tentative detection of the 487.3 GHz line, but at a velocity slightly different from that of the quiescent cloud suggesting that the O_2 was in the postshock gas which had been impacted by the outflow from the newly-formed star in this region[12]. Subsequent Odin observations of the 118.8 GHz line suggested emission at the quiescent cloud velocity, but again with a relatively low fractional abundance compared with theoretical predictions[13].

III. CURRENT STATUS

Oxygen is the third most abundant element (after H and He) and in atomic and molecular form is predicted to play an important role in the cooling of molecular clouds. However, our understanding of the oxygen chemistry still has major problems. As discussed above, the fractional abundances of the oxygen bearing molecules expected to be most abundant in interstellar clouds – H_2O and O_2 – are orders of magnitude less than predicted. On the other hand, the fractional abundance of atomic oxygen may well be much greater than anticipated. All of these measurements are challenging, but together suggest that astrochemical models need significant improvement to explain the data. One possibility[2,5] is that oxygen sticks to grain surfaces, and then is hydrogenated to form H_2O. This molecule remains on the grain surfaces as water ice, which is observed in the infrared. Another possibility is that turbulent diffusion effectively exchanges material characteristic of regions entirely shielded from ultraviolet radiation with that at edges of cloud or clumps where significant UV is present. The result[14] is an increase in the abundance of atomic species deep within clouds and a reduction in the abundance of O_2 and H_2O. Finally, it may be that the abundances seen are a reflection of the "onion skin" nature of molecular clouds in which photodissociation dominates in the outer layers, and grain depletion deep within the cloud. Thus, the region with significant H_2O and O_2 is relatively small, and thus the column densities of these important species are reduced when compared to those of the molecular cloud as a whole.

IV. POSSIBILITIES FOR THE FUTURE

To determine where the oxygen in dense interstellar clouds is to be found, we have to make accurate measurements of abundances of H_2O, O_2, and OI in a good sample of molecular clouds. SWAS and Odin were equipped with heterodyne receivers having high spectral resolution. The **Herschel Space Observatory** (http://herschel.esac.esa.int/), scheduled to be launched late in 2008 or early 2009, will be equipped with a high resolution heterodyne instrument, HIFI, which covers many spectral lines of O_2 and H_2O (but not of OI) with a resolution $R > 10^7$. Its sensitivity is orders of magnitude better than that of the submm receivers on SWAS and Odin. A likely result of the Herschel observations is detection of O_2 and measurement of a sufficient number of lines of H_2O and $H_2{}^{18}O$ that accurate abundances of both of these molecular species are available. A decided improvement in the OI situation should come from the German Receiver for Astronomy at Terahertz Frequencies (GREAT) on the SOFIA aircraft, which will cover both of the OI fine structure lines with spectral resolution sufficient to determine with confidence where within a molecular cloud the OI emission (or absorption) is produced. This instrument, or a successor which ideally would be a focal plane array system, offers the possibility of dramatically increasing our understanding of the quantity and location of interstellar atomic oxygen. Together with the molecular data from Herschel, this will go a long ways to resolving this "oxygen problem", which is critical for understanding interstellar chemistry, dense cloud cooling, and star formation. The research described in this paper was carried out at the Jet Propulsion Laboratory, California Institute of Technology, under a contract with the National Aeronautics and Space Administration.

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