

RADIO-ASTRONOMICAL SPECTROSCOPY OF THE HYPERFINE STRUCTURE OF N_2H^+

P. CASELLI, P. C. MYERS, AND P. THADDEUS

Harvard-Smithsonian Center for Astrophysics, 60 Garden Street, Cambridge, MA 02138; caselli, myers, thaddeus@cfa.harvard.edu

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ABSTRACT

We present high spectral resolution and high-sensitivity observations of the $J = 1 \rightarrow 0$ transition of N_2H^+ at 93 GHz toward the quiescent low-mass cloud core L1512 in Taurus. The relative frequencies of the seven hyperfine components of this transition have been determined with precision ~ 1 kHz, and the absolute frequencies with precision ~ 7 kHz. The hyperfine coupling constants have been determined with precision an order of magnitude higher than previously in the laboratory. Relative intensities of the hyperfine components of N_2H^+ in L1512 as well as in a sample of ~ 60 low-mass cloud cores are not consistent with a single excitation temperature model fit, indicating the presence of excitation anomalies.

Subject headings: ISM: molecules — molecular data

1. INTRODUCTION

N_2H^+ (diazenylium) is one of the few molecular ions observed in interstellar clouds, so it is an important species to trace the ionized gas in dense clouds and to give information about fractional ionization, and the coupling between ions and neutrals in star-forming dense cores. Moreover, N_2H^+ is important for testing models of interstellar chemistry and as a surrogate for the unobservable nonpolar N_2 .

The $J = 1 \rightarrow 0$ transition of N_2H^+ at 93 GHz was first detected by Turner (1974), as an unidentified triplet of lines, toward several warm clouds. The identification of the N_2H^+ ion was soon made by Green, Montgomery, & Thaddeus (1974) on theoretical grounds, and then confirmed by Thaddeus & Turner (1975), who resolved the predicted hyperfine structure due to the inner nitrogen nucleus in the cold source OMC-2 in Orion. Following this early work, N_2H^+ has been extensively observed and mapped in dense clouds, mainly in massive-star-forming regions (Turner & Thaddeus 1977; Womack, Ziurys, & Wyckoff 1992). Recently, Benson et al. (1994, 1995) used the 37 m Haystack antenna to survey the peak position of the low-mass core map in the $(J, K) = (1, 1)$ line of NH_3 (Benson & Myers 1989) for the $J = 1 \rightarrow 0$ line of N_2H^+ at 93 GHz.

N_2H^+ is a linear molecular ion in a stable closed-shell 1Σ configuration; because all electrons are paired, there is no molecular magnetic field except the weak diamagnetic one generated by the molecular rotation. The dominant hyperfine interactions are therefore those between the molecular electric field gradient and the electric quadrupole moments of the two nitrogen nuclei; together these produce a splitting of the $J = 1 \rightarrow 0$ line into seven hyperfine components.

The spectral and spatial resolution now available at millimeter-wavelength telescopes allows accurate measurement of velocity structure in star-forming dense cores. The $1 \rightarrow 0$ transition of N_2H^+ is particularly useful for this purpose because of its generally low optical depth in all hyperfine components. It is therefore important to know the exact frequencies of the hyperfine structure (hfs) of N_2H^+ . The most recent measurement of the hfs has been done in the laboratory by Cazzoli et al. (1985), but the seven hyperfine components of N_2H^+ were not fully resolved owing to pressure broadening.

Because the best interstellar lines are very narrow compared

to all laboratory spectra to date, we obtained a high-sensitivity, high spectral resolution spectrum of N_2H^+ ($1-0$) toward the cold (kinetic temperature $T_k \sim 10$ K) and quiescent dense core L1512 in Taurus. Each of the seven spectral features is resolved with FWHM ~ 0.18 km s $^{-1}$. This width equals the thermal width of N_2H^+ at 20 K, a much lower temperature than can be achieved in the laboratory without recourse to a molecular beam. Such narrow lines, together with the high instrumental resolution (10 kHz; see § 2) used in the observations, allowed us to determine frequencies of the seven hyperfine components and spectral constants of N_2H^+ ($1-0$) with a precision of a few kilohertz. Also, these results place a limit for the first time on the coupling constant of the interaction of the proton spin with the magnetic field due to the molecular rotation.

Observation procedures and frequency estimates are described in § 2. In § 3 we derive N_2H^+ spectral constants. Finally, in § 4 we discuss excitation anomalies observed among the seven hyperfine components.

2. OBSERVATIONS AND N_2H^+ FREQUENCY MEASUREMENTS

The N_2H^+ ($1-0$) spectrum toward L1512 was obtained with the 37 m NEROC Haystack telescope.¹ We observed left and right circular polarization simultaneously, using half the correlator for each polarization. Using a bandwidth of 17.8 MHz, we achieved a frequency resolution of 10.5 kHz, which provided a velocity resolution of 0.034 km s $^{-1}$. System noise temperatures, referenced to above the atmosphere, were about 300 K. The half-power full beamwidth is 27", and the main-beam efficiency is ~ 0.2 , including the effect of the radome. Telescope pointing was checked every few hours by observing available planets by beam-switching; the rms pointing uncertainty was ~ 6 ". Line calibration was done with a blackbody chopper wheel, so as to yield antenna temperature corrected for atmospheric attenuation. The spectra were taken by using overlap frequency switching with an integration time of 10 minutes. We integrated the $1-0$ spectrum for 18 hr, and averaged the two polarizations together. The resulting spectrum is shown in Figure 1a, with the hyperfine transitions

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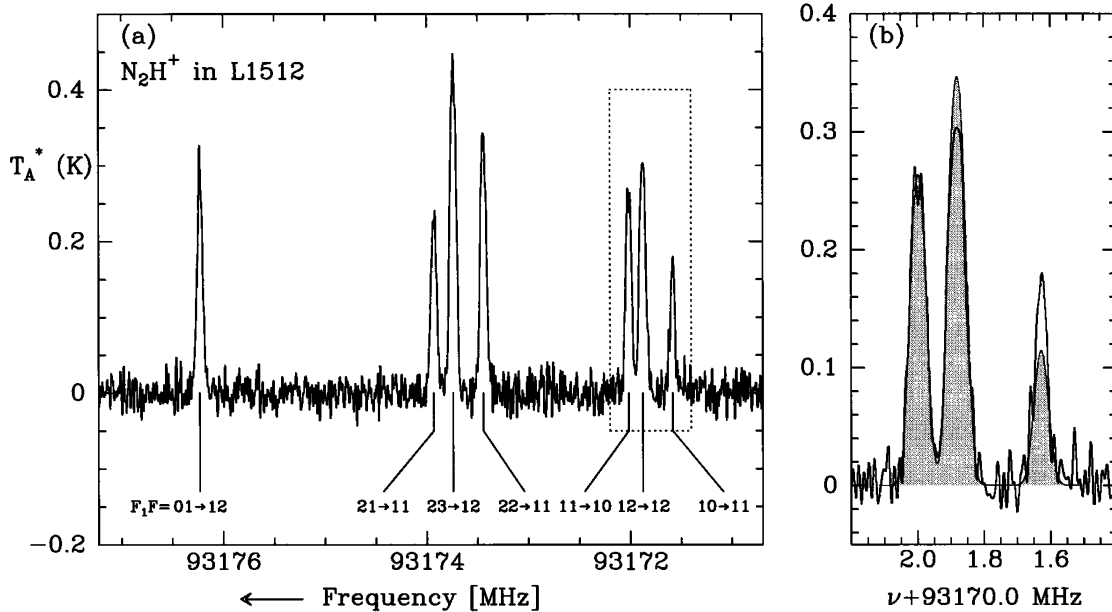


FIG. 1.—(a) N_2H^+ (1–0) spectrum toward L1512 obtained at the Haystack antenna. Each hyperfine component has been labeled with the corresponding quantum numbers F_1F . The spectrum is centered at the frequency of the main component ($\nu_{2,3 \rightarrow 1,2} = 93173.809$ MHz; Cazzoli et al. 1985). (b) The $F_1 = 1 \rightarrow 1$ hyperfine group of N_2H^+ in L1512 superposed with the seven-component hyperfine model-fit spectrum (gray shading) which assumes a single excitation temperature. The $F_1, F = 1, 0 \rightarrow 1, 1$ and $1, 2 \rightarrow 1, 2$ components present excitation anomalies.

indicated. The 1σ level of the noise in the off-line channels is 0.015 K in the unsmoothed spectrum.

We centered the spectrum at the frequency of the main N_2H^+ (1–0) component ($F_1, F = 2, 3 \rightarrow 1, 2$), as given by Cazzoli et al. (1985): 93173.809 MHz. The corresponding LSR velocity of the center of the band was 7.0 km s $^{-1}$. To obtain an accurate measurement of the velocity of L1512, we observed the $2_{1,2} \rightarrow 1_{0,1}$ line of C_3H_2 (85 GHz) in the same position. The rest frequency of the C_3H_2 line is known to 6 kHz from laboratory measurement (Vrtilek, Gottlieb, & Thaddeus 1987), and on the plausible assumption that the C_3H_2 and the N_2H^+ have the same radial velocity exactly, the absolute frequencies of the N_2H^+ hfs can be determined. The C_3H_2 line in L1512 was integrated for 2.5 hr using the 5.9 MHz band-

width and two polarizations converters which give a spectral resolution of 3.5 kHz. The resulting LSR velocity of L1512 is 7.107 ± 0.004 km s $^{-1}$.

The values of LSR velocities and relative errors listed in Table 1 (cols. [2] and [3]) have been calculated by the nonlinear Gaussian fit program in CLASS (Forveille, Guilloteau, & Lucas 1989). The frequencies of the seven N_2H^+ (1–0) hyperfine components and relative uncertainties are listed in columns (4) and (5) of Table 1. The differences between the laboratory frequencies of Cazzoli et al. (1985) and ours are shown in the last column. The uncertainty of about 1 kHz on the measured frequencies does not include the uncertainty on the C_3H_2 ($2_{1,2}-1_{0,1}$) frequency (Table 1), which must be added in quadrature. Absolute frequencies are then measured to about 7 kHz.

TABLE 1
OBSERVED LSR VELOCITIES AND DERIVED FREQUENCIES

Transition (1)	V_{LSR}^a (km s $^{-1}$) (2)	$\sigma_{V_{LSR}^1}$ (km s $^{-1}$) (3)	ν (MHz) (4)	σ_ν^b (MHz) (5)	$\nu_{lab}^c - \nu$ (kHz) (6)
N_2H^+					
$JF_1F \rightarrow J'F_1'F'$					
101 \rightarrow 012	–0.7951	0.0005	93176.2650	0.0011	45.0
121 \rightarrow 011	6.6004	0.0016	93173.9666	0.0012	49.4
123 \rightarrow 012	7.2113	0.0009	93173.7767	0.0012	32.3
122 \rightarrow 011	8.1673	0.0011	93173.4796	0.0012	25.4
111 \rightarrow 010	12.7565	0.0014	93172.0533	0.0012	24.7
112 \rightarrow 012	13.1955	0.0013	93171.9168	0.0012	30.2
110 \rightarrow 011	14.1473	0.0021	93171.6210	0.0013	–2.0
C_3H_2					
$J_{K_aK_c} \rightarrow J'_{K'_aK'_c}$					
$2_{1,2} \rightarrow 1_{0,1}$	7.1074	0.0037	85338.905 ^d	0.006 ^d	...

^a Apparent V_{LSR} values, used to derive hyperfine frequencies ν , are based on rest frequency 93173.809 MHz and corresponding LSR velocity of the center of the band 7.0 km s $^{-1}$.

^b Quoted errors do not take into account the uncertainty on the C_3H_2 ($2_{1,2}-1_{0,1}$) frequency (see text).

^c Laboratory measurement (Cazzoli et al. 1985).

^d Vrtilek, Gottlieb, & Thaddeus 1987.

The separation between any two of the seven features is, however, determined with a precision of about 1 kHz.

Estimates of the N₂H⁺ (1–0) optical depth, excitation temperature, and intrinsic line width have been made using the “hfs method” in CLASS which takes into account molecular hyperfine structure. This procedure gives intrinsic line width $\Delta v = 0.183 \pm 0.001$ km s⁻¹, excitation temperature $T_{\text{ex}} = 4.9 \pm 0.1$ K, total optical depth $\tau_{\text{tot}} = 7.9 \pm 0.3$. Here τ_{tot} is the sum of the peak optical depths of the seven hyperfine components (cf. Benson & Myers 1989, Appendix).

The theoretical line manifold assuming a single excitation temperature is significantly different from that observed. Specifically, the fit to the $F_1, F = 1, 2 \rightarrow 1, 2$ component overestimates the observed intensity, by a factor of ~ 1.2 , while the fit to the $F_1, F = 1, 0 \rightarrow 1, 1$ component underestimates the observed intensity by a factor ~ 2 . This is shown in Figure 1*b*, which is an enlargement of the $F_1 = 1 \rightarrow 1$ hyperfine group of Figure 1*a* together with the fitted spectrum (gray shading). The differences between the observed and fitted spectrum in L1512 are most readily interpreted as excitation anomalies in the hyperfine components (§ 4).

3. DETERMINATION OF N₂H⁺ SPECTRAL CONSTANTS

Neglecting the three direct spin-spin interactions between the nuclei and the spin-rotation interaction of the proton, all probably less than a few kHz (Green et al. 1974), the expression for the hyperfine structure Hamiltonian for N₂H⁺ can be written as

$$H_{\text{hfs}} = H_Q + H_{I,J}, \quad (1)$$

where

$$H_Q = \sum_{k=1}^2 \frac{(eQq)_k}{2I_k(2I_k - 1)J(2J - 1)} \times \left[3(\mathbf{I}_k \cdot \mathbf{J})^2 + \frac{3}{2}(\mathbf{I}_k \cdot \mathbf{J}) - I_k(I_k + 1)J(J + 1) \right], \quad (2)$$

$$H_{I,J} = \sum_{k=1}^2 C_k(\mathbf{I}_k \cdot \mathbf{J}). \quad (3)$$

In the above expressions $(eQq)_1$ and $(eQq)_2$ are the quadrupolar coupling constants for the outer and inner nitrogen, respectively; I_1 and I_2 are the nuclear spins of the two nitrogen atoms; and C_1 and C_2 are the coupling constants of the

TABLE 2
SPECTRAL CONSTANTS OF N₂H⁺ (MHz)

Parameter (1)	This Work (2)	Laboratory ^a (3)
ν_0	93173.4035 ± 0.0005^b	93173.435 ± 0.003
$(eQq)_1$	-5.6902 ± 0.0021	-5.71 ± 0.03
$(eQq)_2$	-1.3586 ± 0.0038	-1.44 ± 0.04
C_1	0.0118 ± 0.0004	0.012 ± 0.004
C_2	0.0087 ± 0.0006	0.011 ± 0.004
C_H	<0.020	...

^a Cazzoli et al. 1985.

^b This estimate excludes the uncertainty on the C₃H₂ frequency. When the C₃H₂ uncertainty is included, ν_0 is effectively determined with an accuracy of 6 kHz. Note: Subscripts 1 and 2 refer to the outer and inner nitrogen, respectively.

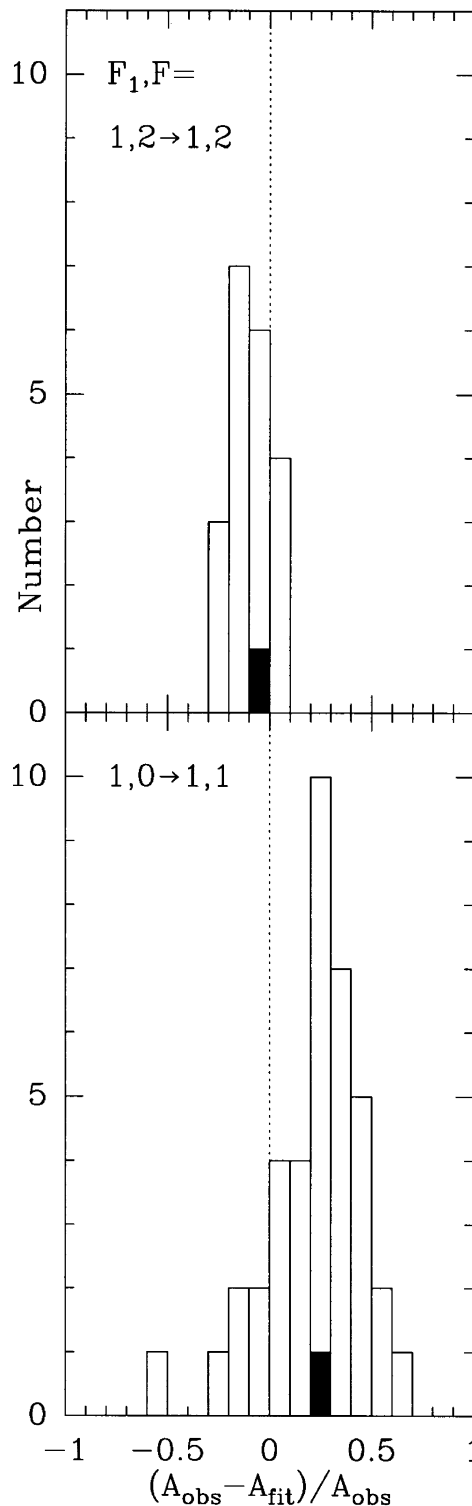


FIG. 2.—Excitation anomalies in the $F_1, F = 1, 2 \rightarrow 1, 2$ and $1, 0 \rightarrow 1, 1$ hyperfine components of N₂H⁺ ($J = 1 \rightarrow 0$) in a sample of 57 low-mass dense cores. The quantity $(A_{\text{obs}} - A_{\text{fit}})/A_{\text{obs}}$ is the difference between the integrated intensity of observed and hyperfine model-fit components, normalized to the observed integrated intensity (A_{obs}). It is a measure of the departure of the observed hyperfine features from a single excitation temperature model fit (see text). The black rectangle indicates the bin for L1512. The histograms confirm that each of the two hyperfine components observed to have anomalous excitation in L1512 is generally anomalous, in the same sense, in a large sample of similar dense cores.

magnetic spin-rotation interactions ($I \cdot J$) of the outer and inner nitrogen, respectively (Thaddeus, Krisner, & Loubser 1964).

The four parameters (eQq)₁, (eQq)₂, C_1 , and C_2 , together with the central line frequency ν_0 ($\equiv 2B_0 - 4D_0$, where B_0 is the rotational constant and D_0 is the centrifugal stretching constant) estimated by Cazzoli et al. (1985), are reported in column (3) of Table 2.

Based on the new observed values of frequencies and relative errors of the hyperfine components of N_2H^+ (1–0) (see Table 1), we calculated new values of the five spectral constants, which are shown in column (2) of Table 2. For this calculation we used the hyperfine fitting program developed by Pickett (1991). As seen from Table 2, the quadrupolar and spin-rotation coupling constants of the two nitrogens are now determined with a precision about an order of magnitude higher than from the laboratory work of Cazzoli et al. (1985). The uncertainty in the C_3H_2 line frequency only affects the central line frequency ν_0 , whose total error is then 6 kHz (see § 2). Our value of ν_0 is less by 31.5 kHz than the laboratory estimate. A shift of about 40 kHz was already known, as Cazzoli et al. (1985) compared their measured frequencies with those deduced from the astronomical observations by Thaddeus & Turner (1975); we confirm this shift and determine it more accurately.

The parameter C_H in Table 2 (row 6) is the coupling constant of the magnetic spin-rotation interaction of the proton. Its value was only roughly estimated to be ~ 4 kHz in magnitude (Green et al. 1974). This further splitting of the N_2H^+ (1–0) line cannot be resolved by our observations toward L1512; to determine an upper limit on C_H it was necessary to fit the manifold of lines by standard least-squares minimization, instead of simply fitting line frequencies. This procedure gave $C_H < 20$ kHz.

4. EXCITATION ANOMALIES

In § 2 we saw that the relative intensities of the seven hyperfine components of N_2H^+ (1–0) in L1512 are not consistent with a single excitation temperature, assuming a single intrinsic line width and allowing the optical depth to take on all the possible values. Assuming equal excitation temperature 4.9 K, best-fit model intensities, and that the optical depth of each component is proportional to its statistical weight, we found that all the N_2H^+ (1–0) components are approximately consistent with a value of $T_{ex} \sim 5$ K, except the $F_{1, F=1, 0 \rightarrow 1, 1}$ component whose excitation temperature is significantly larger (by ~ 1 K). Moreover, the component with the highest value of T_{ex} has the narrowest line width ($\Delta\nu_{1,0 \rightarrow 1,1} = 0.17$ km s⁻¹, about 1.3 times narrower than the average line width of the other six components).

To investigate whether this apparent excitation anomaly is peculiar to L1512, we analyzed the N_2H^+ (1–0) spectra in a sample of low-mass cores (Benson et al. 1994, 1995). In this survey 63 low-mass cores were observed in N_2H^+ at the peak position of the $(J, K) = (1, 1)$ line of NH_3 (Benson & Myers 1989). The observations were also made at the Haystack Observatory under the same conditions as described in § 2. For each source, the $J = 1-0$ transition was integrated for about 40 minutes, using two video converters, which gives a 1σ noise level of ~ 0.04 K in the spectra, smoothed to the effective velocity resolution of 0.034 km s⁻¹.

For all the 57 cores detected in N_2H^+ we calculated the area below each hyperfine component (A_{obs}) limiting the velocity range at the 1σ level of the line. Then the spectra have been fitted using the hfs fitting program (§ 2), giving A_{fit} , the area below the model fit line. For each of the seven hyperfine components we made histograms of the normalized deviation of data and fit, $A_n \equiv (A_{obs} - A_{fit})/A_{obs}$. Four of these histograms have means consistent with zero deviation, indicating no excitation anomaly. The histograms for the $F_{1, F=1, 0 \rightarrow 1, 1}$ and $1, 2 \rightarrow 1, 2$ components, which show significant deviations from $A_n = 0$, are shown in Figure 2. From Figure 2 we conclude that the excitation anomalies observed in the N_2H^+ spectrum of L1512 are general in low-mass cores. The $F_{1, F=0, 1 \rightarrow 1, 2}$ component also significantly deviates from the single excitation temperature model fit, although by a smaller amount than the $1, 0 \rightarrow 1, 1$ component.

It is worth noting that this pattern of anomalous excitation is mainly seen in sources without embedded stars, meaning that infrared pumping of the vibrational modes is unlikely to explain anomalous rotational excitation. Instead the excitation may arise from collisional pumping, if collisional coefficients for each individual hyperfine component of the $J = 1 \rightarrow 0$ transition of N_2H^+ have different values. Hyperfine selective collisional excitation has been discussed in detail by Stutzki & Winnewisser (1985) to interpret observed intensity anomalies in the hyperfine structure of NH_3 and HCN. Another possibility is that the anomalies could arise from different trapping, depending on the fact that the components have different optical depth, and thus get different amounts of radiative excitation, as in the case of HCN studied by Kwan & Scoville (1975).

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REFERENCES

- Benson, P. J., Caselli, P., Chen, H., Tafalla, M., & Myers, P. C. 1995, in preparation
 Benson, P. J., Caselli, P., Myers, P. C., & Goodman, A. A. 1994, in ASP Conf. Ser. 65, Cloud, Cores, and Low Mass Stars, ed. D. P. Clemens & R. Barvainis (San Francisco: ASP), 67
 Benson, P. J., & Myers, P. C. 1989, ApJS, 71, 89
 Cazzoli, G., Corbelli, G., Degli Esposti, C., & Favero, P. G. 1985, Chem. Phys. Lett., 118, 164
 Forveille, T., Guilloteau, S., & Lucas, R. 1989, CLASS Manual (Grenoble: IRAM)
 Green, S., Montgomery, J. A., & Thaddeus, P. 1974, ApJ, 193, L89
 Kwan, J., & Scoville, N. 1975, ApJ, 195, L85
 Pickett, H. M. 1991, J. Mol. Spectrosc., 148, 371
 Stutzki, J., & Winnewisser, G. 1985, A&A, 144, 1
 Thaddeus, P., Krisner, L. C., & Loubser, J. H. N. 1964, J. Chem. Phys., 40, 257
 Thaddeus, P., & Turner, B. E. 1975, ApJ, 201, L25
 Turner, B. E. 1974, ApJ, 193, L83
 Turner, B. E., & Thaddeus, P. 1977, ApJ, 211, 755
 Vrtilik, J. M., Gottlieb, C. A., & Thaddeus, P. 1987, ApJ, 314, 716
 Womack, M., Ziurys, L. M., & Wyckoff, S. 1992, ApJ, 387, 417