The Far Infrared Lines of OH as Molecular Cloud Diagnostics

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Abstract
Future IR missions should give some priority to high resolution spectroscopic observations of the set of far-IR transitions of OH. There are 15 far-IR lines arising between the lowest eight rotational levels of OH, and ISO detected nine of them. Furthermore, ISO found the OH lines, sometimes in emission and sometimes in absorption, in a wide variety of galactic and extragalactic objects ranging from AGB stars to molecular clouds to active galactic nuclei and ultra-luminous IR galaxies. The ISO/LWS Fabry-Perot resolved the 119µm doublet line in a few of the strong sources. This set of OH lines provides a uniquely important diagnostic for many reasons: the lines span a wide wavelength range (28.9µm to 163.2µm); the transitions have fast radiative rates; the abundance of the species is relatively high; the IR continuum plays an important role as a pump; the contribution from shocks is relatively minor; and, not least, the powerful centimeter-wave radiation from OH allows comparison with radio and VLBI datasets. The problem is that the large number of sensitive free parameters, and the large optical depths of the strongest lines, make modeling the full set a difficult job. The SWAS montecarlo radiative transfer code has been used to analyze the ISO/LWS spectra of a number of objects with good success, including in both the lines and the FIR continuum; the DUSTY radiative transfer code was used to insure a self-consistent continuum. Other far IR lines including those from H2O, CO, and [OI] are also in the code. The OH lines all show features which future FIR spectrometers should be able to resolve, and which will enable further refinements in the details of each cloud’s structure. Some examples are given, including the case of S140, for which independent SWAS data found evidence for bulk flows.

1 The Far Infrared Transitions of OH
Storey, Watson and Townes (1981) made the first far infrared detection of OH in the interstellar medium: the two 119µm lambda-doubled lines between the ground and first excited states, which they discovered in absorption from Sag B2, and in emission from the shock in Orion KL. Altogether there are 15 far infrared lines between the lowest 8 rotational levels of OH. The lines (each involving six transitions between the hyperfine-split rotational levels) are at wavelengths of (approximately) 28.9µm, 34.6µm, 43.9µm, 48.8µm, 53.3µm, 65.1µm, 71.2µm, 79.2µm, 84.4µm, 96.3µm, 98.7µm, 115.4µm,
119.9 µm, 134.8 µm, and 163.1 µm. The upper state excitation temperatures for these lines range from 120K to 618K. The dipole moment for OH is large, 1.668 Debye (for comparison the CO dipole moment is 0.112 Debye), and the radiative rates for OH transitions are generally fast. For example, the 119µm fundamental transition rate is about 0.1 sec⁻¹. But the FIR OH transitions also include some cross-ladder lines whose radiative rates are one hundred times weaker, providing a dataset of neighboring, far IR lines which frequently include both optically thin and very optically thick features. The OH analyses have an additional resource from which to draw: the strong hyperfine radio wavelength transitions that OH has in its ground-state, and which have been extensively observed. Maser and/or mega-maser activity is seen in many of the stars and galaxies which ISO observed.

The general properties of interstellar OH are known from thermal OH emission studies done at radio wavelengths, as well as from the far IR observations. Typically OH has the following range of properties: \( \frac{N_{\text{OH}}}{N_{\text{H}_2}} = 0.1 - 3 \times 10^{-7} \); \( N_{\text{OH}} L = 2-100 \times 10^{15} \text{ cm}^{-2} \); \( T_x = 100 - 275 \text{K} \); and \( N_{\text{H}_2} = 0.1 - 3 \times 10^7 \text{ cm}^{-3} \) (e.g., Watson et al. 1985; Jones et al. 1994). In maser galaxies, such as the ones we observed with ISO/LWS, the OH masers regions typically have somewhat different properties: \( \frac{N_{\text{OH}}}{N_{\text{H}_2}} = 10^{-7} - 10^{-8} \); \( N_{\text{OH}} L \sim 10^{15} \text{ cm}^{-2} \); \( T_x = 40 \text{K} - 50 \text{K} \); \( N_{\text{H}_2} \sim 0.1-1 \times 10^4 \text{ cm}^{-3} \) (e.g., Henkel and Wilson, 1990). The presence of OH megamasers allow for VLBI observations in AGN, and results indicate that the sizes of the emitting regions are compact: ~ from a few to tens of parsecs. For example, in Arp220, one of the galaxies I discuss below, they seem to surround the AGN, with \( N_{\text{H}_2} \) densities \( \sim 10^6 \text{ cm}^{-3} \) (Lonsdale et al. 1994; Skinner et al. 1997).

Four of the relatively strong far IR OH transitions involve the ground state. In warm clouds the molecules absorb the strong IR dust continuum, populating effectively some of the higher lying levels. As was conclusively shown by Sylvester et al. (1997), the 18 centimeter radio maser emission in evolved stars is pumped by absorption of the 34µm dust continuum, while in AGN Skinner et al. (1997) proved the effectiveness of the IR pumping of mega-masers in Arp220. The presence of a strong far IR continuum affects all of the far IR lines, to varying degrees, and means (besides making the models more complicated) that the set of far IR OH lines also provide a sensitive measure of the local continuum conditions. One final point is worth noting about OH: unlike other some species commonly used as far IR probes of the interstellar medium, like CO, \( \text{H}_2\text{O} \), or \( \text{OI} \), OH emission from PDRs or shocks does not contribute a relatively dominant amount of luminosity to these other processes. In the cases I model below, just the warm gas from a dusty molecular clouds is adequate to explain the strengths we observe. OH, therefore, has a powerful combination of features that makes it a very useful species for dis-entangling cloud properties across a very wide range of conditions.
2 ISO/LWS Observations of Extragalactic OH

The ISO/LWS Extragalactic Science team has seen OH in fifteen galaxies, and has obtained potentially useful limits on approximately one hundred other galaxies observed by ISO. Our observations include a set on the 34.6µm “IR pump” transition from the OH $^3\Pi_{1/2}$ ground state, which was obtained using the ISO/SWS spectrometer. This line, and the less important 28.9µm line between excited upper states, are the only OH far IR lines not in the LWS wavelength coverage. ISO of course has also seen OH in numerous galactic locations, including Sag A, and Sag B2, and in particular in the evolved star IRC+10420 -- the first source to demonstrate that the 34µm continuum can effectively pump the OH maser lines in these stars. The LWS extragalactic detections of OH are in the following sources: Arp 220, Cen A, IRAS17208-0014, IRAS20100-4156, M82, Mkn 231, Mkn 273, NGC 253, NGC 891, NGC 1068, NGC 1614, NGC 3690A, NGC 4945, NGC 7469, and 3Zw35. Figure 1 shows all the eight OH lines detected in Arp220, along with a sample of the lines detected in other objects to illustrates some of the morphological variety.

2.1 General Characteristics of the Observed Extragalactic OH Lines

Perhaps the most striking observation about the set of extragalactic lines measured is the wide morphological range of behavior they display, even though all arise in infrared bright galaxies with either active star formation, an active nucleus, or perhaps both. In Arp 220, for example, every OH line is seen in absorption except the longest wavelength, 163µm, line which is seen weakly in emission (Fischer et al. 1998). By contrast, NGC 1068, another AGN, has every detected line seen in emission, even the strong 119µm transition between ground and the first excited state (Spinoglio et al. 1999). NGC 253, a nearby starburst, has some OH lines in emission and some in absorption (Bradford et al. 1999), while in M82, the infrared bright, prototype starburst galaxy, the lines’ equivalent widths are so small continuum that even with our high signal-to-noise ratio only the 119µm line has been conclusively seen at all, in absorption (Colbert et al. 1999). From the analysis of this diverse set of line strengths, several useful preliminary generalizations may be drawn for the different categories, as summarized below.

ULIGs: In the case of Arp 220, the VLBI megamaser studies together with the strength of the 34µm pump absorption provide some strong physical constraints. The OH lies in numerous small clouds which surround the AGN, and which are pumped by the local, warm, far IR continuum. Through further modeling I hope to arrive at a better sense of the shape of that continuum: is it starburst-like, or more AGN like, and is it characteristic of all ULIGs?

AGN: In the case of the bright Seyfert galaxy, NGC 1068, analyses of the strong atomic lines (Spinoglio et al. 1999) show the substantial presence of a PDR line emission component, along with the high ionization lines from the AGN component in the ISO beam, and a starburst component, which is seen as well in other AGN. However the [CII]/FIR ratios are strange -- often less than in PDRs. The OH lines, all seen in
Figure 1: The 8 ISO/LWS OH lines seen in Arp 220 (the 34µm SWS-band line is not shown here). Under each OH line in Arp220, an OH line selected from another other ISO galaxy (or IRC+10420) is shown for comparison at the corresponding wavelength to illustrate some of the variety in the intensities observed.
emission, might help sort out the density and geometry of the clouds (for example, to see if the PDR regions have smaller than average filling factors) – and provide clues to their relationship to the active nucleus.

**Infrared Bright Galaxies:** We find that the OH 119 µm ground fundamental transition is always in absorption in these galaxies, as is the 53µm line, while the 163µm feature is always seen in emission. Otherwise there does not appear to be any consistent behavior in the lines from different objects: in some sources they are seen in emission, in others they are in absorption. Saraceno et al. (1996) and Benedetti et al. (2000), among others, have noted there seems to be a dearth of H$_2$O emission in some galactic clouds. Also, the [CII] fluxes are very low, perhaps due to low gas heating (but this is not conclusively demonstrated). They note that the neutral oxygen [OI] 63µm line is often abnormally weak and may be self absorbed. Finally, the SWAS satellite found that O$_2$ is very weak or absent (Goldsmith et al. 2000). OH plays a key role in the chemistry of the ISM, is sensitive to the temperatures and radiation fields, and its abundance and distribution should help in the analyses of all these issues.

3 Modeling of the Far Infrared OH Lines

3.1 The Montecarlo Code for Lines; the “DUSTY” Code for Continuum

I used the one-dimensional montecarlo radiative transfer code developed by the SWAS mission (Ashby et al. private comm) to model the OH line strengths. This code, a modification of the original Bernes code, adds a treatment of continuum photons from dust mixed in with the gas -- a particularly essential feature for OH, which is pumped in many cases by absorption of 34µm continuum. In addition, the code corrects for some previous errors encountered at large optical depths, also an issue of importance for OH which has a very strong matrix element. Finally, the code includes an ability to handle a wide range of molecules besides rigid rotors. The montecarlo code takes as input a series of concentric shells, each of which is specified as to size, gas and dust temperature, H$_2$ density, velocity and velocity width, and molecular abundance relative to H$_2$. The model as a whole also assumes a (specifiable) dust emissivity. In all the modeling, the dust is assumed to be 1% of the gas, and to have the same temperature as the gas everywhere in the cloud. The montecarlo code calculates the populations of the molecular levels in each shell. The output is then fed into a radiative transfer code that calculates the line profiles as seen by an external observer looking at the cloud.

The montecarlo results confirm the fact, noted above, that the OH lines are often optically thick. The peak optical depth at line center for the 119µm line exceeds 100 in some cases. As a result, many of the lines in many situations show self-absorption. As the model is tuned to fit the data by increasing the column density, these features can turn an emission line into an absorption line, one while strengthening the emission from a weaker
The full set of nine line intensities, which span a range of wavelengths and optical depths, enable us to derive a rather detailed self-consistent picture of the cloud conditions solely from their intensity ratios, without the need for velocity information. But, as seen in the example below, there is also a wealth of information in the line shapes.

ISO/LWS also observed lines of CO, H$_2$O, and [OI] in these galaxies, with varying degrees of success. The SWAS montecarlo code can also predict the line emission from these species. In general the model predictions for these lines are in overall agreement with the observations; the uncertainties are due to uncertainties in the ISO line fluxes themselves, in the assumed molecular abundances, and in the amounts of possible line “contamination” from shocks and PDRs in the beam. Overall the results add further confidence to the models. The [OI] 63µm line is clearly self absorbed in several instances, confirming the suspicion that the line intensity is sometimes very weak due to self-absorption (Saraceno et al.)

The montecarlo output is not strictly internally self-consistent; the input parameters need not conserve luminosity between shells, for example. To obtain this self consistency, and to guarantee that the final cloud model was also consistent with the observed far infrared continuum flux, I used the DUSTY code (Ivezic and Elitzur, 1997) to model the continuum and generate a set of shell parameters that provided this consistency. Then I iterated the DUSTY model with the montecarlo line outputs. While this technique does not give a unique solution for the cloud structure, it does provide a canonical model consistent with the observations.

3.2 Some Modeling Results

3.2.1 S140 - A Molecular Cloud with Bulk Inflow Motions
Ashby et al. (2000) used the SWAS satellite to observe S140, and the SWAS montecarlo code to model the shape of the observed submm H$_2$O line. They are able to obtain a detailed, if not entirely unique, model of the cloud. From their set of models they conclude, for example, that the cloud radius is 0.44pc, has an inner temperature of ~70K an inner hydrogen density of 1.4x10$^6$ cm$^{-3}$, a radial profile of temperature which varies like r$^{-0.5}$, and a density profile varying like r$^{-0.8}$. They also conclude that “significant bulk flow” is required to explain the H$_2$O line shape, but because of the small optical depth of the 557 GHz line they could not differentiate between infall and outflow. Although the ISO observations of S140 were only able to set weak limits on the OH lines (Aannestad and Emery, 1998), the detailed nature of the SWAS models made it a useful check.

Taking the SWAS cloud parameters for the case of bulk infall motions, I used the montecarlo code to calculate the strengths and line shapes for the full set of OH lines; I calculated the far IR lines of H$_2$O and the [OI] lines as well, for comparison with the ISO values. The reasonable results obtained from the model of S140, as confirmed with the SWAS (and ISO) observations, provide some confidence in the galaxy modeling. Figure
shows the results for three of the OH lines, on the same scale: the 163µm line (top), the 79µm line (middle), and the 119µm line (bottom). It is clear that high spectral resolution observations of the far IR water lines can readily distinguish infall from outflow, because these lines are optically thicker than the submillimeter line.

3.2.2 Arp220 - The Molecular Cloud Component of a Peculiar Ultra Luminous Galaxy
Arp220 is a particular challenge, because so many OH lines are seen, and every one of them (except the line at 163µm) is seen in absorption -- something that happens in no other known object. Arp220 is also unusual in general in that its spectrum is characterized by numerous molecular absorptions; even the [OI] 63µm fine structure line is seen in absorption, while the [CII] 157µm line is found only in weak emission (e.g., Fischer et al. 1998). Skinner et al. (1997) showed that the 34µm OH absorption could pump the OH megamasers in Arp220, and their analysis supported the model in which many small, dense molecular clouds circulate around the nucleus. Suter et al. (1998) attempted to model the OH line absorptions with some less complex radiative transfer models, and were driven to consider some unusual non-LTE situations to explain the observations; .

I used the SWAS montecarlo code successfully to model (to first order) all of the observed OH lines in Arp220. Figure 3 shows a sample of these model line shapes. In order to get absorption in all the lines, including the 79µm line to the ground state $^2\Pi_{3/2}$ from the lowest level of the $^2\Pi_{1/2}$ ladder, while still getting weak emission at 163 µm, it was necessary to have falling within the ISO/LWS beam a combination small dense clouds, and a few large, giant molecular clouds. Iterating with the DUSTY code provides a way to obtain a continuum shape that fits the observed infrared continuum, though there may also be a continuum component in our beam arising from clouds without much OH. It was not necessary in this process to resort to the non-LTE scenario postulated in Suter et al.

3.3.3 NGC 253 - The OH Emission from a Nearby Infrared Bright Galaxy
In NGC 253, the two strongest OH lines are seen as emission lines: the 79µm and 163µm features, each of which is about twice as strong as the 119µm fundamental absorption (Bradford et al. 1999). Only two other OH lines are also seen in this galaxy, and as a result the model’s constraints are weaker than for Arp220. The montecarlo modeling of these OH lines implies that a few giant molecular clouds, with $r \sim 100$pc, can explain the observations. The clouds have H$_2$ densities averaging approximately $3 \times 10^3$ cm$^{-3}$ and an OH abundance relative to H of about $5 \times 10^{-8}$. ISO/LWS also observed the 119µm line in NGC 253 with the high resolution Fabry-Perot, which Bradford (2001) has successfully modeled.

3.3.4 NGC 1068 - OH Emission from AGN
NGC1068 is a remarkable extragalactic source in its OH spectrum, because it is the only galaxy observed in which all the detected transitions are found in emission. The code accurately predicts the observed line flux ratios to 40%. Based on the montecarlo
Figure 2: The hydrogen density distribution in a nominal giant molecular cloud in the galaxy NGC 253. This distribution was used in the montecarlo code modeling. The inner 50 parsecs of the GMC has warm, 250K, gas and dust, at constant density, while the bulk of the cloud has much cooler, 35K material.

Figure 3: Predicted OH line shapes from infalling gas in S140, based on cloud profiles derived from SWAS data. The figure shows the 163 µm line (top), the 79 µm line (middle), and the 119 µm line (bottom). While all three lines show evidence for infall from their highly asymmetric shapes, only the latter two show characteristic absorption: in the redshifted (near side) material. The velocity range across the figure is ±10 km/sec, reflecting the fact that the maximum infall velocity in the model (and seen by SWAS) was 7.2 km/sec.
Figure 4: Montecarlo modeling results of three OH lines in Arp 220. The OH lines at 119\textmu m, 79 \textmu m, and 53 \textmu m are displayed. All the OH lines are seen in absorption in Arp 220, except the weakly emitting 163 \textmu m line – the only known object with this property.
modeling, it seems the clouds that produce these lines in NGC1068 must be relatively small and dense, and heated from the inside. They are about 0.2pc in radius, with densities of ~10^4 cm^{-3} at the outer edges, increasing towards the center with a power law behavior of (R/\text{Ro})^{1.25}. The temperature in the outer shells is about 25K, increasing inwards approximately with a power law dependence (R/\text{Ro})^{1.47}. The total column density of H_2 in each cloud is 1.5x10^{24} cm^{-2}, and the relative abundance of OH in the model is approximately 10^{-7}. OH is taken to be absent in the hotter portions of the cloud, where T>300K. With these high column densities the strong lines of OH are very optically thick, and precise radiative transfer calculations like the present ones are absolutely essential. At a distance of 16.2Mpc, the total number of equivalent number of clouds needed to produce the observed absolute flux in the lines and the continuum is ~3x10^7. The limits to the observed fluxes in all the weaker lines are consistent with this modeling. It is worth noting in this context that in some galaxies the weaker OH lines in NGC 1068, like the 53µm line, are amongst the strongest, but the montecarlo modeling can successfully account for these differences. The montecarlo code also successfully reproduces the continuum emission seen from NGC 1068 to within a factor of 2-3 in absolute flux density across the entire LWS spectrum. The total mass in such an ensemble of clouds in NGC 1068 is approximately 9x10^9 M_☉.

4 Conclusions to Date
What general conclusions might we hope to draw from this large set of ISO OH observations? Although the analysis is still underway, it appears that the infrared luminous galaxies can be grouped into three general categories based on the relative strengths of their infrared OH lines: (1) relatively normal galaxies like NGC 253 and M82, from which the OH lines are seen in both emission and absorption, and which are dominated by starburst activity in giant molecular clouds; (2) NGC 1068 and other AGN, whose OH is seen in emission, and whose clouds must be quite small and dense (hydrogen densities up to 10^8 cm^{-3} in the cloud cores); and (3) Arp220, and perhaps other ULIGs with active starbursts as well as an active nucleus, for which a combination of a few giant molecular clouds and a collection of moderately dense cloudlets are required. (The ISO/LWS spectrum of Mkn 231 is much noisier than Arp 220's, but hints at similar behavior in its OH.) While I have made substantial progress using only the intensities of these lines, velocity resolved spectra will enable even further refinements. Future far infrared missions with sensitive, spectroscopic capabilities should find that the set of OH lines can provide wealth of information needed to unravel the structures of complex clouds.

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