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Far Infrared Line Profiles from Photodissociation Regions and Warm Molecular Clouds

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1. Introduction

This report summarizes the work done under NASA Grant NAG2-1056 awarded to the University of Colorado. The aim of the project was to analyze data obtained over the past several years with the University of Colorado far-infrared heterodyne spectrometer (Betz & Boreiko 1993) aboard the Kuiper Airborne Observatory. Of particular interest were observations of CO and ionized carbon (C II) in photodissociation regions (PDRs) at the interface between UV-ionized H II regions and the neutral molecular clouds supporting star formation. These data, obtained with a heterodyne spectrometer having a resolution of 3.2 MHz, which is equivalent to a velocity resolution of 0.2 km s^{-1} at 60 μm and 1.0 km s^{-1} at 300 μm, were analyzed to obtain physical parameters such as density and temperature in the observed PDR. The publication resulting from the work reported here is appended. No inventions were made nor was any federally owned property acquired as a result of the activities under this grant.

2. Science Results

2.1. Multitransition Study of High J CO in NGC 3576

The CO molecule is uniquely suited as a probe of physical conditions in molecular clouds because it is abundant, durable, and has many transitions energetically accessible at temperatures typical of these regions. Since CO has a relatively low permanent dipole moment of 0.1 D, the small critical density for collisional excitation for the lower J levels

($J \leq 6$) ensures that these levels are usually in LTE, rendering interpretation of intensities relatively straightforward. The higher J transitions occurring in the submillimeter and far infrared selectively probe hotter and denser gas.

We obtained spectrally resolved profiles of the ^{12}CO J = 9 → 8, J = 12 → 11, and ^{13}CO J = 9 → 8 transitions, and obtained an upper limit to the intensity of the ^{12}CO J = 17 → 16 line, in the dense southern hemisphere galactic molecular cloud NGC 3576 using the KAO.

The high-J CO lines are narrower than those seen in ^{12}CO J = 1 → 0 from the molecular cloud or in the 158 μm fine-structure line of C^+ from the PDR with a similar beam size (see next section). This shows that the dense, warm part of the molecular material adjacent to the PDR is compact and has a smaller velocity dispersion than the cooler cloud or the PDR. There is a strong dynamical association, however, as shown by the similar V_{LSR} values for the high and low J CO and the C II lines.

We developed a single-component non-LTE large velocity gradient model for energy levels up to J=32 to extract physical parameters from the spectroscopic data. The ^{12}CO J = 9 → 8 line was found to be optically thick and originates in an extended region characterized by a kinetic temperature of ~60 K. The higher-J lines arise in a compact region with $T_k \geq 150$ K. These results show that a single-component model is clearly inadequate to describe the region, and suggest that the PDR and heating source are behind the molecular cloud (Boreiko & Betz 1997).

2.2. Ionized Carbon in NGC 3576

Photodissociation regions at the interface between H II regions and cooler molecular material are most easily studied via the fine-structure line emission from C^+ and O as well as the rotational lines of the abundant CO molecule. Of particular interest are the fine-structure lines of O I at 63 μm and C II at 158 μm. Since the first ionization potential of C is similar to the dissociation energy of CO while its second ionization potential is

close to that of He, carbon throughout the PDR will be singly ionized. We had observed the 158 μm C II line in the galactic molecular with a spectral resolution of 0.5 km s^{-1} in the galactic molecular cloud/PDR region NGC 3576 from the KAO. The radiation from C II was found to be widespread and a map of the C II emission was constructed. The lines are much wider than those from the high J CO, reflecting the higher turbulence in the PDR. However, there is no evidence of the extended wings that would be expected if shock excitation were important in the region. The line profiles of the C II show absorption from less excited foreground gas, but this gas is intermixed with the PDR (Boreiko & Betz 1997). The warm PDR represents less than 1% of the molecular cloud material.

2.3. OH in Orion

Emission from the far infrared rotational lines of OH near IRc2 has generally been interpreted as coming from shock-excited material. Our previous heterodyne measurements of the 119 μm line of OH with 0.6 km s^{-1} resolution (Betz & Boreiko 1989) showed the presence of strong absorption in the blueshifted half, probably caused by OH in the expanding postshock gas which has density too low to populate the upper state of the observed transition. More recently, we have observed the 163 μm transition of OH (which terminates at the lowest rotational level of the $^2\Pi_{\frac{1}{2}}$ ladder) at high spectral resolution. We were able to observe this OH line simultaneously with the ^{12}CO J = 16 $\rightarrow$ 15 line in opposite sidebands of the spectrometer. The line profiles of the OH and CO appear very similar, with no foreground absorption in either case. Our multitransition study of CO shows that this radiation arises from several physical components of the gas, not just primarily from the shocked region. Therefore the OH also is not confined to the shocked and post-shocked gas. The very different line shapes of the 119 μm and 163 μm transitions require detailed modeling to reproduce, and the simple one- or two-component LVG models used for the multitransition studies of CO were found to be inadequate for the interpretation of the data.

One of the major advantages of heterodyne spectroscopy is the ability to obtain detailed

line profiles with good signal to noise ratio. However, the interpretation of these profiles in terms of fundamental properties of the molecular clouds requires a practical method for modeling the expected line profiles under a range of assumed physical conditions. The validity of any derived conclusions will directly reflect how realistic the models used for profile synthesis are. Simple plane-parallel LVG models neglect the important role of re-emission from molecules far from the line of sight in filling in any absorption features, and consequently will be unable to reproduce the observed 119 μm profile.

The computation of emergent line profiles in a spherically symmetric model of an expanding envelope such as the plateau outflow region near IRc2 is made more tractable if the Sobolev approximation is used. The Doppler shifts along with the spherical symmetry projection effects can radiatively decouple distant parcels of gas. The calculation of energy level populations for a given molecule then depends solely on the local conditions of temperature and density, with the added excitation from nonlocal continuum (dust) radiation. The relevant equations are still nonlinear and require iteration at any point in the envelope, but are much more tractable than the fully coupled case in which line radiation from every radial shell interacts. This escape probability formalism has been the only method previously employed in modeling infrared lineshapes in molecular clouds, with reasonable success. However, Schönberg has shown that the Sobolev approximation fails for large line opacities or opacity gradients (Schönberg 1985). Therefore, for the analysis of the OH observations, we are adapting the radiative transfer code MMLINE originally developed by Schönberg (1988) and considerably modified by Skinner and Justtanont (Justtanont, Skinner, & Tielens 1994). In this code, the coupled equations of radiative transfer and molecular energy level populations are solved correctly, including non-local interaction effects, in the comoving frame using an approximate Newton-Raphson technique (Schönberg & Hempe 1986). This technique has been shown to be robust and converge monotonically and quickly, independent of initial level populations. The excitation of the molecule is calculated from radiative excitation from the central star, from the dust envelope, and from collisions with H_2 molecules as well as from line photons, taking into

account the Doppler velocities throughout the region. Level populations are then iterated until a self-consistent solution is obtained throughout the circumstellar envelope. Finally a line profile is calculated for a given beam size and offset from the center of the source. The original code was set up specifically for the CO molecule with a constant abundance ratio and monotonic velocity profile. We are modifying it for OH and generalizing it for a variable abundance and velocity structure, as well as removing physical assumptions specific to circumstellar outflows, for which the code was originally designed. Also some errors in the code have been corrected such that the effects on the line profile of the continuum throughout the model region are included. This work is approaching completion, and the code will then be applied to a model of the outflow and shock around IRc2, so that the calculated line profiles of OH and CO, as well as their spatial distributions, can be compared with the measured ones. The model that best reproduces the observed line shapes will provide information on physical conditions and OH and CO abundances within the outflow and shock region around IRc2.

REFERENCES

Betz, A. L., & Boreiko, R. T. 1989, ApJ, 346, L101-L104

Betz, A. L., & Boreiko, R. T. 1993, in ASP Conf. Ser. 41, Astronomical Infrared Spectroscopy, ed. S. Kwok, (San Francisco:ASP), 349

Boreiko, R. T., & Betz, A. L. 1997, ApJS, 111, 409-417

Boreiko, R. T., & Betz, A. L. 1996, ApJ, 464, L83-L86

Justtanont, K., Skinner, C. J., & Tielens, A. G. G. M. 1994, ApJ, 435, 852-863

Schönberg, K. 1985, A&A, 148, 405-411

Schönberg, K. 1988, A&A, 195, 198-207

Schönberg, K., & Hempe, K. 1986, A&A, 163, 151-158