# A Spectral Atlas of the $v_{12}$ Fundamental of ${ }^{13} \mathrm{C}^{12} \mathrm{CH}_{6}$ in the $12 \mu \mathrm{~m}$ Region 

Mark Weber, Dennis Reuter, J. Marcos Sirota, and John Hillman NASA Goddard Space Flight Center<br>Greenbelt, Maryland<br>William E. Blass<br>Department of Physics<br>University of Tennessee

National Aeronautics and
Space Administration
Goddard Space Flight Center
Greenbelt, Maryland 20771


#### Abstract

The recent discovery of the minor isotopomer of ethane, ${ }^{13} \mathrm{C}^{12} \mathrm{CH}_{6}$, in the planetary atmospheres of Jupiter and Neptune, added ethane to the molecules which can be used to determine isotopic ${ }^{12} \mathrm{C} /{ }^{12} \mathrm{C}$ ratios for the jovian planets. The increased spectral resolution and coverage of the IR and far-IR instruments to be carried on the Cassini mission to Saturn and Titan may enable the detection of the minor isotopomer. Accurate frequency and cross-section measurements of the $\nu_{12}$ fundamental under controlled laboratory condition are important to interpret current and future planetary spectra. High resolution spectra of the minor isotopomer ${ }^{13} \mathrm{C}^{12} \mathrm{CH}_{6}$ have been recorded in the $12.2 \mu \mathrm{~m}$ region using the Kitt Peak Fourier Transform (FTS) and the Goddard Tunable Diode Laser spectrometer (TDL). In a global fit to 19 molecular constants in a symmetric top Hamiltonian, transition frequencies of the $\nu_{12}$ fundamental ranging up to $J=35$ and $K=20$ have been determined with a standard deviation of less than $0.0005 \mathrm{~cm}^{-1}$. From selected line intensity measurements, a vibrational dipole moment for the $\nu_{12}$ fundamental has been derived. Observed and calculated spectra covering the region from $740 \mathrm{~cm}^{-1}$ to $910 \mathrm{~cm}^{-1}$ are presented. A compilation of transition frequencies, line intensities, and lower state energies are included for general use in the astronomical community.


## Introduction

The current spectroscopic study of the minor isotopomer ${ }^{13} \mathrm{C}^{12} \mathrm{CH}_{6}$ is motivated by its recent discovery as a constituent in the atmosphere of Jupiter by Wiedemann et al.(1). Employing a cryogenic echelle array spectrometer, Orton et al.(2) identified traces of ${ }^{13} \mathrm{C}$ ethane in Neptune's atmosphere. In both cases a near-terrestrial isotopic ${ }^{12} \mathrm{C} /{ }^{13} \mathrm{C}$ ratio has been found (1,2). Laboratory measurements of frequencies and intensities are important for future identification and atmospheric modeling of ${ }^{13} \mathrm{C}^{12} \mathrm{CH}_{6}$ in the outer planetary atmospheres using for instance high resolution heterodyne remote sensing.

Regular ethane and its deuterated species have been studied in some detail in the mid- and far-infrared (3-9). The minor isotopomer ${ }^{13} \mathrm{C}^{12} \mathrm{CH}_{6}$ has been investigated in the $2700 \mathrm{~cm}^{-1}$ region of the $\nu_{3}+\nu_{4}$ overtone (equivalent to $\nu_{2}+\nu_{6}$ in normal ethane) by Lafferty et al.(10). More recently, in studies of the $12 \mu \mathrm{~m}$ region Kurtz et al.(11) obtained the ratio of the integrated intensity of the ${ }^{r} Q_{0}$-branch of the $\nu_{12}$ band of ${ }^{13} \mathrm{C}^{12} \mathrm{CH}_{6}$ with respect to the equivalent $\nu_{9}$ band of normal ethane. These studies were based on high resolution ( $0.0025 \mathrm{~cm}^{-1}$ ) data recorded with the 1 m McMath FTS instrument at the National Solar Observatory in Kitt Peak, Arizona. The same laboratory data have been analyzed to assign rotation-torsional transitions in the $\nu_{12}$ fundamental and to determine ground state rotational constants from lower state combination differences (12).

More recently, the analysis has been extended to determine upper state constants for the $\nu_{12}$ fundamental of the minor isotopomer and to derive barriers to internal rotation in the ground and vibrational excited state (13). In this publication, a complete line by line compilation of calculated frequencies, lower state energies, and line strengths are published. From the molecular parameters a spectral atlas has been produced covering the region from 740 to $910 \mathrm{~cm}^{-1}$.

## Experimental Details

Several spectra at room and typical planetary temperatures ( 101 K and 161 K ) were recorded using the $1-\mathrm{m}$ Fourier transform spectrometer at the Kitt Peak National Solar Observatory (11,12). This instrument was operated in a double-pass configuration yielding a spectral resolution of $0.0025 \mathrm{~cm}^{-1}$ (14). The ${ }^{13} \mathrm{C}^{12} \mathrm{CH}_{6}$ sample was provided in a $99 \%$ purified form by Matheson Co. No traces of the major isotopomer have been found in the unapodized FTS spectra: Calibration to absolute wavenumbers was done using wellisolated $P$ - and $R$-branch lines of the $\nu_{2}^{1 e}$ and $2 \nu_{2}^{0 e}$ band of $\mathrm{N}_{2} \mathrm{O}$ at $580 \mathrm{~cm}^{-1}$ and 1168 $\mathrm{cm},^{-1}$ respectively (12).

Details of the tunable diode laser system at NASA Goddard Space Flight Center can be found in Ref. (15). Several $Q$-branches ranging from $K \Delta K=-6$ to 6 were measured to obtain complementary information on observed torsional splittings (13). These spectra were recorded with gas pressures of $p=1.5$ Torr and an absorption cell length of $\ell=30 \mathrm{~cm}$. Relative wavenumber calibrations were obtained using a 3 inch solid Ge etalon ( 0.01623 $\mathrm{cm}^{-1}$ fringe spacing). A total of 68 splittings from the diode laser observations (Table II)

Table I. Molecular constants of ${ }^{13} \mathrm{C}^{12} \mathrm{CH}_{6}$ in $\mathrm{cm}^{-1}$. $\mathrm{C}_{\sigma}$ is the torsional Coriolis interaction parameter connecting the $v_{12}=1$ state with the $v_{6}=3$ state. $\sigma_{F}$ is the weighted standard deviation of the overall fit. 2307 transitions and torsional splitting values survived the fit. For convenience parameters are also given in Hz .

| $\nu_{o}$ | 820.931 394(42) |  |  |
| :---: | :---: | :---: | :---: |
| $B_{\text {o }}$ | $0.6497649(91)$ | 19 479.46(27) | MHz |
| $A_{0}$ | $2.66852 \dagger$ | $80000.2 \dagger$ | MHz |
| $D_{o}^{J}$ | $0.99385(67) \times 10^{-6}$ | 29.795(20) | kHz |
| $D_{o}^{J K}$ | $2.6088(87) \times 10^{-6}$ | 78.08(21) | kHz |
| $D_{o}^{K}$ | $9.54 \times 10^{-6} \dagger \dagger$ | $286 \dagger \dagger$ | kHz |
| $\alpha_{12}^{B}$ | $1.29618(50) \times 10^{-3}$ | 38.858(15) | MHz |
| $\alpha_{12}^{A}$ | $-7.7964(11) \times 10^{-3}$ | -233.730(33) | MHz |
| $\beta_{12}^{J}$ | $3.07(10) \times 10^{-9}$ | 92.0(39) | Hz |
| $\beta_{12}{ }^{\text {J }}$ | $-2.063(81) \times 10^{-8}$ | -618(24) | Hz |
| $\beta_{12}^{K}$ | $-1.868(20) \times 10^{-7}$ | -5600(60) | Hz |
| $(A \zeta)_{12}^{z}$ | $0.696191(18)$ | 20871.28 (54) | MHz |
| $\eta_{12}^{J}$ | $-2.024(21) \times 10^{-6}$ | -60.68(63) | kHz |
| $\eta_{12}^{K}$ | $2.3911(30) \times 10^{-5}$ | 716.83(90) | kHz |
| $q_{12}^{o}$ | $-1.72670(83) \times 10^{-3}$ | 51.765(25) | MHz |
| $q_{12}^{J}$ | $9.07(88) \times 10^{-9}$ | 272(26) | Hz |
| $V_{6}^{(0)}$ | 1026.888(79) | $30785.3(24)$ | GHz |
| $V_{6}^{(12)}$ | 1088.61(77) | 32 635(24) | GHz |
| $F_{1 J}$ | $-1.542(12) \times 10^{-2}$ | -462.3(36) | MHz |
| $F_{1 K}$ | $-0.947(11) \times 10^{-2}$ | -283.9(33) | MHz |
| $C_{\sigma}$ | $3.6510(28) \times 10^{-2}$ | 1094.54(84) | MHz |
| $\begin{aligned} & \sigma_{F} \\ & \text { data } \end{aligned}$ | $5.5 \times 10^{-4} \quad 2307$ | $2447^{16 \mathrm{MHz}}$ |  |

$\dagger$ Moazzen-Ahmadi et al.(9)
$\dagger \dagger$ Duncan et al.(16)
were added to the FTS data in the global fit to determine molecular constants for $\nu_{12}$.

## Global Least Squares Fit

An iterative bi-weighted non-linear least squares fit of the upper and lower state energies has been carried out simultaneously. The upper state Hamiltonian included off-diagonal $\ell$-resonance terms within the $v_{12}=1$ state and off-diagonal torsional Coriolis interaction terms connecting with the excited torsional state of $v_{6}=3$. The results of the global fit are summarized in Table I (13). A more detailed account of the fitting procedure and the Hamiltonian used can be found in Ref. (13).

Of the 21 parameters employed in the upper and lower state Hamiltonian, the rotational constants $A_{o}$ and $D_{o}^{K}$ have been fixed to $2.66852 \mathrm{~cm}^{-1}(9)$ and $9.54 \times 10^{-6} \mathrm{~cm}^{-1}(16)$, respectively. The rotation-torsional constants $F_{1 J}$ and $F_{1 K}$ in the $v_{12}=1$ state were fixed to the ground state value. Observed torsional splittings recorded with the TDL spectrometer have been weighted by an extra factor of 4 corresponding to the enhancement in spectral resolution over the FTS data.

The intrinsic and unperturbed torsional splitting between the components of the torsional doublets as calculated from the upper and lower state barriers is $1.53 \times 10^{-3}$ $\mathrm{cm},^{-1}$ which is not resolved in the current FTS data. For $K=3 n$ transitions with relative intensities of $2: 1$, both peaks of the doublets can be measured from the FTS data if they are separated by more than about $4.5 \times 10^{-3} \mathrm{~cm}^{-1}$ and for $K \neq 3 n$ (4:1 relative intensities) by more than $7.0 \times 10^{-3} \mathrm{~cm} .^{-1}$ Therefore, most torsional doublets could not be resolved, except near the crossing region which occurs at $K \Delta K=-18$. Most transition frequencies, particularly in the $R$-branches $(\Delta K=1)$ and as $J$ approaches $K$, represent rather an average of the doublets. In order to avoid "frequency pulling" (5), transition frequencies of the $K=3 n$ series have been calculated using a weighted average of the two calculated frequencies of the doublets. The weights were chosen according to their statistical weights. Simulated spectra showed that such a weighting scheme yields a good approximation. In cases where one of the components of the doublets is rather weak, the average of the frequencies tends to be closer to the frequency of the strong component and therefore observed frequencies of unresolved $K \neq 3 n$ torsional doublets (with 4:1 relative intensity ratio) have been assigned to the stronger component of the doublet.

## Intensity Analysis

Forty-two individual lines of the $\nu_{12}$ band observed with the FTS have been measured to retrieve their intensities. Only those lines whose torsional components were sufficiently separated (mostly ${ }^{p} P_{K}(J)$ lines) permitting a measurement of both components were included in the analysis. Since the intensity retrieval is constrained to a limited region, no attempts were made to determine the $F$-factors. Some of the very weak intensities have been discarded if their peak strength was below $10 \%$. The lines were fitted to a convolution

Table II. Torsional Splittings $\Delta_{\text {obs }}$ measured with the TDL for the $\nu_{12}$ fundamental of ${ }^{13} C^{12} \mathrm{CH}_{6}$.

| $\Delta K$ | $\Delta J$ | $K$ |  | $\begin{aligned} & \Delta_{\text {obs }} \quad \mathrm{o-c} \\ & {\left[\mathrm{~cm}^{-1}\right]} \end{aligned}$ | $\Delta K$ | $\Delta J$ | K | $J$ | $\begin{gathered} \left.\Delta_{\text {obs }} \quad \mathrm{cm}^{-1}\right] \end{gathered}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| -1 | 0 | 6 | 12 | 0.005320 .00029 | -1 | 0 | 2 | 17 | 0.006540 .00028 |
| -1 | 0 | 6 | 13 | 0.006070 .00035 | -1 | 0 | 2 | 18 | 0.007510 .00076 |
| -1 | 0 | 6 | 14 | 0.006740 .00030 | -1 | 0 | 2 | 19 | $0.00696-0.00029$ |
| -1 | 0 | 6 | 15 | 0.007500 .00030 | 1 | 0 | 1 | 10 | 0.002830 .00046 |
| -1 | 0 | 6 | 16 | 0.008480 .00049 | 1 | 0 | 2 | 9 | 0.002630 .00013 |
| -1 | 0 | 6 | 17 | 0.009150 .00033 | 1 | 0 | 2 | 10 | 0.003090 .00036 |
| -1 | 0 | 6 | 18 | 0.009910 .00024 | 1 | 0 | 2 | 11 | 0.003410 .00042 |
| -1 | 0 | 6 | 19 | 0.01049-0.00006 | 1 | 0 | 2 | 12 | 0.003710 .00044 |
| -1 | 0 | 4 | 17 | 0.008520 .00107 | 1 | 0 | 3 | 12 | $0.00240-0.00007$ |
| -1 | 0 | 4 | 18 | 0.008280 .00018 | 1 | 0 | 3 | 13 | 0.002860 .00022 |
| -1 | 0 | 4 | 19 | 0.008930 .00016 | 1 | 0 | 3 | 14 | 0.002950 .00013 |
| -1 | 0 | 4 | 20 | 0.009710 .00026 | 1 | 0 | 3 | 15 | $0.00281-0.00021$ |
| -1 | 0 | 4 | 21 | 0.010230 .00007 | 1 | 0 | 3 | 16 | $0.00311-0.00011$ |
| -1 | 0 | 4 | 22 | 0.011010 .00014 | 1 | 0 | 3 | 17 | 0.00334-0.00010 |
| -1 | 0 | 3 | 10 | 0.00247-0.00015 | 1 | 0 | 3 | 18 | 0.003790 .00012 |
| -1 | 0 | 3 | 11 | 0.002950 .00011 | 1 | 0 | 3 | 19 | $0.00368-0.00024$ |
| -1 | 0 | 3 | 12 | $0.00320 \quad 0.00012$ | 1 | 0 | 3 | 21 | 0.00415-0.00029 |
| -1 | 0 | 3 | 13 | 0.003540 .00020 | 1 | 0 | 3 | 22 | 0.00457-0.00015 |
| -1 | 0 | 3 | 14 | 0.00359-0.00002 | 1 | 0 | 5 | 16 | 0.003000 .00011 |
| -1 | 0 | 3 | 15 | 0.004120 .00023 | 1 | 0 | 5 | 17 | 0.003250 .00018 |
| -1 | 0 | 3 | 17 | $0.00398-0.00051$ | 1 | 0 | 5 | 18 | $0.00320-0.00007$ |
| -1 | 0 | 3 | 18 | 0.00457-0.00025 | 1 | 0 | 5 | 19 | 0.003610 .00013 |
| -1 | 0 | 3 | 19 | 0.005170 .00002 | 1 | 0 | 5 | 20 | 0.00351-0.00019 |
| -1 | 0 | 3 | 20 | $0.00512-0.00036$ | 1 | 0 | 5 | 21 | 0.00357-0.00035 |
| -1 | 0 | 3 | 21 | $0.00540-0.00043$ | 1 | 0 | 6 | 10 | 0.002400 .00031 |
| -1 | 0 | 3 | 22 | 0.00577-0.00042 | 1 | 0 | 6 | 11 | 0.002750 .00048 |
| -1 | 0 | 3 | 23 | 0.00584-0.00071 | 1 | 0 | 6 | 12 | 0.002870 .00040 |
| -1 | 0 | 3 | 24 | $0.00595-0.00096$ | 1 | 0 | 6 | 13 | 0.003120 .00044 |
| -1 | 0 | 3 | 25 | $0.00651-0.00077$ | 1 | 0 | 6 | 14 | 0.003530 .00063 |
| -1 | 0 | 2 | 12 | 0.004270 .00021 | 1 | 0 | 6 | 15 | 0.003640 .00050 |
| -1 | 0 | 2 | 13 | $0.00488 \quad 0.00042$ | 1 | 0 | 6 | 16 | 0.003930 .00053 |
| -1 | 0 | 2 | 14 | 0.005380 .00050 | 1 | 0 | 6 | 18 | 0.004410 .00046 |
| -1 | 0 | 2 | 15 | 0.005620 .00029 | 1 | 0 | 6 | 19 | 0.004680 .00043 |
| -1 | 0 | 2 | 16 | 0.006010 .00022 | 1 | 0 | 6 | 20 | 0.005060 .00050 |

Table III. Measured Line Intensities of the $\nu_{12}$ band $\left(822 \mathrm{~cm}^{-1}\right)$ of ${ }^{13} \mathrm{C}^{12} \mathrm{CH}_{6}$ at 294 K .

| $J$ | $\Delta J$ | $K$ | $\Delta K$ |  | $\begin{gathered} \nu_{i} \\ {\left[\mathrm{~cm}^{-1}\right]} \end{gathered}$ | $\begin{array}{r} S_{i} \times 10 \\ {\left[\mathrm{~cm}^{-2} \mathrm{~atm}\right.} \end{array}$ | $\begin{gathered} (\mathrm{o}-\mathrm{c}) / \mathrm{o} \\ ] \% \end{gathered}$ | $W_{i}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 24 | -1 | 8 | -1 | 2 | 769.1331 | 3.664 | -4.1 | 1.010 |
| 22 | -1 | 9 | -1 | 3 | 769.3221 | 4.289 | -3.7 | 1.006 |
| 18 | -1 | 11 | -1 | 1 | 769.7383 | 5.201 | -3.1 | 1.001 |
| 24 | -1 | 6 | -1 | 0 | 774.1979 | 4.520 | 0.8 | 1.016 |
| 22 | -1 | 7 | -1 | 1 | 774.3451 | 5.187 | -3.8 | 1.010 |
| 20 | -1 | 8 | -1 | 2 | 774.5033 | 5.901 | -5.5 | 1.005 |
| 18 | -1 | 9 | -1 | 3 | 774.6752 | 7.217 | 3.8 | 1.003 |
| 18 | -1 | 9 | -1 | 1 | 774.6813 | 3.808 | 9.0 | 1.002 |
| 16 | -1 | 10 | -1 | 2 | 774.8591 | 7.580 | 1.4 | 1.001 |
| 15 | -1 | 8 | -1 | 2 | 781.1717 | 9.667 | -2.5 | 1.002 |
| 19 | -1 | 4 | -1 | 2 | 786.0276 | 8.304 | 1.0 | 1.017 |
| 22 | -1 | 2 | -1 | 2 | 787.1992 | 6.327 | 3.5 | 1.062 |
| 18 | -1 | 4 | -1 | 2 | 787.3652 | 8.625 | -3.6 | 1.015 |
| 21 | -1 | 2 | -1 | 2 | 788.5452 | 6.427 | -4.6 | 1.056 |
| 17 | -1 | 4 | -1 | 2 | 788.7006 | 9.790 | 1.5 | 1.013 |
| 18 | 0 | 2 | -1 | 2 | 815.8488 | 14.295 | 2.5 | 0.944 |
| 18 | 0 | 2 | -1 | 0 | 815.8856 | 3.517 | 1.0 | 0.943 |
| $R_{v}^{2}=7.45(29) \times 10^{-4}(\text { Debye })^{2}$ |  |  |  |  |  |  |  |  |
| $S_{\mathrm{band}}=\sum_{i} S_{\mathrm{i}}=15.93(62) \mathrm{cm}^{-2} \mathrm{~atm}^{-1} @ 294 \mathrm{~K}$ |  |  |  |  |  |  |  |  |

of a Doppler spectrum in absorption with an appropriate FTS instrument function whose amplitude modulation function of the interferogram is a cosine truncated by the length of the mirror $\operatorname{scan}(17)$.

The retrieved intensities (Table III) were subjected to a least squares fit to the usual equation

$$
\begin{equation*}
S_{i}=\frac{8 \pi^{3}}{3 h c} \frac{L_{o} T_{o}}{T p_{o}} \gamma_{a} g_{J K} \frac{\exp \left(-E_{v r t}^{\prime \prime} / k T\right)}{Q_{v} Q_{r} Q_{t}}\left[1-\exp \left(-\frac{h c \nu_{i}}{k T}\right)\right] L_{r} R_{v}^{2} W_{i} \tag{1}
\end{equation*}
$$

where $S_{i}$ is the line intensity in units of $\mathrm{cm}^{-2} \mathrm{~atm}^{-1} h$ Planck's constant; $k$ the Boltzmann
constant; $c$ the speed of light; $L_{o}$ Loschmidt's number at standard temperature $T_{o}=273.15$ K and pressure $p_{o}=1 \mathrm{~atm} ; T$ the ambient temperature; $E_{v r t}^{\prime \prime}$ the lower state energy, and $Q_{v}$, $Q_{r}$, and $Q_{t}$ are the vibrational, rotational, and torsional partition function, respectively. $\gamma_{a}$ is the isotopic abundance of the species which equals 1 for a purified sample.

The last three terms in Eq. (1) represent the effective square dipole moment, where $R_{v}^{2}$ is the square vibrational transition moment and $L_{r}$ the Hönl-London factor (18). The perturbation factor $W_{i}$ is a correction factor to the rigid-rotor intensity caused by combined $\ell$-resonance within the $v_{12}=1$ state and the torsional Coriolis interaction between $v_{12}=1$ and $v_{6}=3$. These factors have been calculated by transforming the rotational transition moment matrix using the unitary eigenvector matrix which also diagonalizes the upper state Hamiltonian. Values for $W_{i}$ are obtained after squaring and normalizing to the square rotational transition moment $L_{r}$ in the unperturbed limit. Due to the mixing effects, ${ }^{p} P,{ }^{r} Q$, and ${ }^{p} R$ type transitions are enhanced in their intensities, while ${ }^{r} P,{ }^{p} Q$, and ${ }^{r} R$ transitions are depleted.

The partition functions at $T=294 \mathrm{~K}$ were calculated to be: $Q_{r}=18,613, Q_{v}=$ 1.058 , and $Q_{t}=4.063$. The fitted square vibrational dipole moment was $R_{v}^{2}=7.45(29) \times$ $10^{-4} \mathrm{D}^{2}$, which is about $11 \%$ less than the value derived from the major isotopomer(5). This result is also in agreement with earlier analysis of the integrated strength of the ${ }^{r} Q_{0}$ branch(11).

## The Line Atlas

In Appendix A calculated line parameters for transitions of the $\nu_{12}$ fundamental are listed. The line parameters for each transition are the rotational quantum numbers $J, K, \Delta K$, and $\Delta J$ and the torsional quantum number $\sigma$, calculated frequency $\nu_{i}$ in $\mathrm{cm}^{-1}$, observed minus calculated frequency (o-c) given in the last digits, lower state (ground state) energy $E_{i}$ in $\mathrm{cm}^{-1}$, line intensity in $\mathrm{cm}^{-2} \mathrm{~atm}^{-1} @ 296 \mathrm{~K}$, and the perturbation factor $W_{i}$. Line parameters have been calculated up to $K=20$ and $J=35$. The intensities have been converted from 294 K to the standard temperature $T=296 \mathrm{~K}$ using the exact expression in Eq. (1). For general conversion to other temperatures, for instance planetary temperatures, values for the torsional partition function have been calculated in the range of 100 K to 400 K using a ground state torsional barrier height of $1026.88 \mathrm{~cm}^{-1}$ (Table IV).

The observed FTS spectrum of ${ }^{13} \mathrm{C}^{12} \mathrm{CH}_{6}$ is shown in Appendix B. The experimental conditions were $p=1.05$ Torr, $\ell=150 \mathrm{~cm}$, and $T=294 \mathrm{~K}$. Below the observed spectrum in each panel the calculated spectrum under the same experimental condition is shown in two ways, first on a scale from $0 \%$ to $100 \%$ transmission and, secondly, from $90 \%$ to $100 \%$ transmission. The calculated Doppler spectra has been properly convolved with an appropriate instrumental profile as outlined as follows.

The approximate FTS apparatus function in interferogram space due to the aperture

Table IV.The torsional partition function $Q_{1}$ as a function of temperature $T$.

| $T$ <br> $[\mathrm{~K}]$ | $Q_{t}$ | $T$ <br> $[\mathrm{~K}]$ | $Q_{t}$ | $T$ <br> $[\mathrm{~K}]$ | $Q_{t}$ |
| :--- | :--- | :--- | :--- | :--- | :--- |
| 100 | 3.049 | 200 | 3.456 | 300 | 4.105 |
| 110 | 3.072 | 210 | 3.513 | 310 | 4.178 |
| 120 | 3.100 | 220 | 3.572 | 320 | 4.251 |
| 130 | 3.132 | 230 | 3.633 | 330 | 4.326 |
| 140 | 3.168 | 240 | 3.696 | 340 | 4.401 |
| 150 | 3.209 | 250 | 3.761 | 350 | 4.477 |
| 160 | 3.252 | 260 | 3.827 | 360 | 4.553 |
| 170 | 3.299 | 270 | 3.895 | 370 | 4.631 |
| 180 | 3.349 | 280 | 3.964 | 380 | 4.709 |
| 190 | 3.401 | 290 | 4.034 | 390 | 4.787 |
|  |  | 296 | 4.077 | 400 | 4.866 |

effect can be written as (17)

$$
\begin{equation*}
A(\delta)=\cos \left(b \frac{\delta}{L}\right) ; \quad|\delta| \leq L \tag{2}
\end{equation*}
$$

where $\delta$ is the optical path difference in the two arms of the interferometer and $L$ the maximum optical path difference. The form of Eq. (2) introduces a self-apodization in the observed spectra. The Fourier transform of $A(\delta)$ is then given by

$$
\begin{align*}
A(\nu) & =L\left\{\frac{\sin (2 \pi \nu L+b)}{2 \pi \nu L+b}+\frac{\sin (2 \pi \nu L-b)}{2 \pi \nu L-b}\right\} \\
& =L\{\operatorname{sinc}(2 \pi \nu L+b)+\operatorname{sinc}(2 \pi \nu L-b)\} \tag{3}
\end{align*}
$$

The parameters used were $L=173 \mathrm{~cm}$ and $b=0.818$ as determined from a least squares fit of the line profiles. This apparatus function was convolved with a calculated Doppler spectrum to simulate the observed FTS spectra, i.e. the normalized transmission $\tau$ at frequency $\nu$ is

$$
\begin{equation*}
\tau(\nu)=\int_{-\infty}^{\infty} d \nu^{\prime} A\left(\nu^{\prime}-\nu\right) \exp \left(-\sum_{i} S_{i} f\left(\nu^{\prime}-\nu_{i}\right) x\right) \tag{4}
\end{equation*}
$$

$S_{i}$ is the line strength of the transition at frequency $\nu_{i}, x=p \ell$ the optical density, and $f\left(\nu-\nu_{i}\right)$, the unit area line profile, here a Doppler profile. The convolution integral has been calculated by numerical summation with proper truncation to a finite sum of
intensities, the apparatus function, and line shapes in the far wing.
The spectra shown in Appendix B extends from $740 \mathrm{~cm}^{-1}$ to $910 \mathrm{~cm}^{-1}$. The top spectrum shows the observed FTS spectrum, the middle and bottom trace the calculated spectrum in different scales. Observed lines which do not appear in the calculated spectra belong either to the $\nu_{6}+\nu_{12} \leftarrow \nu_{6}$ vibration-torsional hotband, which is equivalent to the $\nu_{4}+\nu_{9} \leftarrow \nu_{4}$ band of normal ethane, or are outside the range of calculated quantum numbers.

## References

[1] G. Wiedemann, G.L. Bjoraker, and D.E. Jennings, Astrophys. J. 383, L29 (1991).
[2] G.S. Orton, J.H. Lacy, J.M. Achtermann, P. Parmar, and W.E. Blass, Icarus 100, 541 (1992).
[3] S.J. Daunt, W.E. Blass, G.W. Halsey, K. Fox, R.J. Lovell, H. Flicker, and J.D. King, J. Mol. Spectrosc. 86, 327 (1981).
[4] J. Susskind, D. Reuter, D.E. Jennings, S.J. Daunt, W.E. Blass, and G.W. Halsey, J. Chem. Phys. 77, 2728 (1982).
[5] L. Henry, A. Valentin, W.J. Lafferty, J.T. Hougen, V. Malathy Devi, P.P. Das, K.N. Rao, J. Mol. Spectrosc, 100, 260 (1983).
[6] S.J. Daunt, A.K. Atakan, W.E. Blass, G.W. Halsey, D.E. Jennings, D.C. Reuter, J. Susskind, and J.W. Brault, Astrophys. J. 280, 921 (1984).
[7] N. Moazzen-Ahmadi, H.P. Gush, M. Halpern, H. Jagannath, A. Leung, and I. Ozier, J. Chem. Phys. 88, 563 (1988).
[8] W.E. Blass, G.W. Halsey, J. Susskind, D.C. Reuter, and D.E. Jennings, J. Mol. Spectrosc. 141, 334 (1990).
[9] N. Moazzen-Ahmadi, A.R.W. Kellar, J.W.C. Johns, and I. Ozier, J. Chem. Phys. 97, 3981 (1992).
[10] W.J. Lafferty and E.K. Plyler, J. Res. Nat. Bur. Stand. A 67, 225 (1963).
[11] J. Kurtz, D.C. Reuter, D.E. Jennings, and J.J. Hillman, J. Geophys. Res. 96, 17489 (1991).
[12] M. Weber, W.E. Blass, D.C. Reuter, D.E. Jennings, and J.J. Hillman, J. Mol. Spectrosc. 159, 388 (1993).
[13] M. Weber, D.C. Reuter, J.M. Sirota, W.E. Blass, and J.J. Hillman, J. Chern. Phys., To be Published (1994).
[14] D.E. Jennings, R. Hubbard, J.W. Brault, Appl. Opt. 24, 3438 (1985).
[15] J.M. Sirota, D.C. Reuter, and M.J. Mumma, Appl. Opt. 32, 2117 (1993).
[16] J.L. Duncan, R.A. Kelly, G.D. Nivellini, and F. Tullini, J. Mol. Spectrosc. 98 , 87 (1983).
[17] V. Dana and A. Valentin, Appl. Opt. 27, 4450 (1988).
[18] H.C. Allen Jr., P.C. Cross, Molecular Vib-Rotors,Wiley and Sons, New York-London, 1963.

## Appendix A

## Table of Calculated $\nu_{12}$ Transitions of ${ }^{13} \mathbf{C}^{12} \mathbf{C H}_{6}$

## Legend:

$K, J \quad$ Lower state rotational quantum number, i.e. $K$," $J^{\prime \prime}$
$\Delta K, \Delta J \quad$ Difference in rotational quantum number of upper and lower state, i.e. $\Delta K=$ $K^{\prime}-K,{ }^{\prime \prime} \Delta J=J^{\prime}-J .{ }^{\prime \prime}$ The $\ell$ quantum number of the upper state can be deduced from the selction rules $\Delta K=\Delta \ell$
$\sigma \quad$ Torsional quantum number with selection rule $\Delta \sigma=0$
$\nu_{i} \quad$ Calculated transition frequency in $\mathrm{cm}^{-1}$
oc
Observed minus calculated frequency in the last five digits. Transitions marked with an asterisk (*) were excluded from the global fit
$E_{i}^{\prime \prime} \quad$ Lower state energy in $\mathrm{cm}^{-1}$
$S_{i} \quad$ Line intensity in $\mathrm{cm}^{-2} \mathrm{~atm}^{-1} @ 296 \mathrm{~K}$
$W_{i} \quad$ Intensity perturbation factor (dimensionless)




|  |  <br>  <br>  <br>  <br>  <br>  <br>  <br>  <br>  <br> NONOM－mーNONm－ONOM－MーNONOMーmHNONMーONmーO <br>  <br>  $\qquad$ $\qquad$ |
| :---: | :---: |
|  |  <br> ת <br>  <br> ศ $\infty$ <br>  <br>  <br>  <br>  <br>  <br>  <br>  <br>  $\qquad$ |


| $\Delta K$ | - | $K \quad J$ | $\sigma$ | $\frac{\nu_{i}}{75630246}$ | O-c | ${ }^{E_{i}^{\prime \prime}}$ | $S_{i}$ | $W_{i}$ | $\Delta K$ | $\Delta J$ | $K \quad J$ | $\sigma$ | $\nu_{i}$ | $0-\mathrm{c}$ | $E_{i}^{\prime \prime}$ | $S_{i}$ | $W_{i}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| -1 | -1 | 1128 | 3 | 756.30246 | 119 | 769.784 | . $3494 \mathrm{E}-03$ | 1.008 | -1 | -1 | 1519 | 3 | 758.74099 | -12 | 699.673 | . $2190 \mathrm{E}-02$ | 1.000 |
| -1 | -1 | 1128 | 1 | 756.31776 | -73 | 769.779 | .1396E-02 | 1.007 | -1 | -1 | 1519 | 1 | 758.74887 | -12 | 699.667 | . $1095 \mathrm{E}-02$ | 1.000 |
| -1 | -1 | 1619 | 2 | 756.37599 | -7 | 762.057 | . $1707 \mathrm{E}-02$ | 1.000 | -1 | -1 | 1028 | 2 | 758.76208 | 26 | 727.492 | . $1638 \mathrm{E}-02$ | 1.010 |
| -1 | -1 | 1619 | 0 | 756.43974 | -71 | 762.051 | . $4136 \mathrm{E}-03$ | . 969 | -1 | -1 | 1028 | 0 | 758.79209 | 15 | 727.487 | . $4088 \mathrm{E}-03$ | 1.008 |
| -1 | -1 | 1226 | 2 | 756.56676 | 21 | 744.953 | .8043E-03 | 1.005 | -1 | -1 | 1126 | 3 | 759.00301 | 1 | 698.640 | . $4796 \mathrm{E}-03$ | 1.006 |
| -1 | -1 | 1226 | 0 | 756.60362 | -12 | 744.947 | . $1604 \mathrm{E}-02$ | 1.002 | -1 | -1 | 1126 | 1 | 759.01647 | -46 | 698.635 | .1918E-02 | 1.006 |
| -1 | -1 | 1717 | 3 | 756.68894 |  | 780.560 | . $4112 \mathrm{E}-03$ | 1.000 | -1 | -1 | 1617 | 2 | 759.03793 | -32 | 714.162 | . $2147 \mathrm{E}-02$ | 1.000 |
| -1 | -1 | 1717 | 1 | 756.69055 | -51 | 780.555 | . $1645 \mathrm{E}-02$ | 1.000 | -1 | -1 | 1617 | 0 | 759.06445 | -97 | 714.156 | . $5283 \mathrm{E}-03$ | . 984 |
| -1 | -1 | 735 | 3 | 756.71364 |  | 914.341 | . $1643 \mathrm{E}-03$ | 1.035 | -1 | -1 | 635 | 2 | 759.24183 | 51 | 888.158 | . $3600 \mathrm{E}-03$ | . 1.044 |
| -1 | -1 | 735 | 1 | 756.72876 | -113 | 914.335 | .6573E-03 | 1.035 | -1 | -1 | 1224 | 2 | 759.25857 | 36 | 678.967 | . $1080 \mathrm{E}-02$ | 1.003 |
| -1 | -1 | 1324 | 3 | 756.83512 | 17 | 729.306 | .4450E-03 | 1.003 | -1 | -1 | 635 | 0 | 759.26666 | -4 | 888.152 | .7200E-03 | 1.044 |
| -1 | -1 | 1324 | 1 | 756.84876 | -28 | 729.301 | . $1778 \mathrm{E}-02$ | 1.002 | -1 | -1 | 1224 | 0 | 759.29035 | -18 | 678.962 | . $2155 \mathrm{E}-02$ | 1.001 |
| -1 | -1 | 833 | 2 | 756.93956 | 17 | 855.389 | .8769E-03 | 1.024 | -1 | -1 | 733 | 3 | 759.44561 | 25 | 825.181 | .2439E-03 | 1.030 |
| -1 | -1 | 833 | 0 | 756.96872 | $-103$ | 855.384 | .2190E-03 | 1.023 | -1 | -1 | 733 | 1 | 759.45957 | -94 | 825.175 | . $9756 \mathrm{E}-03$ | 1.030 |
| -1 | -1 | 1422 | 2 | 757.11805 | 20 | 722.839 | . $1893 \mathrm{E}-02$ | 1.001 | -1 | -1 | 1322 | 3 | 759.51896 | 55 | 668.484 | .5853E-03 | 1.002 |
| -1 | -1 | 1422 | 0 | 757.15916 | 21 | 722.834 | . $4705 \mathrm{E}-03$ | . 995 | -1 | -1 | 1322 | 1 | 759.53020 | -23 | 668.479 | .2339E-02 | 1.001 |
| -1 | -1 | 931 | 3 | 757.16674 | 60 | 805.609 | . $1126 \mathrm{E}-02$ | 1.017 | -1 | -1 | 831 | 2 | 759.66210 | 26 | 771.368 | .1272E-02 | 1.020 |
| -1 | -1 | 931 15 | 1 | 757.18184 | -72 | 805.603 | .5623E-03 | 1.016 | -1 | -1 | 831 | 0 | 759.68881 | $-28$ | 771.363 | .3180E-03 | 1.020 |
| -1 | -1 | 1520 | 3 | 757.40650 | 97 | 725.561 | . $1941 \mathrm{E}-02$ | 1.000 | -1 | -1 | 1420 | 2 | 759.79311 | 11 | 667.184 | .2443E-02 | 1.001 |
| -1 | -1 | 1029 | 2 | 757.40863 | $-117$ | 764.998 | . $1387 \mathrm{E}-02$ | 1.011 | -1 | -1 | 1420 | 0 | 759.82486 | -36 | 667.179 | .6077E-03 | . 996 |
| -1 | -1 | 1520 | 1 | 757.41603 | -2 | 725.555 | . $9703 \mathrm{E}-03$ | 1.000 | -1 | -1 | 929 | 3 | 759.88076 | 57 | 726.733 | . $1596 \mathrm{E}-02$ | 1.014 |
| -1 | -1 | 1029 | 0 | 757.44033 | 3 | 764.993 | . $3461 \mathrm{E}-03$ | 1.009 | -1 | -1 | 929 | 1 | 759.89440 | -37 | 726.728 | .7972E-03 | 1.013 |
| -1 | -1 | $\begin{array}{ll}11 & 27 \\ 11 & 27\end{array}$ | 3 | 757.65363 | 51 | 733.568 | . $4107 \mathrm{E}-03$ | 1.007 | -1 | -1 | 1518 | 3 | 760.07364 | -31 | 675.076 | . $2457 \mathrm{E}-02$ | 1.000 |
| -1 | -1 | 1127 | 1 | 757.66801 | -64 | 733.563 | . $1641 \mathrm{E}-02$ | 1.006 | -1 | -1 | 1518 | 1 | 760.07990 | 64 | 675.071 | . $1229 \mathrm{E}-02$ | 1.000 |
| -1 | -1 | 1618 | 2 | 757.70787 | -28 | 737.463 | .1920E-02 | 1.000 | -1 | -1 | 1027 | 2 | 760.11374 | 23 | 691.274 | . $1923 \mathrm{E}-02$ | 1.009 |
| -1 | -1 | 1618 | 0 | 757.75474 | $-130$ | 737.458 | . $4679 \mathrm{E}-03$ | . 975 | -1 | -1 | 1027 | 0 | 760.14204 | 6 | 691.268 | . $4798 \mathrm{E}-03$ | 1.007 |
| -1 | -1 | 1225 | 2 | 757.91356 | 6 | 711.316 | .9348E-03 | 1.004 | -1 | -1 | 1125 | 3 | 760.35059 | 63 | 665.000 | . $5566 \mathrm{E}-03$ | 1.005 |
| -1 | -1 | 1225 7 | 0 | 757.94790 | -19 | 711.310 | .1864E-02 | 1.001 | -1 | -1 | 1125 | 1 | 760.36313 | 158 | 664.994 | .2226E-02 | 1.005 |
| -1 | -1 | 734 | 3 | 758.08054 |  | 869.120 | .2008E-03 | 1.032 | -1 | -1 | 1616 | 2 | 760.36612 | -141 | 692.152 | . $2391 \mathrm{E}-02$ | 1.000 |
| -1 | -1 | 734 13 | 1 | 758.09508 | -95 | 869.114 | .8031E-03 | 1.032 | -1 | -1 | 1616 | 0 | 760.36773 |  | 692.146 | .5977E-03 | 1.000 |
| -1 | -1 | 1323 13 | 3 | 758.17794 | -10 | 698.250 | . $5116 \mathrm{E}-03$ | 1.002 | -1 | -1 | 1223 | 2 | 760.60177 | 21 | 647.908 | . $1241 \mathrm{E}-02$ | 1.003 |
| -1 | -1 | 1323 832 | 1 | 758.19038 | -36 | 698.245 | .2044E-02 | 1.001 | -1 | -1 | 634 | 2 | 760.60976 | 19 | 842.934 | . $4393 \mathrm{E}-03$ | 1.041 |
| -1 | -1 | 832 832 | 2 | 758.30173 | 14 | 812.737 | $.1060 \mathrm{E}-02$ | 1.022 | -1 | -1 | 1223 | 0 | 760.63096 | 34 | 647.903 | .2474E-02 | 1.000 |
| -1 | -1 | 832 14 | 0 | 758.32968 | 35 | 812.731 | . $2649 \mathrm{E}-03$ | 1.022 | -1 | -1 | 634 | 0 | 760.63366 | -236* | 842.928 | . $8786 \mathrm{E}-03$ | 1.041 |
| -1 | -1 | 1421 | 2 | 758.45649 | 12 | 694.367 | .2157E-02 | 1.001 | -1 | -1 | 732 | 3 | 760.80883 |  | 782.526 | . $2943 \mathrm{E}-03$ | 1.028 |
| -1 | -1 | 1421 930 | 0 | 758.49299 | -17 | 694.361 | . $5360 \mathrm{E}-03$ | . 995 | -1 | -1 | 732 | 1 | 760.82221 | -73 | 782.520 | .1177E-02 | 1.028 |
| -1 | -1 | 930 930 | 3 | 758.52465 | 64 | 765.529 | .1344E-02 | 1.015 | -1 | -1 | 1321 | 3 | 760.85814 | 61 | 640.008 | . $6649 \mathrm{E}-03$ | 1.001 |
| -1 | -1 | 930 | 1 | 758.53902 | -53 | 765.523 | . $6721 \mathrm{E}-03$ | 1.015 | -1 | -1 | 1321 | 1 | 760.86820 | -28 | 640.003 | .2660E-02 | 1.001 |










|  | 区 <br> 战 <br>  <br>  <br>  <br>  <br>  <br>  <br> NOMールーNOM－NNONOM－NONONONOM－NONNONONON <br>  <br>  <br>  |
| :---: | :---: |
|  |  <br>  <br>  <br>  <br>  <br>  Nod <br>  <br>  <br>  |




| $\Delta K$ |  | $K \quad J$ | $\sigma$ | $\nu_{i}$ | O-C | $E_{i}^{\prime \prime}$ | $S_{i}$ | $W_{i}$ | $\Delta K \Delta J$ | $K \quad J$ | $\sigma$ | $\nu_{i}$ | O-c | $E_{i}^{\prime \prime}$ | $S_{i}$ | $W_{i}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| -1 | -1 | 711 | 3 | 788.99033 |  | 184.443 | . $3316 \mathrm{E}-02$ | 1.001 | -1 -1 | 416 | 0 | 790.04012 |  | 208.612 | . $2543 \mathrm{E}-02$ | 1.011 |
| -1 | -1 | 711 | 1 | 788.99297 | -48 | 184.438 | . $1326 \mathrm{E}-01$ | 1.001 | -1 0 | 1228 | 0 | 790.05895 | $-60$ | 816.084 | . $1021 \mathrm{E}-02$ | . 976 |
| -1 | -1 | 89 | 2 | 789.10590 | 40 | 187.466 | .1419E-01 | 1.000 | -1 0 | 1227 | 2 | 790.08025 |  | 779.878 | . $5838 \mathrm{E}-03$ | . 983 |
| -1 | -1 | 89 | 0 | 789.10809 |  | 187.461 | . $3547 \mathrm{E}-02$ | 1.000 | -1 -1 | 514 | 3 | 790.11636 |  | 186.593 | .2896E-02 | 1.005 |
| 1 | -1 | 024 | 2 | 789.31508 |  | 388.794 | . $2021 \mathrm{E}-02$ | 1.000 | $\begin{array}{ll}-1 & -1\end{array}$ | 514 | 1 | 790.11994 | -40 | 186.588 | . $1158 \mathrm{E}-01$ | 1.005 |
| 1 | -1 | 024 | 0 | 789.31671 | -9 | 388.789 | .4042E-02 | 1.000 | -1 0 | 1227 | 0 | 790.12196 | -242* | 779.872 | . $1162 \mathrm{E}-02$ | . 978 |
| -1 | 0 | 1235 | 2 | 789.48924 |  | 1105.565 | . $1639 \mathrm{E}-03$ | . 969 | -1 0 | 1226 | 2 | 790.14319 | -22 | 744.953 | .6571E-03 | . 984 |
| -1 | 0 | 1235 | 0 | 789.54764 |  | 1105.559 | . $3258 \mathrm{E}-03$ | . 963 | -1 0 | 1226 | 0 | 790.18249 | 40 | 744.947 | .1309E-02 | . 980 |
| -1 | 0 | 1234 | 2 | 789.57170 |  | 1060.361 | .1977E-03 | . 971 | -1 0 | 1225 | 2 | 790.20372 |  | 711.316 | .7329E-03 | . 986 |
| -1 | 0 | 1234 | 0 | 789.62829 |  | 1060.355 | . $3931 \mathrm{E}-03$ | . 965 | -1 -1 | 612 | 2 | 790.20940 |  | 173.779 | .6418E-02 | 1.002 |
| -1 | 0 | 1233 | 2 | 789.65169 |  | 1016.439 | .2367E-03 | . 973 | -1 -1 | 612 | 0 | 790.21380 | $-112$ | 173.773 | . $1284 \mathrm{E}-01$ | 1.002 |
| -1 | 0 | 1233 | 0 | 789.70639 |  | 1016.433 | .4706E-03 | . 967 | -1 0 | 1225 | 0 | 790.24056 | $-150$ | 711.310 | . $1458 \mathrm{E}-02$ | . 981 |
| -1 | 0 | 1232 | 2 | 789.72922 |  | 973.800 | . $2808 \mathrm{E}-03$ | . 974 | -1 0 | 1224 | 2 | 790.26186 | 73 | 678.967 | . $8080 \mathrm{E}-03$ | . 987 |
| 1 | $-1$ | 432 | 2 | 789.74801 | 70 | 716.040 | .7554E-03 | . 898 | -1 0 | 1224 | 0 | 790.29618 | $246 *$ | 678.962 | . $1609 \mathrm{E}-02$ | . 983 |
| 1 | -1 | 534 | 3 | 789.74805 |  | 820.778 | .1152E-03 | . 904 | -1 1 | 710 | 3 | 790.30986 |  | 170.182 | . $3478 \mathrm{E}-02$ | 1.000 |
| 1 | -1 | 330 | 3 | 789.75521 | 616* | 620.467 | .1177E-02 | . 886 | $\begin{array}{ll}-1 & -1\end{array}$ | 710 | 1 | 790.31218 | -36 | 170.177 | . $1391 \mathrm{E}-01$ | 1.000 |
| 1 | -1 | 534 | 1 | 789.75544 |  | 820.773 | . $4604 \mathrm{E}-03$ | . 903 | -1 0 | 1223 | 2 | 790.31761 |  | 647.908 | .8816E-03 | . 989 |
| 1 | -1 | 432 | 0 | 789.75850 |  | 716.034 | . 1884E-03 | . 896 | -1 0 | 1223 | 0 | 790.34937 | 8 | 647.903 | . $1756 \mathrm{E}-02$ | . 985 |
| 1 | -1 | 330 | 1 | 789.76225 |  | 620.461 | . $5879 \mathrm{E}-03$ | . 885 | -1 0 | 1222 | 2 | 790.37098 | -12 | 618.139 | .9492E-03 | . 990 |
| 1 | -1 | 228 | 2 | 789.77905 | -92 | 534.060 | . $1726 \mathrm{E}-02$ | . 859 | -1 0 | 1222 | 0 | 790.40015 | -22 | 618.134 | . $1891 \mathrm{E}-02$ | . 986 |
| -1 | 0 | 1232 | 0 | 789.78195 |  | 973.794 | . $5588 \mathrm{E}-03$ | . 969 | -1 -1 | 88 | 2 | 790.42081 | 33 | 175.797 | .1493E-01 | 1.000 |
| 1 | -1 | 228 | 0 | 789.78930 |  | 534.055 | . $4306 \mathrm{E}-03$ | . 857 | -1 0 | 1221 | 2 | 790.42198 | -84 | 589.660 | .1008E-02 | . 991 |
| -1 | 0 | 1231 | 2 | 789.80430 |  | 932.445 | . $3308 \mathrm{E}-03$ | . 976 | $\begin{array}{ll}-1 & -1\end{array}$ | 88 | 0 | 790.42236 |  | 175.792 | . $3734 \mathrm{E}-02$ | 1.000 |
| -1 | -1 | 122 | 3 | 789.81299 |  | 329.949 | . $1531 \mathrm{E}-02$ | 1.136 | -1 0 | 1221 | 0 | 790.44853 | 33 | 589.655 | .2011E-02 | . 988 |
| -1 | -1 | 122 | 1 | 789.81783 | -38 | 329.944 | . $6129 \mathrm{E}-02$ | 1.137 | -1 0 | 1220 | 2 | 790.47060 | 7 | 562.472 | .1055E-02 | . 992 |
| 1 | -1 | 126 | 3 | 789.82316 |  | 456.836 | .5642E-03 | . 775 | -1 0 | 1220 | 0 | 790.49452 | -18 | 562.467 | . $2104 \mathrm{E}-02$ | . 989 |
| 1 | -1 | 126 | 1 | 789.83014 | -39 | 456.830 | . $2254 \mathrm{E}-02$ | . 774 | -1 0 | $12 \quad 19$ | 2 | 790.51687 | 23 | 536.576 | . $1086 \mathrm{E}-02$ | . 994 |
| -1 | 0 | 1231 | 0 | 789.85497 |  | 932.439 | .6583E-03 | . 971 | -1 0 | 1219 | 0 | 790.53815 | 23 | 536.570 | . $2165 \mathrm{E}-02$ | . 991 |
| -1 | 0 | 1230 | 2 | 789.87693 |  | 892.374 | . $3864 \mathrm{E}-03$ | . 978 | -1 0 | 1218 | 2 | 790.56078 | -335* | 511.971 | . $1094 \mathrm{E}-02$ | . 995 |
| -1 | -1 | 220 | 2 | 789.88891 | -14 | 280.299 | .7243E-02 | 1.050 | -1 0 | 1218 | 0 | 790.57943 | 5 | 511.966 | . $2182 \mathrm{E}-02$ | . 992 |
| -1 | -1 | 220 | 0 | 789.89618 | 118 | 280.294 | .1812E-02 | 1.051 | -1 0 | 1217 | 2 | 790.60234 | 34 | 488.659 | .1075E-02 | . 996 |
| -1 | 0 | 1230 | 0 | 789.92547 |  | 892.369 | .7682E-03 | . 972 | -1 0 | 1217 | 0 | 790.61838 | 20 | 488.653 | . $2146 \mathrm{E}-02$ | . 994 |
| -1 | 0 | 1229 | 2 | 789.94713 |  | 853.589 | . $4476 \mathrm{E}-03$ | . 980 | -1 0 | 1216 | 2 | 790.64156 | $-176 *$ | 466.639 | .1023E-02 | . 997 |
| -1 | -1 | 318 | 3 | 789.95736 | 136 | 239.857 | .8683E-02 | 1.023 | -1 0 | 1216 | 0 | 790.65502 | -11 | 466.634 | . $2041 \mathrm{E}-02$ | . 995 |
| -1 | -1 | 318 | 1 | 789.96187 |  | 239.851 | .4342E-02 | 1.023 | -1 0 | 1215 | 2 | 790.67844 | -2 | 445.913 | .9301E-03 | . 998 |
| -1 | 0 | 1229 | 0 | 789.99346 | 109 | 853.584 | .8897E-03 | . 974 | -1 0 | 1215 | 0 | 790.68937 | 9 | 445.908 | .1857E-02 | . 996 |
| -1 | 0 | 1228 | 2 | 790.01490 |  | 816.090 | .5133E-03 | . 981 | $1 \begin{array}{ll}1 & -1\end{array}$ | 023 | 2 | 790.70328 |  | 357.717 | . $2254 \mathrm{E}-02$ | 1.000 |
| -1 | -1 | 416 | 2 | 790.03389 | -9 | 208.618 | .1017E-01 | 1.011 | $1-1$ | 023 | 0 | 790.70490 | -16 | 357.712 | . $4508 \mathrm{E}-02$ | 1.000 |




|  |  <br>  <br>  <br>  <br>  N <br>  <br>  <br>  <br>  <br>  <br>  |
| :---: | :---: |
|  |  <br>  <br>  <br>  <br>  <br>  <br>  <br>  <br>  <br> 品 <br>  |




|  |  <br>  <br>  <br> 象 <br>  <br>  <br>  <br>  NOM-NOM-NONOMNOーNOMNTONONOMHNONONONOON <br>  <br>  <br>  |
| :---: | :---: |
|  |  <br>  <br>  <br>  <br>  <br>  <br>  <br>  <br> NONOONNONONONONONONOONONONNONOM-NM-NOO <br>  <br>  $0000-1000000000000070000007000170171071$ |







|  |  <br>  성 <br>  <br>  <br>  ※ <br>  <br>  NONOM－NONNOOMーツーNONNONOOONNールーNONNOON <br>  <br>  <br>  |
| :---: | :---: |
|  |  <br>  <br>  －© <br>  <br>  <br> O स <br>  <br>  <br> OMNOーNMーONO－NONNOONNO－NONOMNNOMNNNHO <br>  <br>  |



|  |  <br>  <br>  <br>  <br>  <br>  <br> 效 <br>  <br>  <br>  <br>  $\qquad$ |
| :---: | :---: |
|  |  |










|  |  <br>  <br>  <br>  <br>  <br>  <br>  <br>  <br>  <br>  <br>  <br>  |
| :---: | :---: |
|  |  <br>  <br>  <br>  <br>  $\stackrel{*}{\circ}$ <br>  <br>  <br>  ONOMーNONONONONNTMNOMONNNOOMONM-NONNOON <br>  <br>  <br>  |




|  |  <br>  <br>  <br>  <br>  <br> $\vec{\sim}$ <br> 8 <br> 分 8 <br>  F <br>  <br>  －NTONONーMーONOMーNOMーNONONOMーNONONONONO <br>  <br>  |
| :---: | :---: |
|  |  <br> 知 <br>  <br>  <br>  <br> 会 <br>  <br>  <br>  <br>  ※た <br>  |




| $E_{i}^{\prime \prime}$ | $S_{i}$ | $W_{i}$ |
| ---: | :---: | :---: |
| 620.467 | $.3964 \mathrm{E}-02$ | 1.101 |
| 620.461 | $.1982 \mathrm{E}-02$ | 1.101 |
| 581.661 | $.4600 \mathrm{E}-02$ | 1.094 |
| 581.655 | $.2302 \mathrm{E}-02$ | 1.095 |
| 668.484 | $.3767 \mathrm{E}-04$ | .970 |
| 668.479 | $.1507 \mathrm{E}-03$ | .970 |
| 544.141 | $.5304 \mathrm{E}-02$ | 1.088 |
| 544.135 | $.2652 \mathrm{E}-02$ | 1.088 |
| 982.758 | $.3197 \mathrm{E}-04$ | 1.053 |
| 853.589 | $.1150 \mathrm{E}-03$ | 1.050 |
| 1121.055 | $.6790 \mathrm{E}-04$ | 1.056 |
| 733.568 | $.9875 \mathrm{E}-04$ | 1.047 |
| 982.752 | $.1279 \mathrm{E}-03$ | 1.053 |
| 733.563 | $.3954 \mathrm{E}-03$ | 1.048 |
| 622.699 | $.6482 \mathrm{E}-03$ | 1.045 |
| 507.909 | $.6068 \mathrm{E}-02$ | 1.082 |
| 507.903 | $.3034 \mathrm{E}-02$ | 1.082 |
| 521.000 | $.1014 \mathrm{E}-02$ | 1.042 |
| 853.584 | $.2300 \mathrm{E}-03$ | 1.050 |
| 622.694 | $.1620 \mathrm{E}-03$ | 1.045 |
| 520.995 | $.5073 \mathrm{E}-03$ | 1.042 |
| 428.473 | $.1516 \mathrm{E}-02$ | 1.039 |
| 1121.050 | $.1691 \mathrm{E}-04$ | 1.052 |
| 428.468 | $.3790 \mathrm{E}-03$ | 1.039 |
| 472.965 | $.6888 \mathrm{E}-02$ | 1.076 |
| 472.959 | $.3444 \mathrm{E}-02$ | 1.076 |
| 783.655 | $.9816 \mathrm{E}-04$ | .967 |
| 783.649 | $.2454 \mathrm{E}-04$ | .967 |
| 345.134 | $.5408 \mathrm{E}-03$ | 1.036 |
| 345.129 | $.2163 \mathrm{E}-02$ | 1.036 |
| 439.310 | $.7758 \mathrm{E}-02$ | 1.070 |
| 439.304 | $.3882 \mathrm{E}-02$ | 1.071 |
| 270.983 | $.1474 \mathrm{E}-02$ | 1.033 |
| 270.978 | $.2951 \mathrm{E}-02$ | 1.034 |
| 157.217 | $.3151 \mathrm{E}-04$ | .989 |
| 157.212 | $.1261 \mathrm{E}-03$ | .989 |
| 406.944 | $.8675 \mathrm{E}-02$ | 1.065 |
| 206.036 | $.9611 \mathrm{E}-03$ | 1.031 |
|  |  |  |




| $\Delta K$ | $\Delta J$ | $K$ 3 | $\sigma$ | $\frac{\nu_{i}}{828.89121}$ | $\mathrm{o}-\mathrm{C}$ | $\frac{E_{i}^{\prime \prime}}{}{ }^{\prime \prime}$ | $\frac{S_{i}}{4337 \mathrm{E}-02}$ | $W_{i}$ | $\Delta K$ |  | K J | $\sigma$ | $\nu_{i}$ | O-c | $E_{i}^{\prime \prime}$ | $S_{i}$ | $W_{i}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| -1 | 1 | 515 | 1 | 828.89493 | -623* | 406.938 206.030 | . $4337 \mathrm{E}-02$ | 1.065 | 1 | -1 | 1015 | 2 | 829.36449 |  | 357.250 | .2831E-03 | . 980 |
| 1 | 0 | 323 | 3 | 828.94431 | 129 | 375.868 | . $.9621 \mathrm{E}-02$ | 1.031 | 1 |  | 1015 | 0 | 829.36666 |  | 357.244 | .7077E-04 | . 980 |
| 1 | 0 | 323 | 1 | 828.94932 |  | 375.862 | . $4810 \mathrm{E}-02$ | 1.060 | 1 | 0 | 314 | 3 | 829.36712 | -26 | 154.319 | .1626E-01 | 1.022 |
| -1 | 1 | 413 | 2 | 828.95616 | 42 | 150.290 | . $4790 \mathrm{E}-02$ | 1.060 1.028 | 1 |  | 314 | 1 | 829.36994 |  | 154.314 | .8136E-02 | 1.023 |
| -1 | 1 | 413 | 0 | 828.96179 |  | 150.284 | .1199E-02 | 1.028 | 1 |  | 173 | 3 | 829.39947 |  | 9.804 | . $2196 \mathrm{E}-02$ | . 996 |
| 1 | -1 | 1526 | 3 | 828.97168 |  | 907.982 | . $6020 \mathrm{E}-04$ | 1.029 | 1 |  | 1730 | 3 | 829.39985 |  | 1184.040 | .4782E-05 | . 959 |
| 1 | -1 | 1526 | 1 | 828.97452 |  | 907.976 | . $3010 \mathrm{E}-04$ | . 964 | 1 |  | $\begin{array}{ll}1 & 3 \\ 3\end{array}$ | 1 | 829.40113 | 111 | 9.799 | . $8785 \mathrm{E}-02$ | . 996 |
| 1 | 0 | 322 | 3 | 829.00050 | 138 | 346.082 | . $1058 \mathrm{E}-01$ | . 1.055 | 1 | 0 | 313 17 | 3 | 829.40225 | -89 | 136.170 | .1633E-01 | 1.019 |
| 1 | 0 | 322 | 1 | 829.00523 |  | 346.077 | . $5290 \mathrm{E}-02$ | 1.055 | 1 | -1 | 1730 3 | 1 | 829.40299 |  | 1184.034 | .1913E-04 | . 959 |
| -1 | 1 | 311 | 3 | 829.02802 | 1 | 103.758 | . $5730 \mathrm{E}-02$ | 1.027 | 1 | 0 | 313 3 | 1 | 829.40489 |  | 136.165 | .8166E-02 | 1.019 |
| -1 | 1 | 311 | 1 | 829.03109 |  | 103.752 | . $2865 \mathrm{E}-02$ | 1.027 | 1 | 0 | 312 312 | 3 | 829.43494 | -24 | 119.316 | . $1618 \mathrm{E}-01$ | 1.016 |
| 1 | -1 | 811 | 2 | 829.03168 |  | 214.690 | .2332E-03 | 1.027 | 1 | 0 | 312 311 | 1 | 829.43741 |  | 119.311 | .8096E-02 | 1.017 |
| 1 | -1 | 811 | 0 | 829.03350 |  | 214.685 | . $5830 \mathrm{E}-04$ | . 986 | 1 | 0 | 311 | 3 | 829.46518 | -21 | 103.758 | . $1578 \mathrm{E}-01$ | 1.014 |
| 1 | 0 | 321 | 3 | 829.05445 | 211* | 317.588 | . $1154 \mathrm{E}-01$ | . 1.050 | 1 | 0 | 11 | 1 | 829.46749 |  | 103.752 | . $7890 \mathrm{E}-02$ | 1.014 |
| 1 | 0 | 321 | 1 | 829.05889 |  | 317.582 | .5769E-02 | 1.050 | 1 | 0 | 310 | 3 | 829.49294 | -23 | 89.495 | . $1509 \mathrm{E}-01$ | 1.011 |
| 1 | 0 | 320 | 3 | 829.10612 | 211* | 290.385 | .1247E-01 | 1.045 | 1 | 0 | 10 | 1 | 829.49511 |  | 89.489 | .7546E-02 | 1.011 |
| -1 | 1 | 29 | 2 | 829.10953 | -129 | 66.437 | . $6591 \mathrm{E}-02$ | 1.026 | 1 | 0 | 39 | 3 | 829.51823 | -26 | 76.527 | .1412E-01 | 1.009 |
| 1 | 0 | 320 | 1 | 829.11030 |  | 290.380 | . $6240 \mathrm{E}-02$ | 1.046 | 1 | 0 | $\begin{array}{ll}3 & 9 \\ 3\end{array}$ | 1 | 829.52027 |  | 76.522 | . $7061 \mathrm{E}-02$ | 1.009 |
| -1 | 1 | 29 | 0 | 829.11286 |  | 66.432 | .1648E-02 | 1.026 | 1 | -1 | 38 17 | 3 | 829.54102 | $-20$ | 64.856 | . $1283 \mathrm{E}-01$ | 1.007 |
| 1 | 0 | 319 | 3 | 829.15550 | -12 | 264.475 | . $1337 \mathrm{E}-01$ | 1.026 | 1 | -1 | 1117 | 3 | 829.54171 |  | 442.323 | .6177E-04 | . 978 |
| 1 | 0 | 319 | 1 | 829.15942 |  | 264.469 | .6683E-02 | 1.041 | 1 | -1 | 38 | 1 | 829.54294 |  | 64.851 | .6417E-02 | 1.007 |
| 1 | -1 | 1628 | 2 | 829.18304 |  | 1041.445 | . $3486 \mathrm{E}-04$ | 1.041 .961 | 1 | -1 | 1117 | 1 | 829.54381 |  | 442.317 | .2468E-03 | . 977 |
| 1 | -1 | 1628 | 0 | 829.18663 |  | 1041.439 | .8716E-05 | . 961 |  | 0 | 7 | 3 | 829.56131 | -25 | 54.481 | $.1121 \mathrm{E}-01$ | 1.005 |
| 1 | -1 | 913 | 3 | 829.19366 |  | 281.372 | . $2844 \mathrm{E}-03$ | . 983 | 1 | 0 |  | 1 | 829.56312 |  | 54.476 | .5610E-02 | 1.006 |
| 1 | -1 | 913 | 1 | 829.19550 |  | 281.367 | . $1422 \mathrm{E}-03$ | . 983 | 1 | 0 |  | 3 | 829.57908 | -28 | 45.403 | .9222E-02 | 1.004 |
| -1 | 1 | 17 | 3 | 829.19747 |  | 281.3679 | .1844E-02 | .983 1.030 | 1 | 0 |  | 1 | 829.58080 |  | 45.398 | . $4611 \mathrm{E}-02$ | 1.004 |
| -1 | 1 | 17 | 1 | 829.19962 | 242* | 38.334 | . $7377 \mathrm{E}-02$ | 1.030 | 1 | 0 |  | 3 | 829.59432 | -42 | 37.621 | .6801E-02 | 1.003 |
| 1 | 0 | 318 | 3 | 829.20255 | $-173^{*}$ | 239.857 | . $1419 \mathrm{E}-01$ | 1.030 1.037 | 1 |  |  | 1 | 829.59597 |  | 37.616 | . $3401 \mathrm{E}-02$ | 1.003 |
| 1 | 0 | 318 | 1 | 829.20623 |  | 239.851 | . $7096 \mathrm{E}-02$ | 1.037 |  |  |  | 3 | 829.60704 | -34 | 31.136 | $.3825 \mathrm{E}-02$ | 1.002 |
| 1 | 0 | 317 | 3 | 829.24726 | 2 | 216.532 | .1492E-01 | 1.033 |  |  |  | 1 | 829.60863 |  | 31.131 | .1912E-02 | 1.002 |
| 1 | 0 | 317 | 1 | 829.25070 |  | 216.526 | . $7460 \mathrm{E}-02$ | 1.033 1.033 |  |  |  | 2 | 829.62562 |  | 1335.746 | .4970E-05 | . 956 |
| 1 | 1 | 05 | 2 | 829.25836 |  | 19.458 | . $3926 \mathrm{E}-02$ | 1.033 1.000 |  |  |  | 0 | 829.62961 |  | 1335.740 | .9940E-05 | . 956 |
| 1 | 1 | 05 | 0 | 829.25989 | 30 | 19.453 | .7852E-02 | 1.000 |  |  |  | 2 | 829.72778 |  | 536.576 | .9747E-04 | . 975 |
| 1 | 0 | 316 | 3 | 829.28960 | -7 | 194.500 | .1552E-01 | 1.029 |  |  |  | 0 | 829.73034 |  | 536.570 | .1947E-03 | . 974 |
| 1 | 0 | 316 | 1 | 829.29283 | -55 | 194.495 | .7761E-02 | 1.029 |  |  |  | 3 | 829.85647 |  | 1496.556 | . $1226 \mathrm{E}-05$ | . 953 |
| 1 | 0 | 315 | 3 | 829.32956 |  | 173.762 | . $1599 \mathrm{E}-01$ | 1.026 |  |  |  | 1 | 829.85992 |  | 1496.550 | .4903E-05 | . 953 |
| 1 | 0 | 315 | 1 | 829.33258 |  | 173.757 | .7993E-02 | 1.026 | -1 |  |  | 3 | 829.86331 |  | 1024.109 | .2812E-04 | 1.056 |
|  |  |  |  |  |  |  | . 995 L -02 | 1.020 | -1 | 1 | 1434 | 2 | 829.86872 |  | 1164.968 | .5879E-04 | 1.059 |















| $\Delta K$ | ${ }^{\text {d }}$ | $K \quad J$ <br> 1021 | $\sigma$ | $\frac{\nu_{i}}{84846819}$ | $\frac{0-\mathrm{c}}{36}$ | $\frac{E_{i}^{\prime \prime}}{}{ }^{\prime \prime}$ | $S_{i}$ | $W_{i}$ | $\Delta K \Delta$ | J | K J | $\sigma$ | $\nu_{i}$ | O-c | $E_{i}^{\prime \prime}$ | $S_{i}$ | $W_{i}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 0 | 1021 | 2 | 848.46819 | 36 | 501.023 | . $3651 \mathrm{E}-02$ | 1.012 | 1 | 1 | 510 | 3 | 849.19291 |  | 121.773 | . $4310 \mathrm{E}-02$ | . 997 |
| 1 | 0 | 1021 | 0 | 848.47184 |  | 501.017 | .9127E-03 | 1.012 | -1 | 1 | 123 | 3 | 849.19323 |  | 359.736 | . $1527 \mathrm{E}-02$ | 1.212 |
| 1 | 0 | 1020 | 2 | 848.52348 | 47 | 473.830 | .3847E-02 | 1.011 | 1 | 1 | 510 | 1 | 849.19500 | 29 | 121.768 | .1724E-01 | . 997 |
| 1 | 0 | 1020 | 0 | 848.52688 |  | 473.824 | .9617E-03 | 1.011 | -1 | 1 | 123 | 1 | 849.19871 | -342* | 359.730 | . $6118 \mathrm{E}-02$ | 1.214 |
| -1 | 1 | 531 | 3 | 848.55213 |  | 692.801 | .2782E-03 | 1.093 | 1 | 1 | 68 | 2 | 849.41512 |  | 119.325 | . $9430 \mathrm{E}-02$ | . 999 |
| -1 | 1 | 531 | 1 | 848.56390 | -33 | 692.795 | .1114E-02 | 1.094 | 1 | 1 | 68 | 0 | 849.41704 | 82 | 119.319 | .1886E-01 | . 999 |
| 1 | 0 | 1019 | 2 | 848.57618 | 131 | 447.929 | .3993E-02 | 1.010 | -1 | 1 | 634 | 2 | 849.60169 |  | 842.934 | . $2824 \mathrm{E}-03$ | 1.096 |
| 1 | 1 | 216 | 2 | 848.57778 | -28 | 184.412 | .1105E-01 | . 960 | -1 | 1 | 634 | 0 | 849.62736 |  | 842.928 | . $5653 \mathrm{E}-03$ | 1.097 |
| 1 | 0 | 1019 | 0 | 848.57935 |  | 447.923 | .9983E-03 | 1.010 | 1 | 1 | 119 | 3 | 849.64499 |  | 248.339 | .1907E-02 | . 875 |
| 1 | 1 | 216 | 0 | 848.58277 |  | 184.407 | . $2759 \mathrm{E}-02$ | . 959 | 1 | 1 | 119 | 1 | 849.64991 | -39 | 248.334 | .7620E-02 | . 874 |
| 1 | 0 | 1018 | 2 | 848.62630 | 35 | 423.320 | . $4070 \mathrm{E}-02$ | 1.008 | -1 | 1 | 532 | 3 | 849.75282 |  | 734.176 | .2382E-03 | 1.098 |
| 1 | 0 | 1018 | 0 | 848.62925 |  | 423.314 | . $1018 \mathrm{E}-02$ | 1.008 | -1 | 1 | 532 | 1 | 849.76507 | -63 | 734.170 | .9537E-03 | 1.099 |
| 1 | 0 | 1017 | 2 | 848.67383 | 30 | 400.003 | .4070E-02 | 1.007 | 1 | 1 | 217 | 2 | 849.82748 | 17 | 206.444 | .1032E-01 | . 955 |
| -1 | 0 | 1017 419 | 0 | 848.67656 |  | 399.998 | .1017E-02 | 1.007 | 1 | 1 | 217 | 0 | 849.83289 |  | 206.439 | .2577E-02 | . 954 |
| 1 | 0 | 429 1016 | 2 | 848.70936 | -14 | 595.767 | . $1780 \mathrm{E}-02$ | 1.099 | -1 | 1 | 430 | 2 | 849.91585 | -125 | 634.573 | . $1546 \mathrm{E}-02$ | 1.105 |
| 1 | 0 | 1016 | 0 | 848.72128 |  | 377074 | .3969E-02 | 1.006 | -1 | 1 | 430 | 0 | 849.93336 |  | 634.567 | . $3868 \mathrm{E}-03$ | 1.106 |
| -1 | 1 | 429 | 0 | 848.72613 |  | 595.762 | . 4455 E | 1.006 | 1 | 1 | 315 | 3 | 850.02726 | -3 | 173.762 | . $1264 \mathrm{E}-01$ | . 980 |
| 1 | 0 | 1015 | 2 | 848.76107 | 56 | 357.250 | . $3748 \mathrm{E}-02$ | 1.005 |  | 1 | 315 | 1 | 850.03047 |  | 173.757 | .6322E-02 | . 980 |
| 1 | 0 | 1015 | 0 | 848.76340 |  | 357.244 | . $9369 \mathrm{E}-03$ | 1.005 | -1 | 1 | 28 | 3 | 850.07981 | 35 | 544.141 | .2412E-02 | 1.117 |
| 1 | 1 | 314 | 3 | 848.77297 | -1 | 154.319 | .1336E-01 | . 983 | 1 | 1 | 328 | 1 | 850.08855 | 20 | 544.135 | .1207E-02 | 1.118 |
| 1 | 1 | 314 | 1 | 848.77597 |  | 154.314 | .6682E-02 | . 983 | 1 | 1 | 22 | 2 | 850.17865 |  | 327.931 | . $3074 \mathrm{E}-02$ | 1.000 |
| 1 | 0 | 1014 | 2 | 848.80077 | 26 | 337.813 | .3385E-02 | 1.004 | 1 | 1 | 413 | 2 | 850.18024 | 9 | 327.925 | .6149E-02 | 1.000 |
| 1 | 0 | 1014 | 0 | 848.80293 |  | 337.808 | .8463E-03 | 1.004 | 1 | 1 | 413 | 2 | 850.23905 | 41 | 150.290 | .1475E-01 | . 991 |
| 1 | 0 | 1013 | 2 | 848.83785 | 9 | 319.671 | .2858E-02 | 1.003 | -1 | 1 | 226 | 2 | 850.24239 850.25141 |  | 150.284 | . $3688 \mathrm{E}-02$ | . 991 |
| 1 | 0 | 1013 | 0 | 848.83984 |  | 319.666 | .7144E-03 | 1.003 | -1 | 0 | 1135 | 3 | 850.26235 | 10 | 462.883 1059.286 | .3653E-02 | 1.144 |
| -1 | 1 | 327 | 3 | 848.86798 | 348* | 507.909 | .2739E-02 | 1.110 | -1 | 1 | 226 | 0 | 850.26286 | -215* | 1059.286 462.877 | $.1187 E-03$ $.9149 E-03$ | 1.034 1.146 |
| 1 | 0 | 1012 | 2 | 848.87231 | -84 | 302.824 | .2139E-02 | 1.002 | 1 | 0 | 1135 | 1 | 850.26796 |  | 1059.280 | . $4747 \mathrm{E}-03$ | 1.146 1.034 |
| 1 | 0 | 1012 | 0 | 848.87414 |  | 302.818 | . $5347 \mathrm{E}-03$ | 1.002 | 1 | 0 | 1134 | 3 | 850.35354 |  | 1014.078 | . $1426 \mathrm{E}-03$ | 1.034 1.032 |
| -1 | 1 | 327 | 1 | 848.87635 |  | 507.903 | .1371E-02 | 1.111 | 1 | 0 | 1134 |  | 850.35892 |  | 1014.072 | . $5705 \mathrm{E}-03$ | 1.032 |
| 1 | 0 | 1011 | 2 | 848.90414 | 31 | 287.271 | .1199E-02 | 1.001 | -1 | 1 | 124 | 3 | 850.41242 |  | 390.813 | .1389E-02 | 1.032 1.228 |
| 1 | 0 | 1011 | 0 | 848.90582 |  | 287.265 | .2997E-03 | 1.001 | -1 | 1 | 124 | 1 | 850.41812 | -125 | 390.807 | . $5567 \mathrm{E}-02$ | 1.228 1.230 |
| 1 | 1 | 412 | 2 | 848.97959 | 275* | 133.436 | . $1544 \mathrm{E}-01$ | . 993 | 1 | 0 | 1133 | 3 | 850.44228 |  | 970.152 | . $1701 \mathrm{E}-03$ | 1.230 1.030 |
| 1 | 1 | 412 | 0 | 848.98267 |  | 133.431 | . $3855 \mathrm{E}-02$ | . 992 | 1 | 0 | 1133 |  | 850.44743 |  | 970.146 | . $6802 \mathrm{E}-03$ | 1.030 |
| 1 | 1 | 021 | 2 | 848.98514 |  | 299.435 | . $3380 \mathrm{E}-02$ | 1.000 | 1 | 1 | 511 | 3 | 850.45760 |  | 136.035 | . $4149 \mathrm{E}-02$ | 1.030 |
| 1 | 1 | 021 | 0 | 848.98672 | $-333^{*}$ | 299.430 | . $6761 \mathrm{E}-02$ | 1.000 | 1 | 1 | 511 | 1 | 850.45983 | -45 | 136.030 | . $1659 \mathrm{E}-01$ | . 9996 |
| -1 | 1 | 225 | 2 | 849.03470 | -19 | 429.227 | . $4085 \mathrm{E}-02$ | 1.134 | 1 | 0 | 1132 | 3 | 850.52853 |  | 927.509 | 2012E-03 | . 996 |
| -1 | 1 | 225 | 0 | 849.04562 | 26 | 429.221 | .1023E-02 | 1.136 | 1 | 0 | 1132 | 1 | 850.53346 |  | 927.503 | . $8046 \mathrm{E}-03$ | 1.028 |








| $\Delta K \Delta J$ | $K \quad J$ | $\sigma$ | $\nu_{i}$ | O-c | $E_{i}^{\prime \prime}$ | $S_{i}$ | $W_{i}$ | $\Delta K \Delta J$ | K J | $\sigma$ | $\nu_{i}$ | O-C | $E_{i}^{\prime \prime}$ | $S_{i}$ | $W_{i}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 11 | 1010 | 2 | 863.16196 | 8 | 273.013 | . $1432 \mathrm{E}-01$ | 1.000 | 10 | 1633 | 2 | 864.88128 |  | 1241.703 | . $1562 \mathrm{E}-03$ | 1.018 |
| 11 | 1010 | 0 | 863.16363 |  | 273.008 | . $3579 \mathrm{E}-02$ | 1.000 | 10 | 1633 | 0 | 864.88628 |  | 1241.697 | . $3906 \mathrm{E}-04$ | 1.018 |
| 11 | 130 | 3 | 863.22160 |  | 604.343 | . $4063 \mathrm{E}-03$ | . 706 | 10 | 1632 | 2 | 864.97082 |  | 1199.083 | . $1828 \mathrm{E}-03$ | 1.017 |
| 1 | 619 | 2 | 863.22916 |  | 318.921 | . $4721 \mathrm{E}-02$ | . 988 | 10 | 1632 | 0 | 864.97557 |  | 1199.078 | . $4571 \mathrm{E}-04$ | 1.017 |
| 11 | 130 | 1 | 863.23163 | 88 | 604.337 | . $1620 \mathrm{E}-02$ | . 704 | 10 | 1631 | 2 | 865.05775 |  | 1157.747 | . $2116 \mathrm{E}-03$ | 1.015 |
| 11 | 619 | 0 | 863.23370 | -119 | 318.916 | .9443E-02 | . 988 | 10 | 1631 | 0 | 865.06224 |  | 1157.741 | . $5291 \mathrm{E}-04$ | 1.015 |
| 11 | 228 | 2 | 863.40157 | 62 | 534.060 | . $2851 \mathrm{E}-02$ | . 875 | 11 | 816 | 2 | 865.06227 | 77 | 305.413 | . $1111 \mathrm{E}-01$ | . 996 |
| 11 | 228 | 0 | 863.41308 |  | 534.055 | .7120E-03 | . 874 | 11 | 816 | 0 | 865.06541 |  | 305.407 | . $2776 \mathrm{E}-02$ | . 996 |
| 11 | 717 | 3 | 863.51650 |  | 297.199 | .2718E-02 | . 994 | 11 | 425 | 2 | 865.13179 | 12 | 453.420 | .4851E-02 | . 958 |
| 11 | 717 | 1 | 863.51942 | -52 | 297.193 | . $1087 \mathrm{E}-01$ | . 994 | 1.1 | 425 | 0 | 865.13966 |  | 453.415 | . $1211 \mathrm{E}-02$ | . 957 |
| 11 | 326 | 3 | 863.64163 | 215* | 472.965 | . $4131 \mathrm{E}-02$ | . 934 | 0 | 1630 | 2 | 865.14204 |  | 1117.695 | . $2428 \mathrm{E}-03$ | 1.014 |
| 11 | 326 | 1 | 863.64791 |  | 472.959 | .2063E-02 | . 933 | 0 | 1630 | 0 | 865.14629 |  | 1117.689 | . $6069 \mathrm{E}-04$ | 1.014 |
| 11 | 815 | 2 | 863.81297 | 42 | 284.679 | . $1204 \mathrm{E}-01$ | . 997 | 10 | 1629 | 2 | 865.22370 |  | 1078.927 | .2755E-03 | 1.013 |
| 11 | 815 | 0 | 863.81589 |  | 284.674 | . $3011 \mathrm{E}-02$ | . 997 | 0 | 1629 | 0 | 865.22772 |  | 1078.921 | .6886E-04 | 1.013 |
| 11 | 424 | 2 | 863.90642 | 2 | 421.055 | . $5541 \mathrm{E}-02$ | . 962 | 0 | 1628 | 2 | 865.30272 |  | 1041.445 | . $3090 \mathrm{E}-03$ | 1.012 |
| 11 | 424 | 0 | 863.91383 |  | 421.050 | . $1384 \mathrm{E}-02$ | . 961 | 0 | 1628 | 0 | 865.30650 |  | 1041.439 | .7724E-04 | 1.012 |
| 11 | 1913 | 3 | 864.11504 | -19 | 281.372 | . $1290 \mathrm{E}-01$ | . 999 | 11 | 914 | 3 | 865.36981 | -12 | 299.516 | . $1199 \mathrm{E}-01$ | . 998 |
| 11 | 1913 | 1 | 864.11709 |  | 281.367 | . $6452 \mathrm{E}-02$ | . 999 | 11 | 914 | 1 | 865.37199 |  | 299.510 | . $5994 \mathrm{E}-02$ | . 998 |
| 11 | 1034 | 2 | 864.12423 |  | 770.409 | .5409E-03 | 1.000 | 0 | 1627 | 2 | 865.37908 |  | 1005.249 | . $3422 \mathrm{E}-03$ | 1.011 |
| 11 | 1034 | 0 | 864.12591 | 202* | 770.403 | .1082E-02 | 1.000 | 0 | 1627 | 0 | 865.38264 |  | 1005.243 | . $85555 \mathrm{E}-04$ | 1.011 |
| 11 | 1522 | 3 | 864.18105 |  | 378.344 | . $1759 \mathrm{E}-02$ | . 977 | 1 | 523 | 3 | 865.41125 |  | 408.128 | . $1561 \mathrm{E}-02$ | . 975 |
| 1 | 1522 | 1 | 864.18544 | -41 | 378.339 | . $7036 \mathrm{E}-02$ | . 977 | 11 | 523 | 1 | 865.41589 | -74 | 408.122 | .6237E-02 | . 974 |
| 1 | $1 \quad 1011$ | 2 | 864.42520 | 33 | 287.271 | .1343E-01 | 1.000 | 0 | 1626 | 2 | 865.45278 |  | 970.340 | . $3735 \mathrm{E}-03$ | 1.009 |
| 1 | 11011 | 0 | 864.42701 |  | 287.265 | . $3357 \mathrm{E}-02$ | 1.000 | 0 | 1626 | 0 | 865.45613 |  | 970.334 | .9337E-04 | 1.009 |
| 11 | 1131 | 3 | 864.44442 |  | 644.436 | . $3355 \mathrm{E}-03$ | . 688 | 0 | 1625 | 2 | 865.52382 |  | 936.718 | . $4017 \mathrm{E}-03$ | 1.008 |
| 11 | 1131 | 1 | 864.45503 | -77 | 644.431 | . $1338 \mathrm{E}-02$ | . 686 | 0 | 1625 | 0 | 865.52695 |  | 936.712 | . $1004 \mathrm{E}-03$ | 1.008 |
| 1 | 1620 | 2 | 864.46758 |  | 344.829 | . $4270 \mathrm{E}-02$ | . 987 | 0 | 1624 | 2 | 865.59218 |  | 904.384 | .4245E-03 | 1.007 |
| 11 | 1620 | 0 | 864.47246 | -22 | 344.824 | . $8531 \mathrm{E}-02$ | . 986 | 0 | 1624 | 0 | 865.59511 |  | 904.379 | . $1061 \mathrm{E}-03$ | 1.007 |
| 11 | 1229 | 2 | 864.62032 | 65 | 571.580 | .2421E-02 | . 866 | 0 | 1623 | 2 | 865.65786 |  | 873.339 | . $4393 \mathrm{E}-03$ | 1.006 |
| 11 | 1229 | 0 | 864.63252 |  | 571.575 | .6040E-03 | . 864 | 0 | 1623 | 0 | 865.66060 |  | 873.334 | . $1098 \mathrm{E}-03$ | 1.006 |
| 10 | 01635 | 2 | 864.69437 |  | 1330.789 | .1111E-03 | 1.021 | 11 | 132 | 3 | 865.66555 |  | 685.815 | .2750E-03 | . 670 |
| 10 | 01635 | 0 | 864.69990 |  | 1330.783 | .2778E-04 | 1.021 | 11 | 132 | 1 | 865.67678 | -180* | 685.810 | . $1097 \mathrm{E}-02$ | . 668 |
| 1 | 1718 | 3 | 864.76029 |  | 320.520 | .2483E-02 | . 993 | 1 | 1012 | 2 | 865.68552 | 36 | 302.824 | . $12565 \mathrm{E}-01$ | 1.000 |
| 1 | 1718 | 1 | 864.76338 | -51 | 320.514 | . $9933 \mathrm{E}-02$ | . 993 | 11 | 1012 | 0 | 865.68750 |  | 302.818 | . $3139 \mathrm{E}-02$ | 1.000 |
| 10 | $\begin{array}{lll}0 & 1634\end{array}$ | 2 | 864.78913 |  | 1285.605 | .1323E-03 | 1.019 | 11 | 621 | 2 | 865.70306 | -91 | 372.029 | . $3832 \mathrm{E}-02$ | . 985 |
| 10 | $0 \quad 1634$ | 0 | 864.79439 |  | 1285.599 | . $3308 \mathrm{E}-04$ | 1.019 | 11 | 621 | 0 | 865.70827 | 1 | 372.023 | . $7664 \mathrm{E}-02$ | . 985 |
| 1 | 1327 | 3 | 864.86272 | -26 | 507.909 | . $3565 \mathrm{E}-02$ | . 928 | 0 | 1622 | 2 | 865.72085 |  | 843.583 | . $4430 \mathrm{E}-03$ | 1.005 |
| 11 | 1327 | 1 | 864.86935 |  | 507.903 | .1783E-02 | . 928 | 10 | 1622 | 0 | 865.72340 |  | 843.578 | . $1108 \mathrm{E}-03$ | 1.005 |


|  |  <br>  <br>  <br>  <br> ㄲ <br> 䓵 <br> Y <br> 俞 <br> Tis <br>  <br>  <br>  <br>  |
| :---: | :---: |
|  |  <br>  <br>  <br>  <br>  <br>  <br>  N <br>  <br>  <br>  <br>  |








| $\Delta K \Delta J$ | $K \quad J$ | $\sigma$ | $\nu_{i}$ | O-C | $E_{i}^{\prime \prime}$ | $S_{i}$ | $W_{i}$ | $\Delta K \Delta J$ | K | $K J \quad \sigma$ | $\sigma$ | $\nu_{i}$ | O-C | $E_{i}^{\prime \prime}$ | $S_{i}$ | $W_{i}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 11 | 1426 | 2 | 894.46451 | 139 | 849.626 | . $1351 \mathrm{E}-02$ | . 996 | 1 | 1 | 1819 | 2 | 897.61990 |  | 898.839 | . $6229 \mathrm{E}-03$ | 1.000 |
| 11 | 1426 | 0 | 894.46856 |  | 849.621 | .3379E-03 | . 996 | 1 | 1 | 1819 | 0 | 897.62177 | 70 | 898.834 | . $1246 \mathrm{E}-02$ | 1.000 |
| 11 | 1719 | 3 | 894.66321 |  | 828.449 | .4151E-03 | 1.000 | 1 | 1 | 1624 | 2 | 897.85751 | 31 | 904.384 | . $1125 \mathrm{E}-02$ | . 998 |
| 11 | 1719 | 1 | 894.66509 | -37 | 828.444 | . $1661 \mathrm{E}-02$ | 1.000 | 1 | 1 | 1624 | 0 | 897.86062 |  | 904.379 | . $2812 \mathrm{E}-03$ | . 998 |
| 11 | 1231 | 2 | 894.73947 |  | 932.445 | .4336E-03 | . 988 | 1 | 1 | 1429 | 2 | 898.09013 | -44 | 958.240 | . $8237 \mathrm{E}-03$ | . 993 |
| 11 | 1231 | 0 | 894.74557 | 89 | 932.439 | . $8671 \mathrm{E}-03$ | . 988 | 1 | 1 | 1429 | 0 | 898.09494 |  | 958.234 | .2059E-03 | . 993 |
| 11 | 1524 | 3 | 894.93541 | -16 | 842.018 | .1447E-02 | . 998 | 1 | 1 | 1234 | 2 | 898.32033 |  | 1060.361 | .2420E-03 | . 985 |
| 11 | 1524 | 1 | 894.93820 |  | 842.012 | .7235E-03 | . 998 | 1 | 1 | 1234 | 0 | 898.32739 |  | 1060.355 | . $4834 \mathrm{E}-03$ | . 984 |
| 11 | 1329 | 3 | 895.20362 |  | 903.911 | .2553E-03 | . 992 | 1 | 1 | 1722 | 3 | 898.35145 |  | 909.965 | . $28388 \mathrm{E}-03$ | . 999 |
| 11 | 1329 | 1 | 895.20762 | 117 | 903.905 | . $1021 \mathrm{E}-02$ | . 992 | 1 | 1 | 1722 | 1 | 898.35370 | -95 | 909.959 | . $1135 \mathrm{E}-02$ | . 999 |
| 11 | 1622 | 2 | 895.41363 | 68 | 843.583 | . $1487 \mathrm{E}-02$ | . 999 | 1 | 1 | 1527 | 3 | 898.57853 | 30 | 942.895 | . $9127 \mathrm{E}-03$ | . 996 |
| 11 | 1622 | 0 | 895.41635 |  | 843.578 | .3719E-03 | . 999 | 1 | 1 | 1527 | 1 | 898.58179 |  | 942.889 | . $4563 \mathrm{E}-03$ | . 996 |
| 11 | 1134 | 3 | 895.47069 |  | 1014.078 | .1444E-03 | . 982 | 1 | 1 | 1332 | 3 | 898.80169 |  | 1024.109 | . $1476 \mathrm{E}-03$ | . 989 |
| 11 | 1134 | 1 | 895.47628 |  | 1014.072 | .5775E-03 | . 982 | 1 | 1 | 1332 | 1 | 898.80628 |  | 1024.103 | . $5903 \mathrm{E}-03$ | . 989 |
| 11 | 1427 | 2 | 895.67633 | 51 | 884.544 | . $1153 \mathrm{E}-02$ | . 995 | 1 | 1 | 1820 | 2 | 898.85201 |  | 924.717 | .5512E-03 | 1.000 |
| 11 | 1427 | 0 | 895.68062 |  | 884.538 | .2882E-03 | . 995 | 1 | 1 | 1820 | 0 | 898.85404 | 58 | 924.711 | . $1102 \mathrm{E}-02$ | 1.000 |
| 11 | 1720 | 3 | 895.89585 |  | 854.331 | . $3678 \mathrm{E}-03$ | 1.000 | 1 | 1 | 1625 | 2 | 899.07455 | 38 | 936.718 | . $9699 \mathrm{E}-03$ | . 998 |
| 11 | 1720 | 1 | 895.89785 | -51 | 854.325 | .1471E-02 | 1.000 | 1 | 1 | 1625 | 0 | 899.07787 |  | 936.712 | . $2425 \mathrm{E}-03$ | . 998 |
| 11 | 1232 | 2 | 895.93639 |  | 973.800 | . $3592 \mathrm{E}-03$ | . 987 | 1 | 1 | 1430 | 2 | 899.29208 | 184* | 997.017 | .6905E-03 | . 993 |
| 11 | 1232 | 0 | 895.94280 | 257* | 973.794 | .7185E-03 | . 987 | 1 | 1 | 1430 | 0 | 899.29716 |  | 997.011 | . $1726 \mathrm{E}-03$ | . 993 |
| 11 | 1525 | 3 | 896.15305 | 7 | 874.356 | .1248E-02 | . 997 | 1 | 1 | 1723 | 3 | 899.57438 |  | 939.717 | .2473E-03 | . 999 |
| 11 | 1525 | 1 | 896.15600 |  | 874.350 | .6240E-03 | . 997 | 1 | 1 | 1723 | 1 | 899.57675 | -9 | 939.711 | .9892E-03 | . 999 |
| 11 | 1818 | 2 | 896.38456 |  | 874.252 | .7004E-03 | 1.000 | 1 | 1 | 1528 | 3 | 899.78633 | 26 | 979.096 | .7730E-03 | . 995 |
| 11 | 1818 | 0 | 896.38628 | 73 | 874.247 | $.1401 \mathrm{E}-02$ | 1.000 | 1 | 1 | 1528 | 1 | 899.78975 |  | 979.090 | .3865E-03 | . 995 |
| 11 | 11330 | 3 | 896.40627 |  | 942.692 | .2140E-03 | . 991 | 1 | 1 | 1333 | 3 | 899.99442 |  | 1066.744 | . $1214 \mathrm{E}-03$ | . 988 |
| 11 | $1 \begin{array}{ll}13 & 30\end{array}$ | 1 | 896.41047 | -98 | 942.686 | .8562E-03 | . 991 | 1 | 1 | 1333 | 1 | 899.99922 |  | 1066.738 | . $4856 \mathrm{E}-03$ | . 988 |
| 1.1 | 11623 | 2 | 896.63720 | -17 | 873.339 | .1297E-02 | . 998 | 1 | 1 | 1821 | 2 | 900.08088 |  | 951.885 | . $4851 \mathrm{E}-03$ | 1.000 |
| 11 | 11623 | 0 | 896.64011 |  | 873.334 | . $3241 \mathrm{E}-03$ | . 998 | 1 | 1 | 1821 | 0 | 900.08307 | 50 | 951.880 | .9702E-03 | 1.000 |
| 1 1 | $1 \quad 1428$ | 2 | 896.88488 | 30 | 920.749 | .9775E-03 | . 994 | 1 | 1 | 1626 | 2 | 900.28830 | 103 | 970.340 | .8306E-03 | . 997 |
| 11 | 11428 | 0 | 896.88942 |  | 920.743 | .2444E-03 | . 994 | 1 | 1 | 1626 | 0 | 900.29184 |  | 970.334 | .2076E-03 | . 997 |
| 11 | 11721 | 3 | 897.12527 |  | 881.503 | . $3238 \mathrm{E}-03$ | . 999 | 1 | 1 | 1431 | 2 | 900.49071 | -74 | 1037.079 | . $5746 \mathrm{E}-03$ | . 992 |
| 11 | 11721 | 1 | 897.12739 | -3 | 881.497 | . $1295 \mathrm{E}-02$ | . 999 | 1 | 1 | 1431 | 0 | 900.49606 |  | 1037.073 | .1437E-03 | . 992 |
| 11 | 11233 | 2 | 897.13001 |  | 1016.439 | . $2958 \mathrm{E}-03$ | . 986 | 1 | 1 | 1919 | 3 | 900.59113 |  | 973.230 | . $2288 \mathrm{E}-03$ | 1.000 |
| 11 | 11233 | 0 | 897.13674 |  | 1016.433 | . $5915 \mathrm{E}-03$ | . 986 | 1 | 1 | 1919 | 1 | 900.59282 |  | 973.224 | . $9154 \mathrm{E}-03$ | 1.000 |
| 11 | 11526 | 3 | 897.36743 | -25 | 907.982 | .1071E-02 | . 997 | 1 | 1 | 1724 | 3 | 900.79403 |  | 970.758 | . $2143 \mathrm{E}-03$ | . 999 |
| 11 | 1526 | 1 | 897.37053 |  | 907.976 | .5350E-03 | . 996 | 1 | 1 | 1724 | 1 | 900.79653 | -63 | 970.752 | .8571E-03 | . 999 |
| 11 | 11331 | 3 | 897.60563 |  | 982.758 | .1783E-03 | . 990 | 1 | 1 | 1529 | 3 | 900.99081 | 28 | 1016.583 | . $6514 \mathrm{E}-03$ | . 995 |
| 11 | $1 \quad 1331$ | 1 | 897.61003 | -101 | 982.752 | .7132E-03 | . 990 | 1 | 1 | 1529 | 1 | 900.99441 |  | 1016.577 | . $3257 \mathrm{E}-03$ | . 995 |




## Appendix B

## Observed and Calculated FTS Spectra of $\nu_{12}{ }^{13} \mathbf{C}^{12} \mathbf{C H}_{6}$

Top trace:
Observed at $p=1.05$ Torr, $\ell=1.5 \mathrm{~m}$ and $T=294 \mathrm{~K}$.

## Middle trace:

Calculated at $p=1.05$ Torr, $\ell=1.5 \mathrm{~m}$ and $T=294 \mathrm{~K}$. Spectrum shown on a scale from $0 \%$ to $100 \%$ transmission.

## Bottom trace:

Same as middle trace. Spectrum shown on a blown up scale from $90 \%$ to $100 \%$ transmission.

(






( wavenumber $\left(\mathrm{cm}^{-1}\right)$

$\underset{\text { wavenumber }\left(\mathrm{cm}^{-1}\right)}{ }$


B-5
c-2









## B-8









```
~yn
```







B-12



B-14



B-16












B-18



B-19









rrprorror




























## 





B-32

## 



## 













## 




## 



## 

## $\rightarrow \sqrt{\sim}$







## Moverion






## ,

## 






## 











































"prompromprommpmirng
















## 










qurmprormprormorn









B-72


## 




## 



## mormorns







B-79








$\underset{904.0}{\text { wavenumber }\left(\mathrm{cm}^{-1}\right)}$




| 1. AGENCY USE ONLY (Leave blank) | 2. REPORT DATE <br> April 1994 | 3. REPORT TYPE AND DATES COVERED <br> Technical Memorandum |
| :--- | :--- | :--- |

4. TITLE AND SUBTITLE

A Spectral Atlas of the $v_{12}$ Fundamental of ${ }^{13} \mathrm{C}^{12} \mathrm{CH}_{6}$ in the $12 \mu \mathrm{~m}$ Region
5. FUNDING NUMBERS
6. AUTHOR(S)

Mark Weber, Dennis Reuter, J. Marcos Sirota, William Blass, John Hillman
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)

Goddard Space Flight Center
Greenbelt, Maryland 20771
9. SPONSORINGMONITORING AGENCY NAME(S) AND ADDRESS(ES)

National Aeronautics and Space Administration
Washington, D.C. 20546-0001
8. PERFORMING ORGANIZATION REPORT NUMBER

94B00067
10. SPONSORINGMONTTORING AGENCY REPORT NUMBER

## 11. SUPPLEMENTARY NOTES

William E. Blass: Department of Physics, University of Tennessee

12a. DISTRIBUTIONAVAILABILTYY STATEMENT
Unclassified-Unlimited
Subject Category 72
Report available from the NASA Center for AeroSpace Information, 800 Elkridge
Landing Road, Linthicum Heights, MD 21090; (301) 621-0390.

12h. DISTRIBUTION CODE

## 13. ABSTRACT (Maximum 200 words)

The recent discovery of the minor isotopomer of ethane, ${ }^{13} \mathrm{C}^{12} \mathrm{CH}_{6}$, in the planetary atmospheres of Jupiter and Neptune, added ethane to the molecules which can be used to determine isotopic ${ }^{12} \mathrm{C}^{12} \mathrm{C}$ ratios for the jovian planets. The increased spectral resolution and coverage of the IR and far-IR instruments to be carried on the Cassini mission to Saturn and Titan may enable the detection of the minor isotopomer. Accurate frequency and cross-section measurements of the $\mathrm{v}_{12}$ fundamental under controlled laboratory condition are important to interpret current and future planetary spectra. High resolution spectra of the minor isotopomer ${ }^{13} \mathrm{C}^{12} \mathrm{CH}_{6}$ have been recorded in the $12.2 \mu \mathrm{~m}$ region using the Kitt Peak Fourier Transform (FTS) and the Goddard Tunable Diode Laser spectrometer (TDL). In a global fit to 19 molecular constants in a symmetric top Hamiltonian, transition frequencies of the $\mathrm{v}_{12}$ fundamental ranging up to $\mathrm{J}=35$ and $\mathrm{K}=20$ have been determined with a standard deviation of less than $0.0005 \mathrm{~cm}^{-1}$. From selected line intensity measurements, a vibrational dipole moment for the $v_{12}$ fundamental has been derived. Observed and calculated spectra covering the region from $740 \mathrm{~cm}^{-1}$ and to $910 \mathrm{~cm}^{-1}$ are presented. A compilation of transition frequencies, line intensities, and lower state energies are included for general use in the astronomical community.

| 14.SUBJECT TERMS <br> Kitt Peak Fourier Transform, Goddard Tunable Diode Lasers, Molecular Spectroscopy, <br> Infrared Spectrum | 15. NUMBER OF PAGES <br> 178 |  |
| :--- | :--- | :---: |
| 17. SECURITY CLASSIFICATION <br> OF REPORT <br> Unclassified | 18. SECURITY CLASSIFICATION <br> OF THIS PAGE <br> Unclassified | 19. SECURITY CLASSIFICATION <br> OF ABSTRACT <br> Unclassified | | 20. LIMITATION OF ABSTRACT |
| :---: |
| Unlimited |

