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LETTER TO THE EDITOR

Spectroscopic parameters and rest frequencies of isotopic methylidynium, CH$^+$

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ABSTRACT

Context. Astronomical observations toward Sagittarius B2(M) as well as other sources with APEX have recently suggested that the rest frequency of the $J = 1-0$ transitions of ^{13}CH$^+$ is too low by about 80 MHz.
Aims. Improved rest frequencies of isotopologs of methylidynium should be derived to support analyses of spectral recording obtained with the ongoing *Herschel* mission or the upcoming SOFIA.
Methods. Laboratory electronic spectra of four isotopologs of CH$^+$ have been subjected to one global least-squares fit. Laboratory data for the $J = 1-0$ ground state rotational transitions of CH$^+$, ^{13}CH$^+$, and CD$^+$, which became available during the refereeing process, have been included in the fit as well.
Results. An accurate set of spectroscopic parameters has been obtained together with equilibrium bond lengths and accurate rest frequencies for six CH$^+$ isotopologs: CH$^+$, ^{13}CH$^+$, ^{13}CD$^+$, CD$^+$, ^{14}CH$^+$, and CT$^+$.
Conclusions. The present data will be useful for the analyses of *Herschel* or SOFIA observations of methylidynium isotopic species.

Key words. molecular data – radio lines: ISM – submillimeter: ISM – ISM: molecules

1. Introduction

The first three molecules detected in space in the 1930s were methylidynium, CH$^+$, methylidyne, CH, and cyanogen, CN. Douglas & Herzberg (1941) identified three absorption lines, which had been observed toward several stars, as belonging to the A $^1\Pi-X$ $^1\Sigma^+$ electronic transition of CH$^+$. They were assigned to the $R(0)$ ($\equiv J = 1-0$) transitions of the $v = 0-0$, $1-0$, and $2-0$ vibrational bands.

The $J = 2-1$, $3-2$, and $4-3$ rotational transitions were identified by Cernicharo et al. (1997) in spectra recorded with the Long Wavelength Spectrometer of the Infrared Space Observatory toward the planetary nebula NGC 7027. The observation of the $J = 1-0$ rotational transitions at 835 137.5 MHz (Amano 2010) is hampered by a telluric line of molecular oxygen close by Drouin et al. (2010, and references therein) and thus requires observations from space, e.g. with the recently launched *Herschel* satellite or with the Stratospheric Observatory For Infrared Astronomy (SOFIA).

Recently, Falgarone et al. (2005) reported on the observation of the $J = 1-0$ transition of ^{13}CH$^+$ in absorption toward the star-forming region G10.6-0.4. They deduced 830 132 (3) MHz as the prefered rest frequency based on scaling from the CH$^+$ laboratory rest frequency. Alternative rest frequencies of 830 107 (1) or 830 193 (4) MHz were excluded. Very recently, Menten et al. (2010) carried out an absorption study with the Atacama Pathfinder EXperiment (APEX) of light hydride species toward the evolved massive star-forming region Sagittarius (Sgr for short) B2(M). They detected low-lying rotational transitions of ^{13}CH$^+$, H^{35}Cl, H^{37}Cl, and, for the first time, of SH$^+$. Similar studies have been carried out toward additional sources

(F. Wyrowski, private communication). A comparison of the line profiles among these species together with observations of additional species at lower frequencies suggested a rest frequency of about 830 210 MHz, approximately 80 MHz higher than the prefered rest frequency from Falgarone et al. (2005), but in reasonable agreement with an alternative rest frequency of 830 193 (4) MHz they had dismissed.

Pearson & Drouin (2006) obtained a value of 835 078.950 (75) MHz as the $J = 1-0$ transition frequency of CH$^+$, about 5 MHz lower than they deduced from analyses of the A $^1\Pi-X$ $^1\Sigma^+$ electronic spectra of four isotopologs (Carrington & Ramsay 1982; Bembenek 1997a; Bembenek et al. 1987; Bembenek 1997b).

During the refereeing process of this manuscript I received $J = 1-0$ transition frequencies for CH$^+$, ^{13}CH$^+$, and CD$^+$, very recently obtained by Amano (2010). While the latter two frequencies (~830 216 and 453 522 MHz) were rather close to predictions made from the spectroscopic parameters of the respective isotopolog (Bembenek 1997a; Bembenek et al. 1987), the CH$^+$ frequency (835 137.5 MHz) was almost 40 MHz higher than that deduced from a more recent analysis of the CH$^+$ electronic spectrum (Hakalla et al. 2006), but almost 70 MHz higher than measurements by Pearson & Drouin (2006) indicated. Because no further rotational data and no infrared transitions have been reported thus far, determinations of methylidynium rest frequencies still rely quite heavily on the electronic spectra.

In the current work, I present a combined reanalysis of the A $^1\Pi-X$ $^1\Sigma^+$ electronic spectra of four isotopic species of CH$^+$ together with the available rotational transitions to derive reliable rest frequencies for CH$^+$ isotopologs.

2. Analysis and discussion

The ro-vibrational energy levels of a diatomic molecule AB can be represented by the Dunham expression

$$E(v, J)/h = \sum_{i,j} Y_{ij}(v + 1/2)^i J^j (J + 1)^j, \tag{1}$$

where the Y_{ij} are the Dunham parameters. In electronic states different from Σ states, i.e. in states with orbital angular momentum $\Lambda > 0$, the expansion in $J(J+1)$ is commonly replaced by an expansion in $J(J+1)-\Lambda^2$, see e.g. (Watson 1980). Obviously, the two are the same for Σ states with $\Lambda = 0$, such as the ground electronic state of CH$^+$. The A state is a $^1\Pi$ electronic state with $\Lambda = 1$, and the expansion has been carried out in $J(J+1)-1$; an expansion in $J(J+1)$ can be found also, see e.g. the case of the $^2\Pi$ radical BrO (Drouin et al. 2001).

The energy levels in a $^1\Pi$ electronic state are modified by a λ-doubling which can be expressed as

$$E^\lambda(v, J)/h = \pm J(J+1)/2 \sum_{i,j} q_{ij}(v + 1/2)^i J^j (J + 1)^j, \tag{2}$$

where the λ-doubling parameters q_{ij} scale with $\mu_c^{-2-(i+2j)/2}$ (Brown et al. 1979).

Watson (1973, 1980) has shown that several isotopic species of AB can be fit jointly by constraining the Y_{ij} to

$$Y_{i,j} = U_{i,j}\left(1 + \frac{m_e \Delta_{ij}^A}{M_A} + \frac{m_e \Delta_{ij}^B}{M_B}\right)\mu_c^{-(i+2j)/2}, \tag{3}$$

where $U_{i,j}$ is isotope invariant, m_e is the mass of the electron, $\mu_c = M_A M_B/(M_A + M_B nm_e)$ is the charge-corrected reduced mass of AB and n is the charge of AB, M_A is the mass of atom A, and Δ_{ij}^A is a Born-Oppenheimer breakdown (BOB) term. $U_{ij}\mu^{-(i+2j)/2}\Delta_{ij}^A m_e/M_A$ is sometimes abbreviated as δ_{ij}^A. Moreover, it is noteworthy that both Δ_{ij}^A and δ_{ij}^A are defined negatively in some papers. Obviously, Δ_{ij}^B and δ_{ij}^B are defined equivalently.

A specific transition of the $A\,^1\Pi-X\,^1\Sigma^+$ electronic spectrum of CH$^+$ is well described by the isotopolog, the vibrational quantum numbers in the upper and lower electronic states, the lower state rotational quantum number J and whether the transition belongs to the R, Q, or P-branch in which the upper state rotational quantum number is $J + 1$, J, and $J-1$, respectively; J is commonly given in parentheses.

None of the investigations of the $A-X$ electronic spectrum of CH$^+$ and its isotopologs provided uncertainties for individual lines, only estimates of average precision and accuracy. In the present work the initial uncertainties were estimated for each isotopolog and each vibronic band separately based on average residuals between observed frequencies and those calculated from the spectroscopic parameters. During the analysis, the uncertainties were adjusted to yield an rms error very close to the theoretical value of 1.0, usually slightly lower. Transitions with residuals between observed and calculated frequencies much higher than the average were omitted from the fit. These may have been weak lines with very low or very high values of J or accidentally overlapped lines. For each isotopolog and each vibronic band the finally ascribed uncertainty will be given below in parentheses in units of 0.001 cm^{-1} together with the lines from the original literature, which have been omitted from the fit. Lines already discarded in the original analyses were usually

Table 1. Experimentally determined spectroscopic parameters[a] (cm^{-1}, MHz) of methylidynium, ^{12}CH$^+$ in its $X\,^1\Sigma^+$ and $A\,^1\Pi$ electronic states from a global fit involving four isotopologs.

Parameter	Value
$X\,^1\Sigma^+$	
$U_{10}\mu^{-1/2}$	2 860.387 (22)
$U_{10}\mu^{-1/2}\Delta_{10}^C m_e/M_C$	−0.147 (18)
$U_{10}\mu^{-1/2}\Delta_{10}^H m_e/M_H$	−2.672 (13)
$U_{20}\mu^{-1}$	−59.369 7 (61)
$U_{20}\mu^{-1}\Delta_{20}^H m_e/M_H$	0.051 0 (62)
Y_{30}	0.225 46 (106)
$U_{01}\mu^{-1}$	427 360.68 (121)
$U_{01}\mu^{-1}\Delta_{01}^C m_e/M_C$	−155.80 (21)
$U_{01}\mu^{-1}\Delta_{01}^H m_e/M_H$	−2 146.22 (177)
$U_{11}\mu^{-3/2}$	−14 917.7 (57)
$U_{11}\mu^{-3/2}\Delta_{11}^H m_e/M_H$	58.6 (27)
Y_{21}	91.8 (41)
Y_{31}	−3.84 (66)
$U_{02}\mu^{-2}$	−42.468 (21)
$U_{02}\mu^{-2}\Delta_{02}^H m_e/M_H$	0.563 (20)
Y_{12}	0.960 (34)
Y_{22}	−0.045 (10)
$Y_{03} \times 10^3$	4.264 (86)
$Y_{13} \times 10^3$	−0.726 (53)
$Y_{04} \times 10^{6c}$	−0.4
$C(^{13}C)$	1.091 (28)
$A\,^1\Pi$	
$U_{00}(H)^b$	23 639.326 (23)
$U_{00}\Delta_{10}^C m_e/M_C(H)^b$	−19.620 (24)
$U_{00}(D)^b$	23 786.537 (24)
$U_{00}\Delta_{10}^C m_e/M_C(D)^b$	−26.436 (26)
$U_{10}\mu_c^{-1/2}(H)$	1 864.379 (14)
$U_{10}\mu_c^{-1/2}\Delta_{10}^C m_e/M_C(H)$	0.106 (12)
$U_{10}\mu_c^{-1/2}(D)$	1 367.473 (17)
$U_{10}\mu_c^{-1/2}\Delta_{10}^C m_e/M_C(D)$	−0.180 (19)
$Y_{20}(H)$	−115.884 7 (48)
$Y_{20}(D)$	−60.815 4 (47)
$Y_{30}(H)$	2.639 48 (85)
$Y_{30}(D)$	0.776 92 (78)
$U_{01}\mu_c^{-1}$	356 717.5 (63)
$U_{01}\mu_c^{-1}\Delta_{01}^C m_e/M_C$	−9.2 (53)
$U_{01}\mu_c^{-1}\Delta_{01}^H m_e/M_H$	−316.4 (24)
$U_{11}\mu_c^{-3/2}$	−27 562.7 (70)
$U_{11}\mu_c^{-3/2}\Delta_{11}^H m_e/M_H$	24.06 (147)
Y_{21}	−634.8 (49)
Y_{31}	137.76 (95)
Y_{02}	−58.166 (26)
Y_{12}	−2.502 (61)
Y_{22}	−0.252 (44)
Y_{32}	0.149 3 (87)
$Y_{03} \times 10^3$	−0.876 (84)
$Y_{13} \times 10^3$	−0.911 (63)
q_{00}	1 234.25 (108)
q_{10}	−96.53 (82)
q_{01}	−0.643 6 (98)
q_{11}	−0.020 3 (79)

Notes. [a] The vibrational parameters Y_{i0} as well as related parameters are given in cm^{-1}; all other Y_{ij} as well as related parameters are given in MHz. Numbers in parentheses are one standard deviation in units of the least significant figures. [b] Determined with respect to the lowest allowed energy levels of each electronic state. [c] Estimated, see text.

omitted here as well; these lines will not be mentioned specifically.

The fit was started with the CH$^+$ data from Carrington & Ramsay (1982) and Hakalla et al. (2006), and the initial parameters were taken from the latter work. As the Y_{0i} got smaller by factors of $\sim-10\,000$, Y_{04} was estimated as -0.4 Hz. Hakalla et al. (2006) measured the $v = 0-0$ (5 ($\times0.001$ cm^{-1}), $R(17)$), $0-1$ (5, $-$), and $2-1$ (9, $P(14)$) bands, while Carrington & Ramsay (1982) obtained data for the $v = 0-0$ (5, $P(6)$), $0-1$ (6, $Q(14)$), $1-0$ (12, $R(3)$), $1-1$ (7, $P(7,8)$), $1-2$ (6, $P(7)$), $1-3$ (4, $R(5)$), $2-1$ (5, $-$), and $3-1$ (7, $Q(9)$, $P(2)$) bands. The CH$^+$ $J = 1-0$ rotational transition predicted from this data set is $835\,093.42 \pm 5.25$ MHz, almost exactly 10 MHz higher than what Pearson & Drouin (2006) obtained and about 14.5 MHz higher than the line these authors measured in the laboratory. Inclusion of data from three additional isotopologs, as described below, shifted the prediction to somewhat higher frequencies, $\sim835\,112$ MHz being the highest as long the the weights of the CH$^+$ data were not reduced.

Scaling these parameters directly with μ_c yields $830\,146.97$ MHz for the ^{13}CH$^+$, $J = 1-0$ transition. In contrast, predictions from Bembenek (1997a) yield a value approximately 80 MHz higher, suggesting a large BOB term for Y_{01} will be necessary at least in the ground electronic state. Inclusion of data from the $v = 0-0$ (4, $-$) band confirmed this. These data also required a BOB term for Y_{01} as well as for the term value T of the excited electronic A state, though the latter value appeared to be too high to be considered a BOB term in the usual sense. The $J = 1-0$ ground state rotational transition was now predicted at $830\,206.82 \pm 5.85$ MHz, 60 MHz higher than from direct scaling as a result of large effects caused by the breakdown of the Born-Oppenheimer approximation. The $v = 0-1$ (4, $-$), $2-0$ (8, $R(8)$) and $2-1$ (12, $-$) bands were included without much difficulty. In the $v = 1-0$ (6, $-$) band, in which already several lines were not used in the original fits, the $R(5,9)$ and $P(3,4,10)$ lines were omitted in addition in the present work. In the $v = 1-1$ (9, $-$) band, $R(6,7)$ are in fact $R(7,8)$, similarly the J values have to be revised one up for $Q(7,8)$. Moreover, $R(7,9,10)$ were omitted from the fit. With more vibronic bands included, a correction term for Y_{10} was also employed in the fit.

The CD$^+$ data from Bembenek et al. (1987) proved to be much more difficult to reproduce. Not only were BOB terms required for the Y_{01} and Y_{10}, as for ^{13}CH$^+$, but also for Y_{20}, Y_{11}, and Y_{02} in both electronic states. The correction term to T turned out to be very large again. The $v = 0-0$ (4, $-$), $0-1$ (4, $R(12)$), $1-0$ (3, $R(11)$), $P(2,6,12,13)$), $1-2$ (9, $-$), $2-1$ (6, $-$), and $3-1$ (5, $Q(1)$, $P(6,11)$) bands were used in the fit. The $v = 1-3$ band was measured but not used in the fit by Bembenek et al. (1987), it is on average about 0.09 cm^{-1} too low. In addition, $v = 2-0$ was also not used in the present fit as it was about 0.03 cm^{-1} too low. Its inclusion in the fit would have afforded *both* $v = 2-1$ and $v = 3-1$ to be omitted from the fit.

Lastly, ^{13}CD$^+$ data from Bembenek (1997b) were included in the fit, namely the $v = 0-0$ (6, $P(12,13,14)$) and $1-0$ (4, $-$) bands. The band origins were not quite compatible with the other data. In combination with the considerable corrections required for T, this was interpreted as a sign of the perturbation of the A electronic state. Therefore, separate term values as well as Y_{i0} were used for CH$^+$ and CD$^+$. In addition, different carbon BOB terms were required for T and Y_{10}.

The referee of this manuscript pointed out new laboratory measurements of the $J = 1-0$ rotational transitions of CH$^+$, ^{13}CH$^+$, and CD$^+$ which I received soon thereafter from the

Table 2. Derived spectroscopic parameters^a (cm^{-1}, MHz, unitless) of methylidynium, ^{12}CH$^+$ in its $X\ ^1\Sigma^+$ and $A\ ^1\Pi$ electronic states from a global fit involving four isotopologs.

Parameter	Value
$X\ ^1\Sigma^+$	
Y_{10}	2 857.569 2 (92)
Δ_{10}^{C}	-1.120 (137)
Δ_{10}^{H}	$-1.715\,9$ (86)
Y_{20}	$-59.318\,7$ (60)
Δ_{20}^{H}	-1.578 (188)
Y_{01}	425 058.66 (248)
Δ_{01}^{C}	$-7.974\,9$ (105)
Δ_{01}^{H}	$-9.226\,3$ (76)
Y_{11}	$-14\,859.0$ (67)
Δ_{11}^{H}	-7.222 (33)
Y_{02}	-41.905 (20)
Δ_{02}^{H}	-24.36 (86)
$A\ ^1\Pi$	
$T(\mathrm{H})^b$	23 619.707 (5)
$T(\mathrm{D})^b$	23 760.102 (5)
$Y_{10}(\mathrm{H})$	1 864.485 (8)
$\Delta_{10}^{\mathrm{C}}(\mathrm{H})$	1.244 (145)
$Y_{10}(\mathrm{D})$	1 367.294 (8)
$\Delta_{10}^{\mathrm{C}}(\mathrm{D})$	-2.876 (306)
Y_{01}	356 391.8 (29)
Δ_{01}^{C}	-0.56 (33)
Δ_{01}^{H}	-1.630 (12)
Y_{11}	$-27\,538.7$ (71)
Δ_{11}^{H}	-1.604 (98)

Notes. $^{(a)}$ The electronic term values T, and the vibrational parameters Y_{i0} are given in cm^{-1}; all other Y_{ij} are given in MHz; the Δ_{ij}^{X} are unitless. Numbers in parentheses are one standard deviation in units of the least significant figures. $^{(b)}$ Determined with respect to the lowest allowed energy levels of each electronic state.

author (Amano 2010). The ^{13}CH$^+$ and CD$^+$ frequencies were close to the predictions based on parameters from Bembenek (1997a); Bembenek et al. (1987) as well as predictions from present fits which only included data from the electronic spectra. In contrast, the CH$^+$ frequency was higher than predictions from the current fits by between 25 and 45 MHz. The CH$^+$ and ^{13}CH$^+$ lines showed large Zeeman splitting in a magnetic field, which, as already mentioned by Amano (2010), requires a high g_J-value for a $^1\Sigma^+$ molecule. This in turn leads to high Δ_{01} BOB terms for CH$^+$ in the ground electronic state, see below. The large g_J-value is also compatible with the large ^{13}C nuclear spin-rotation splitting of 1.6 MHz in the $J = 1-0$ transition of ^{13}CH$^+$, as already pointed out by Amano (2010).

The fit easily accomodated these rotational data; the rms error of the fit only slightly increased from 0.944 to 0.991. This rather small deterioration of the fit may indicate unfavorable correlation of the parameters, which is reduced by the inclusion of the pure rotational data in the fit. Weighting two vibronic bands of CH$^+$ each from Carrington & Ramsay (1982); Hakalla et al. (2006) slightly lower ($\leq25\%$) yielded rms errors of all vibronic bands very close to 1.0 and an overall rms error of 0.945. The inclusion of the rotational data caused the ^{13}C BOB correction value to $U_{01}\mu^{-1}$ in the ground electronic state to be reduced by almost half, similar changes in magnitude occured in the excited A state ^{13}C BOB term. These changes were mostly compensated

Table 3. Measured (Amano 2010) and calculated low-J rotational transition frequencies[a] (MHz) of six isotopic species of CH^+.

| | Measured | Calculated | |
	$J = 1-0$	$J = 1-0$	$J = 2-1$
CH^+	835 137.504 (20)	835 137.503 (20)	1 669 281.3 (3)
$^{13}CH^+$	830 216.095 (30)[b]	830 216.096 (22)	1 659 450.3 (3)
CD^+	453 521.851 (20)	453 521.851 (20)	906 752.0 (1)
$^{13}CD^+$		448 539.258 (26)	896 793.2 (1)
$^{14}CH^+$		826 012.748 (45)	1 651 053.6 (3)
CT^+		325 443.364 (70)	650 736.8 (1)

Notes. [a] Numbers in parentheses are one standard deviation in units of the least significant figures; see the text for discussion of uncertainties. [b] Value corrected for hyperfine splitting; two lines were measured, see text, each accurate to 30 kHz.

by changes in $U_{01}\mu^{-1}$, to a much lesser extent by the BOB term for H. Changes considerably outside the uncertainties also occured for $U_{02}\mu^{-2}$ and Y_{02} in the X and A state, respectively. All other changes were mostly well within the uncertainties.

The final spectroscopic parameters are given in Table 1; further spectroscopic parameters, which were derived from these parameters, are given in Table 2. Predictions of the $J = 1-0$ and $2-1$ transitions of six isotopologs are given in Table 3 together with the measured ones; these should be useful for astronomical observations as well as for laboratory spectroscopic investigations. The three laboratory rotational transitions (Amano 2010) determine three parameters related to U_{01}. In addition, the weight of each line in the fit is much larger than that of a rovibronic transition. Therefore, it is not surprising that in these cases predicted frequencies and their uncertainties are essentially identical to laboratory values (Amano 2010). More extensive predictions, including those of rovibrational spectra, as well as details of the fit file will be available in the Cologne Database for Molecular Spectroscopy, CDMS,[1] (Müller et al. 2001, 2005). Extrapolations beyond $J = 1-0$ should be viewed with some caution, meaning the actually measured transition frequency may be more than three times the predicted uncertainty away from the calculated position, especially for the CH^+ main isotopolog because the rotational transition was rather far away from prediction absed on electronic spectra. Predictions with $J \geq 10$ should be viewed with great caution.

In contrast to e.g. Carrington & Ramsay (1982), but in agreement with Hakalla et al. (2006), the excited A electronic state could be reproduced in a rather satisfactorily manner using power series in $v + 1/2$ besides $J(J+1)-1$ for each isotopolog individually and, with the exception of the term value and the vibrational spacings, also for the combined data set of four isotopic species. The fact that separate parameters had to be used for CH^+ and CD^+ may be explained by a perturbation of the A state. Essentially all parameters Y_{ij} with $j > 0$ or related parameters $U_{i,j}\mu_c^{-(i+2j)/2}$ in Table 1 as well as the BOB terms in Table 2 appear to be reasonable.

The Y_{ij} or related parameters for the X ground electronic state in Table 1 again appear rather reasonable. The BOB terms Δ_{i0} in Table 2 are negative and their magnitudes are normal (Watson 1973, 1980; Drouin et al. 2001; Müller et al. 2005, 2007). The BOB terms Δ_{i1}, however, are rather large, but of similar magnitude. Watson (1973) has shown that Δ_{01} has one contribution $g_J m_e/m_p$, where g_J is the rotational g-factor and m_p is the mass of the proton, which may get big for low-lying

electronic states of the same multiplicity, i.e. singlet states in the case of CH^+. Because Y_{11} is the first vibrational correction term to Y_{01} it is probably reasonable that Δ_{11}^H is large in magnitude also. Gauss & Puzzarini (2010) have shown that Δ_{01} can be calculated ab initio and presented results which were compared with experimental data for SiS (Müller et al. 2007), HCl, and HF. Calculations for CH^+ will be very welcome.

Equilibrium structural parameters of 112.77543 (16) and 123.45370 (106) pm have been derived for the X and A electronic state, respectively, in the BO approximation which are very different from 113.08026 (33) and 123.50991 (50) pm obtained for the CH^+ isotopolog under consideration of the breakdown of the BO approximation. The latter values agree fairly well with 113.08843 (30) and 123.5053 (37) pm obtained by Hakalla et al. (2006).

3. Conclusion

The $A\ ^1\Pi-X\ ^1\Sigma^+$ electronic spectra of four isotopologs plus the rotational data for three species have been reproduced rather well with one set of spectroscopic parameters and with only comparatively few transitions omitted from the fit. Considering that the A electronic state has been judged to be perturbed by an unidentified state, the spectroscopic parameters show few peculiarities.

The predicted $J = 1-0$ transition frequencies of the three remaining isotopologs as well as higher-J predictions for all species will be useful for future astronomical observations or laboratory spectroscopic investigations. The data for $^{14}CH^+$ and CT^+ may be useful for determining if ^{14}C or T play a significant role in certain (circumstellar) environments.

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