NEW INTERSTELLAR MOLECULAR DETECTIONS: IMPLICATIONS FOR "SHOCK CHEMISTRY"

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INTRODUCTION: Several new interstellar species have recently been detected in the molecular gas, including rotationally-excited CH, vibrationally-excited HCN, and a new molecular ion, HCNH+. These detections have raised some interesting questions concerning the relative importance of "shock" or "high temperature" chemistry vs. ion-molecule reactions in the synthesis of interstellar molecules in dense clouds.

ROTATIONALLY-EXCITED CH:

The CH radical ($^2\Pi$) was first detected in the interstellar medium in 1973, when the three hyperfine lines of the ground state Λ-doubling transition (F_2, N=1, J=1/2) were observed. Unfortunately, these CH lines almost universally exhibited weak maser action, which made the derivation of the molecule's abundances uncertain. Detection of the excited rotational states of CH were thus of major astrophysical interest, because they would enable better determination of the abundance of the species, certainly one of the building blocks of interstellar chemistry, and because they could provide further data on the maser mechanism of the ground state.

Rotationally-excited CH has thus been the subject of astronomical searches for many years, both at radio and FarIR wavelengths. Only recently, however, with the laboratory measurement of very accurate rest frequencies, has rotationally-excited CH finally been detected (Ziurys and Turner 1985). The first excited rotational state (F_1, N=1, J=3/2) was observed via its Λ-doubling transitions at 700 MHz towards W51, a dense molecular cloud, using the 1000 ft. antenna at Arecibo. Initially only the two main hyperfine components were observed, but subsequent measurements have resulted in the detection of the weaker hyperfine lines.

Additional observations using the 300 ft. telescope at NRAO: Green Bank in April 1984 and 1985 resulted in the detection of the first excited state in other dense molecular clouds, including OriB,

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W3, W33, W43, and K3-50 (Ziurys and Turner 1986a). In several of these sources both main hyperfine transitions were observed and, as in W51, all lines were observed in absorption. Column densities calculated from these excited state observations are on the order of 10^{18} cm^{-2} in several clouds, implying a CH abundance 1000 times higher than what was previously derived from the non-thermal ground state transition. Such abundances have to be present in dense gas as well, for a high gas density is needed to explain the excitation of the first excited state. This CH abundance is about four orders of magnitude larger than what has been predicted by ion-molecule models of interstellar chemistry at the given gas density; contrary to past conclusions, CH may be one of the most abundant interstellar molecules. Such an unexpected high CH concentration is suggestive that the species may be formed by "shock chemistry" in dense clouds. The detection of this excited state of CH also provides further evidence for the proposed Λ-doubling-selective collisional pump of the ground stater maser, the so-called "Gwinn-Townes" model.

VIBRATIONALLY-EXCITED HCN:

Several molecules thus far have been detected in the interstellar medium in vibrationally excited states, including SiO, HCCCN, and CH_3CN. Unfortunately, past studies of vibrationally excited species in space have been somewhat incomplete, involving measurements of ro-vibrational transitions, done in the IR where astronomical sensitivity is limited; or else, they have concerned radio/mm wave observations of rotational lines of low-excitation bending modes of large polyatomics as CH_3CN. Such large species are not very abundant and have many low-lying vibrational states, making transitions originating in such states quite weak. Nonetheless, observations of interstellar molecules in vibrationally excited modes have a definite impact on interstellar chemistry, because they indicate that much molecular material is present at high temperatures. In such gas "shock chemistry" must occur. The role of this type of chemistry in overall interstellar synthesis is one of the important unanswered questions in astrochemistry.

It was therefore most interesting when a search for interstellar vibrationally excited HCH resulted in the detection of the $(0,1^{1c,1d},0)$ ℓ-doublets. The J=3-2 transitions of this bending mode were observed in Orion-KL and late-type carbon star IRC+10216, using the NRAO 12 meter antenna at 265-267 GHz (Ziurys and Turner 1986b). This particular mode lies 1025 K above ground state in energy and has an Einstein A coefficient for decay to ground of 3.7 s^{-1}.

The J=3-2 rotational lines in the (0,1,0) vibrational mode are particularly strong in Orion-KL with $T_R^* \simeq 1.5$ K. Such intensities are somewhat amazing, considering how high this mode lies in energy and its short lifetime. The column density estimated for the excited state gas alone in HCN is 10^{16} cm^{-2}, which is substantial and implies a ground state HCN column density of 10^{18} cm^{-2} and a vibrational temperature of 180 K. Thus, a considerable amount of HCN is present in conditions where shock chemistry must govern chemical abundances.

Also, the particular "clump" of gas which contains the vibrationally excited HCN, known as the "hot core", contains the highest column of HCN in all of the Orion molecular cloud. Yet, because of foreground optical depth effects, this is the first instance in which HCN has been clearly detected in this region.

These observations suggest that other common interstellar molecules may have large abundances in vibrationally excited states, and the extent of vibrational excitation in the ISM, and its affect on interstellar chemistry, may be more widespread than previously thought.

HCNH+:

Although predictions of the ion-molecule reaction scheme of interstellar chemistry have had considerable success, definitive tests of the theory are few. Only four molecular ions have been detected in interstellar gas thus far, and only two of these, HCO+ and N_2H+, have served the theory in a predictive sense. HCNH+, the protenated form of HCN, however, has long been regarded as a definite test of ion-molecule theory, because it is predicted to be intimately involved in the chemistry of such well known and abundant interstellar species HCN and HNC. There were a long series of unsuccessful searches over the past decades for HCNH+, based on crudely known rotational frequencies. Thus it was of interest when Altman, et al., 1984 finally obtained the mid-IR ro-vibrational spectrum of HCNH+, from which accurate rotational transitions could be predicted.

Based on these results, we (Ziurys and Turner, 1986c) have succeeded in detecting interstellar HCNH+. The J=1-0, J=2-1, and J=3-2 rotational transitions of this molecular ion have been observed toward Sgr B2. Using a large velocity gradient model calculation, the column density of HCNH+ has been found to be $\sim 4 \times 10(14)$ cm^{-2}, about one order of magnitude less than that estimated for HCO+ and HCN in this source. Such a column density implies a fractional abundance for HCNH+ in Sgr B2 of $\sim 3 \times 10(-10)$, one to several orders of magnitude greater than the values predicted by ion-molecule models of interstellar chemistry. The high observed abundance of this species, relative to theoretical calculations, suggests that chemical pathways other than the dissociative recombination of HCNH+ may be important in the formation of HCN and HNC. Such pathways may well involve reactions requiring high temperatures.

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