1975ApJ...201L..25T

THE ASTROPHYSICAL JOURNAL, 201:L25–L26, 1975 October 1
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CONFIRMATION OF INTERSTELLAR N_2H^+

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Received 1975 June 2

ABSTRACT

The identification of the new interstellar lines at 93.174 GHz as the molecular ion N_2H^+ has been confirmed by resolving in the source OMC-2 the predicted hyperfine structure of the inner nitrogen nucleus. The hyperfine constants of N_2H^+ derived from the observational data are eqQ(outer N) = -5.666 ± 0.012 MHz, eqQ(inner N) = -1.426 ± 0.021 MHz, and c(outer N) = 0.0147 ± 0.0023 MHz. The rest center frequency of the $J = 1$–0 rotational transition is determined to be 93173.392 ± 0.031 MHz.

Subject headings: molecules, interstellar — radio lines

The radical ion N_2H^+, a molecule never detected spectroscopically in the laboratory, has been proposed on theoretical grounds as the carrier of the triplet of interstellar lines recently discovered at 93.174 GHz (Turner 1974; Green *et al.* 1974). The gist of the identification is that the observed triplet represents the quadrupole hyperfine structure in the lowest rotational transition produced by the outer nitrogen nucleus. The corresponding structure of the inner nitrogen is predicted by Green *et al.* on the basis of an ab initio calculation of the N_2H^+ electronic structure to be about 5 times smaller, and hence incapable of being resolved in the sources studied by Turner. Detection of this hidden structure is the best way of confirming the identification of N_2H^+ short of an actual laboratory measurement of its microwave spectrum, and it is the purpose of this *Letter* to report that additional line structure essentially identical to that predicted has now been observed in OMC-2, the narrow-line molecular source recently discovered in the Orion Nebula (Gatley *et al.* 1974; Morris *et al.* 1974).

Figure 1 shows the lines we observe in OMC-2, the result of a 26 hour integration with the NRAO[1] 36-foot (11 m) telescope. The ordinate is the observed antenna temperature corrected for the beam efficiency and for atmospheric absorption. The instrumental spectral resolution was 100 kHz, the antenna beam width 70″, and the beam efficiency 0.68; the single-sideband noise temperature of the telescope's superheterodyne receiver was about 1600 K. A baseline extremely free of tilt or curvature was obtained by position switching once per minute between the source and a nearby area of clear sky.

It is evident from Figure 1 that the two strongest lines of the 93.174 GHz triplet (F_1 = 2–1 and 1–1) are significantly broadened or split by internal structure, while the weakest line (0–1) is apparently fully resolved,

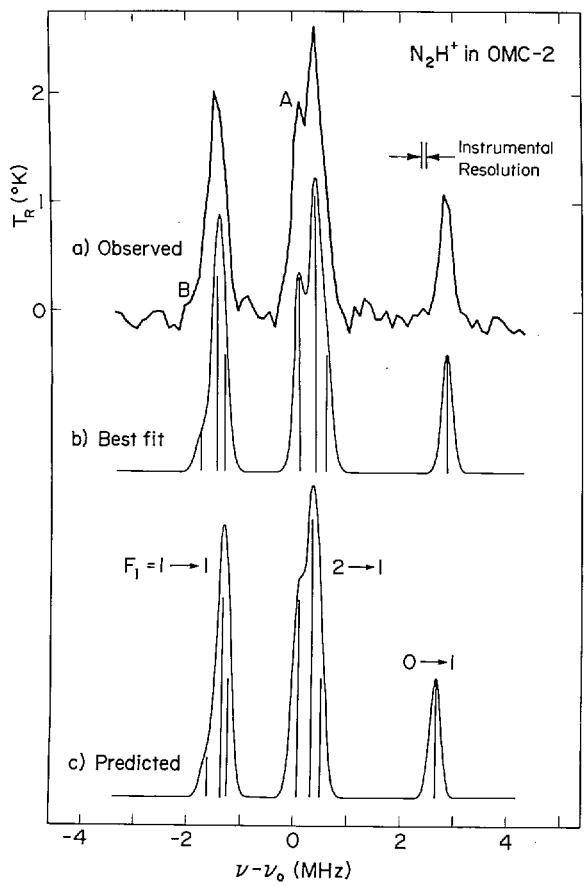

FIG. 1.—The 93.174 GHz lines in OMC-2, compared with theoretical calculations of the hyperfine structure of the $J = 1$–0 transition of N_2H^+.

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and so presumably represents the intrinsic Doppler line width in OMC-2. The shape of this very narrow line is approximately Gaussian; its full width at half-maximum, corrected for the slight broadening produced by the 100 kHz resolution of the spectrometer, is only 230 kHz (0.74 km s^{-1} in radial velocity), making it to our knowledge the narrowest molecular emission line (excluding the maser point sources) so far observed in the direction of an H II region or infrared source. The temperature required for thermal Doppler broadening by this amount is only 340 K for a molecule with the molecular weight of N_2H^+, meaning that even by laboratory standards the spectral resolution in OMC-2 is remarkably good.

The lower theoretical spectrum in Figure 1 is the hyperfine structure (hfs) of the $J = 1$–0 transition of N_2H^+ calculated from the quadrupole constants of Green *et al.* (Table 1). This entirely *a priori* prediction —made, it should be emphasized, without any adjustable parameters at all—is seen to account qualitatively for all the important observational results, in particular (i) the broadening of the two strongest lines, (ii) the splitting of the central line at A, and (iii) the hint of a shoulder on the low-frequency line at B. The relative *peak* intensities of the triplet are predicted to deviate significantly from the ratios 5:3:1 expected for the hfs of a single nitrogen, but the relative *integrated* intensities should maintain these ratios, and this is observed to be the case: numerical integration of the data yields for the integrated intensities $5:2.84 \pm 0.09:1.02 \pm 0.06$, where the uncertainties represent one standard deviation.

The most conspicuous quantitative discrepancy between the observational data and the *a priori* calculation is in the splitting of the central line, which appears to be somewhat larger than predicted. This disagreement is without statistical significance, however, since it is entirely removed by a least-squares adjustment of the hyperfine coupling constants which shifts them by an amount less than the ab initio uncertainties. The resulting best-fit spectrum—to within the statistical uncertainties an essentially exact reproduction of the observational data—is shown in Figure 1*b* (as in Fig. 1*c*, it has been assumed in computing this spectrum that the line width is that of the narrow $F_1 = 0$–1 line), while Table 1 lists the best-fit hyperfine constants, plus the rest center frequency ν_{10} of the $J = 1$–0 transition derived on the assumption that in OMC-2 the radial velocity of N_2H^+ is the same as that of HCN, 11.14 ± 0.10 km s^{-1} with respect to the local standard of rest (Morris *et al.* 1974). The formal standard deviation in determining ν_{10} in the observer's rest frame is only 0.003 MHz, so the quoted uncertainty results almost entirely from the uncertainty in the HCN radial velocity; if the assumption of a common radial velocity is correct, a better determination of the HCN radial velocity in OMC-2 should yield a corresponding improvement in ν_{10} for N_2H^+.

TABLE 1

MICROWAVE CONSTANTS OF N_2H^+

Constant	Predicted (MHz)	Observed (MHz)
$\nu_{10}=2B_0-4D_0$.....	92200 ± 1800	93173.392 ± 0.031
eqQ(outer N).....	-5.3 ± 0.5	-5.666 ± 0.012
eqQ(inner N).....	-1.2 ± 0.5	-1.426 ± 0.021
c(outer N).....	0.012*	0.0147 ± 0.0023

* Value for HCN (Tomasevich 1970).

NOTE.—Uncertainties represent one standard deviation.

Even when N_2H^+ is eventually detected in the laboratory, it may prove difficult because of pressure broadening to equal the high spectral resolution observed in OMC-2, so the astronomical data may represent the best information on the microwave constants of this molecule for some time to come. For this reason we have made a careful check of systematic errors which might affect our results, paying particular attention to the small additional hyperfine interactions expected in N_2H^+.

With one exception, these interactions were found to have a negligible effect on the fit. The three direct spin-spin interactions (the mutual interaction of the nitrogen nuclei, and the interaction of each nitrogen with the proton) can be evaluated rather precisely in terms of the known bond lengths (Green *et al.* 1974) and nuclear moments; the largest amounts to only a few kilohertz, and none were found to have a statistically significant effect on the hyperfine constants in Table 1 when included in our fitting program. The spin-rotation constant of the proton, and that of the inner nitrogen, cannot be easily calculated, but they can be estimated from measurements on HCN and its isotopic species (Maki 1974) to be about 4 kHz in magnitude; these likewise were found to have no significant effect on the fit. The spin-rotation interaction of the outer nitrogen, however, turned out to be significant, partly because it is appreciably larger than that of the other two nuclei, but also because, unlike the other spin-rotation interactions, it tends to alter the separation between the fully resolved members of the triplet; treated as an independent parameter in our least-squares analysis, its coupling constant c(outer N) was determined to be 14.7 ± 2.3 kHz. For comparison, the spin-rotation constant of the nitrogen in the similar molecule HCN is 12.07 ± 0.27 kHz (Tomasevich 1970)—an agreement which may be regarded as slight additional evidence in favor of the identification of N_2H^+.

We wish to thank Linda Gaines for assistance with the data analysis. Further observations of N_2H^+ in a number of astronomical sources will be published elsewhere.

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