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# An Alternative Perturbation Method for the Molecular Vibration-Rotation Problem II- Calculation *ab initio* of observables, application to the dipole moment of methane

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## Abstract

The first article of this series has introduced an alternative perturbation scheme to find approximate solutions of the spectral problem for the rotation-vibration molecular Hamiltonian. The convergence of our method for the methane vibrational ground state rotational energy levels was quicker than that of the traditional method, as expected, and our predictions were quantitative. In this second article, we study the convergence of the calculation *ab initio* of effective dipole moments for methane within the same theoretical frame. The first order of perturbation when applied to the electric dipole moment operator of a spherical top gives the expression used in previous spectroscopic studies. Higher orders of perturbation give corrections corresponding to higher centrifugal distortion contributions and are calculated accurately for the first time. Two potential energy surfaces of the literature have been used for solving the anharmonic vibrational problem by means

of the vibrational mean field configuration interaction approach. Two corresponding dipole moment surfaces were calculated in this work at a high level of theory. The predicted intensities agree better with recent experimental values than their empirical fit. This suggests that our *ab initio* dipole moment surface and effective dipole moment operator are both highly accurate.

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## 1 INTRODUCTION

In Part 1 of this series of papers [1], we have presented a method which generalises Rayleigh-Schrödinger perturbation theory to the case where “eigenvalues” are not element of the field of real numbers but are element of a ring spanned by, non necessarily commuting, operators, and where “eigenfunctions” are not elements of a Hilbert space but element of a module over a ring. The method was applied to the calculation of the rotational levels of methane in its vibrational ground state. The speed of convergence of our approach, where the unperturbed Hamiltonian was the ( $J = 0$ )-Watson Hamiltonian [2,3] in the Eckart frame [4], was found much quicker than that of the traditional approaches starting from the vibrational harmonic Hamiltonian [5–7].

In another study of the same system [8], our approach has been compared numerically to contact transformation methods and the reliability of the predicted rotational energy levels has been further confirmed. The relevance of our calculated rotational wave functions was demonstrated in [9], where the predicted Q-branch spectrum was found accurate enough to usefully complement the HITRAN database [10]. However, in the latter study, we used the effective dipole moment experimental value of Ozier [11] to compute our transition intensities.

The purpose of this article is to calculate purely *ab initio* transition intensities for the R-branch of methane vibrational ground state by using an *ab initio* effective dipole moment operator, computed according to the same perturbation theory [12] already used to derive the effective rotational Hamiltonian. For this purpose, we have calculated our

own high level dipole moment surface (DMS) and have determined the vibrational wave functions by means of the variational vibrational mean field configuration interaction approach [13]. It is important to have such a theoretical reference, independent of any experimental number, because the value of the effective dipole moment of methane is still a debated question. Recent experimental studies have obtained quite different values [14,15]. A precise modelling of the rotational forbidden spectra of methane is of paramount significance, since it can be used to derive methane abundances in Titan, Saturn or Neptune atmosphere for example [16].

The vibrational and/or rotational spectra of methane has been the topics of many theoretical studies, see Refs. [17–29] to quote a few. However, as far as we are aware, only Signorel et al. [30] have investigated its effective rotational dipole moment coefficients.

The rest of the paper is organised as follows: In Section II we introduce the general theoretical setting of our approach and we recall the perturbation formula for effective Hamiltonian and other observables such as the electric dipole moment. In section III we apply the new method to the R-Branch of  $CH_4$  and thoroughly assess the convergence of our results. In conclusion, we compare our *ab initio* results to experimental values.

## **2 AB INITIO EFFECTIVE ROTATIONAL HAMILTONIAN AND DIPOLE MOMENT**

In this section, the theory of effective operators implemented in this work is briefly introduced, in order to make the article self-contained. Effective Hamiltonian theory has a long history, and many reviews of this topics are available, see [31–33] to quote a few. Our generalized Schrödinger equation need not be solved perturbationally, however the perturbative solutions of the present section can be seen as a particular case of Ref. [33] section 8. The specific properties of this particular perturbation theory are detailed in [31], where its origin is traced back to Des Cloizeaux in 1960 [34]. An independent formulation using the wave operator idea can be found in [35]. This theory has also

been shown equivalent [31] to the contact transformation approach of Van Vleck [36], Kemple [37] and Primas [38], provided a minimum distance criterium between the eigenkets of the original and transformed representations is enforced, and to the approach of Buleavski [39]. However, there is one more ingredient in our approach: the fact that tensorial structure of the Hilbert space is compatible with the decomposition of the original Hamiltonian. Note that this ingredient has also been exploited in [32] in the framework of the contact transformation formalism.

### 2.1 Definition of effective operators

Let us consider a molecular rotation-vibration Hamiltonian in the Eckart frame. Let denote by  $X$  the set of vibrational coordinates and their conjugate momenta,  $X = \{(Q_i)_i, (P_k)_k\}$ , and by  $Y$ , the set of Euler angles and their conjugate momenta,  $Y = \{\theta, \chi, \phi, P_\theta, P_\chi, P_\phi\}$ . The operators in  $X$  act on a Hilbert space,  $V_{\mathbf{x}}$ , of square integrable functions of the vibrational degrees of freedoms (DOF), collectively denoted by  $\mathbf{x}$ . Similarly, those in  $Y$  act on a Hilbert space,  $V_{\mathbf{y}}$ , of square integrable functions of the rotational DOF,  $\mathbf{y}$ . The Hilbert space of the whole system is the tensor product,  $V = V_{\mathbf{x}} \otimes V_{\mathbf{y}}$ . In Dirac notation, kets on  $V$  (resp. on  $V_{\mathbf{x}}$ ,  $V_{\mathbf{y}}$ ) will be denoted by  $|\cdots\rangle$ , (resp.  $|\cdots\rangle_{\mathbf{x}}$ ,  $|\cdots\rangle_{\mathbf{y}}$ ). No index is used for the corresponding bra's. The identity on  $V_{\mathbf{x}}$  (respectively  $V_{\mathbf{y}}$ ) is written  $Id_{\mathbf{x}}$  (respectively  $Id_{\mathbf{y}}$ ).

The Hamiltonian of the system,  $H(X, Y)$ , considered in this work will be the Eckart-Watson Hamiltonian for non linear molecules [2]. It can be decomposed as,

$$H(X, Y) = H_0(X) \otimes Id_{\mathbf{y}} + H_1(X, Y), \quad (1)$$

where, in atomic units,  $H_0(X)$  is the ( $J = 0$ )-Hamiltonian,

$$H_0(X) = \frac{1}{2} \sum_k P_k^2 + U + \frac{1}{2} \sum_{\alpha\beta} \mu_{\alpha\beta} \pi_\alpha \pi_\beta - \frac{1}{8} \sum_\alpha \mu_{\alpha\alpha}, \quad (2)$$

and,

$$H_1(X, Y) = \sum_{\alpha\beta} \frac{1}{2} \mu_{\alpha\beta} \otimes \Pi_\alpha \Pi_\beta - \mu_{\alpha\beta} \pi_\alpha \otimes \Pi_\beta. \quad (3)$$

In the equations above,  $U$  is the potential of electronic origin in the Born-Oppenheimer approximation, expressed as a function of the normal coordinates  $Q_i$ ,  $\mu$  is the 3 by 3 effective reciprocal inertia matrix whose series expansion in terms of the normal coordinates is

$$\mu = \sum_{r=0}^{+\infty} \left(\frac{1}{2}\right)^r (r+1) \sum_{k_1, \dots, k_r} I_e^{-1} a_{k_1} I_e^{-1} \dots a_{k_r} I_e^{-1} Q_{k_1} \dots Q_{k_r}, \quad (4)$$

where,  $I_e^{-1}$  is the inverse of the inertia tensor  $I(Q_1, \dots, Q_n)$  at equilibrium and  $(a_k)_k$  the derivatives of the latter with respect to the normal coordinates,

$$a_k = \left( \frac{\partial I}{\partial Q_k} \right)_0. \quad (5)$$

$\pi$  is the so-called "Coriolis coupling operator", it only depends upon the operators in set  $X$ .  $\Pi$  is the total angular momentum, and is the sole quantity depending upon the operators in set  $Y$ .

Let  $(\psi_n)_n$ , (respectively  $(\Psi_K)_K$ ), be a normalized Hilbertian basis set of  $V_{\mathbf{x}}$  (respectively  $V_{\mathbf{y}}$ ), we have:  $Id_{\mathbf{x}} = \sum_n |\psi_n\rangle_{\mathbf{x}} \cdot \langle \psi_n|$ , (respectively  $Id_{\mathbf{y}} = \sum_K |\Psi_K\rangle_{\mathbf{y}} \cdot \langle \Psi_K|$ ). A basis of  $V$  is obtained by taking the tensor product of basis functions,  $(\psi_n \otimes \Psi_K)_{n,K}$ . Since we are free to choose the basis set of  $V_{\mathbf{x}}$ , we can take for  $(\psi_n)_n$  a set of orthonormal eigenvectors of  $H_0$ . We label this set with positive integers and denote the associated eigenvalues by  $(\nu_n)_n$ .

For simplicity, we assume that the eigenstates of  $H_0(X)$  are non-degenerate. The version of the method for (quasi-) degenerate eigenstates of  $H_0(X)$  will be explored in part III of this series of articles.

To solve perturbationally the eigenvalue equation,

$$H(X, Y)\phi = E\phi, \quad (6)$$

we introduce a real parameter,  $\varepsilon \in [0, 1]$ , and the Hamiltonian,

$$H(X, Y, \varepsilon) = H_0(X) \otimes Id_{\mathbf{y}} + \varepsilon H_1(X, Y), \quad (7)$$

such that,  $H(X, Y, 0) = H_0(X) \otimes Id_{\mathbf{y}}$  and  $H(X, Y, 1) = H(X, Y)$ .

So, for  $\varepsilon = 0$ , given our choice for  $(\psi_n)_n$ ,

$$H(X, Y, 0)|\psi_n \otimes \Psi_K\rangle = \nu_n |\psi_n \otimes \Psi_K\rangle \quad \forall K. \quad (8)$$

The eigenspaces are degenerate of dimension,  $\dim V_{\mathbf{y}}$ . Substituting  $|\Psi_K\rangle_{\mathbf{y}}$  by  $|\Psi_K\rangle_{\mathbf{y}} \cdot \langle \Psi_K|$  in  $|\psi_n \otimes \Psi_K\rangle = |\psi_n\rangle_{\mathbf{x}} \otimes |\Psi_K\rangle_{\mathbf{y}}$  of Eq.(8), and summing over  $K$ , one obtains,

$$(H_0(X) \otimes Id_{\mathbf{y}})|\psi_n\rangle_{\mathbf{x}} \otimes Id_{\mathbf{y}} = \nu_n |\psi_n\rangle_{\mathbf{x}} \otimes Id_{\mathbf{y}}. \quad (9)$$

For any fixed  $n$ , (which will be the ground state,  $n = 0$ , in the application), and all  $\varepsilon \in [0, 1]$ , the  $\dim V_{\mathbf{y}}$  eigenstates  $(\psi_n \otimes \Psi_K)_K$  of  $H(X, Y, 0)$  can be related in a one-to-one correspondance to a set of  $\dim V_{\mathbf{y}}$  eigenstates of  $H(X, Y, \varepsilon)$ , denoted by  $(\phi_{n,K}(\varepsilon))_K$ . The  $\phi_{n,K}(\varepsilon)$ 's can be expanded on the tensorial product basis set as,

$$\phi_{n,K}(\varepsilon) = \sum_{n', K'} c_{n', K'}^{n, K}(\varepsilon) \psi_{n'} \otimes \Psi_{K'}. \quad (10)$$

Introducing  $\dim V_{\mathbf{x}}$  linear operators on  $V_{\mathbf{y}}$ ,  $\Psi_{n'}(Y, \varepsilon)$ , by

$$\forall n', \forall \Psi_K, \quad \Psi_{n'}(Y, \varepsilon) \Psi_K := \sum_{K'} c_{n', K'}^{n, K}(\varepsilon) \Psi_{K'}, \quad (11)$$

we can define a so-called "effective wave operator",  $\phi_n(Y, \varepsilon)$ , from  $V_{\mathbf{y}}$  onto  $V_{\mathbf{x}} \otimes V_{\mathbf{y}}$ , by

$$\phi_n(Y, \varepsilon) = \sum_{n'} \psi_{n'} \otimes \Psi_{n'}(Y, \varepsilon). \quad (12)$$

Combining Eqs. (11) and (12), we see from Eq. (10), that the action of the effective wave operator on the basis functions  $\Psi_K$  gives the exact eigenfunctions of  $H(X, Y, \varepsilon)$ ,

$$\phi_{n,K}(\varepsilon) = \phi_n(Y, \varepsilon) \Psi_K. \quad (13)$$

We define another operator on  $V_{\mathbf{y}}$ , called the "effective Hamiltonian",  $E_n(Y, \varepsilon)$ , by its action on the basis functions  $\Psi_K$ ,

$$E_n(Y, \varepsilon)\Psi_K = E_{n,K}(\varepsilon)\Psi_K. \quad (14)$$

Inserting Eqs. (13) and (14) in the eigenvalue equation of  $H(X, Y, \varepsilon)$ , we have for all  $\Psi_K$ ,

$$H(X, Y, \varepsilon)\phi_n(Y, \varepsilon)\Psi_K = \phi_n(Y, \varepsilon)E_n(Y, \varepsilon)\Psi_K. \quad (15)$$

Since the  $\Psi_K$ 's form a basis set, we can write the following identity between operators acting on  $V_{\mathbf{y}}$ ,

$$H(X, Y, \varepsilon)\phi_n(Y, \varepsilon) = \phi_n(Y, \varepsilon)E_n(Y, \varepsilon). \quad (16)$$

For the case of interest,  $\varepsilon = 1$ , we alleviate the notation by ignoring the dependence upon  $\varepsilon$ . The previous eigen-equation for effective operators is rewritten,

$$H(X, Y)\phi_n(Y) = \phi_n(Y)E_n(Y). \quad (17)$$

Applying the operators of both members of Eq.(17) to the  $\Psi_K$ 's basis, Eq.(6) is recovered for the  $(E_{n,K}, \phi_{n,K})_K$  eigenpairs of  $H(X, Y)$ .

The effective wave operator, together with its Hermitic conjugate which satisfies,

$$\phi_n^\dagger(Y)H(X, Y) = E_n^\dagger(Y)\phi_n^\dagger(Y), \quad (18)$$

where the operators act on  $V_{\mathbf{y}}$  on the left, allows one to derive for the laboratory-fixed, dipole moment,  $D(X, Y)$ , acting on  $V_{\mathbf{x}} \otimes V_{\mathbf{y}}$ , an effective Hermitian operator,  $D_n(Y)$ , acting solely on  $V_{\mathbf{y}}$ , by,

$$D_n(Y) = \langle \phi_n^\dagger(Y) | D(X, Y) | \phi_n(Y) \rangle_{\mathbf{x}}. \quad (19)$$

Here the notation  $\langle \cdots \rangle_{\mathbf{x}}$  generalizes that of kets of  $V_{\mathbf{x}}$  and means that integration is carried over the  $\mathbf{x}$ -variables only, for example,

$$\langle \psi_1 \otimes \Psi_1(Y) | \psi_2 \otimes \Psi_2(Y) \rangle_{\mathbf{x}} = \langle \psi_1 | \psi_2 \rangle_{\mathbf{x}} \Psi_1(Y) \Psi_2(Y). \quad (20)$$



Note that, if we impose the normalization condition,

$$\langle \phi_n^\dagger(Y) \phi_n(Y) \rangle_{\mathbf{x}} = Id_{\mathbf{y}}, \quad (21)$$

we obtain easily from Eqs. (17) and (18) that the effective rotational Hamiltonian,  $E_n(Y)$ , is Hermitian,

$$E_n(Y) = E_n^\dagger(Y), \quad (22)$$

and the effective dipole moment  $D_n(Y)$  will also be Hermitian and properly normalized.

## 2.2 Generalized perturbation theory for the effective wave operator equation

In the previous section, we have shown that the "exact" effective wave operator and effective Hamiltonian were solutions of an "eigen equation" for operators, Eq. (17). However, at this stage, the unicity of the solution has not been established. In this section, we show how a Rayleigh-Schrödinger type of perturbational strategy permits to solve Eq. (17), and as a by-product, we obtain that this solution is unique, provided that two reasonable constraints are enforced.

Hereafter, we set  $n = 0$  to fix the ideas, (as if the band of interest was that of the vibrational ground state). We assume that the effective operators,  $\phi_0(Y, \varepsilon)$  and  $E_0(Y, \varepsilon)$ , defined by Eqs. (13) and (14), are smooth (more precisely, analytical) functions of  $\varepsilon$ . So, it is natural to look for solutions  $\phi(Y, \varepsilon)$  and  $E(Y, \varepsilon)$  of Eq. (16) that can be expanded as a power series of  $\varepsilon$ :

$$\phi(Y, \varepsilon) = \psi_0 \otimes Id_{\mathbf{y}} + \varepsilon \phi^{(1)}(Y) + \varepsilon^2 \phi^{(2)}(Y) + \varepsilon^3 \phi^{(3)}(Y) + \varepsilon^4 \phi^{(4)}(Y) + \dots, \quad (23)$$

$$E(Y, \varepsilon) = \nu_0 Id_{\mathbf{y}} + \varepsilon E^{(1)}(Y) + \varepsilon^2 E^{(2)}(Y) + \varepsilon^3 E^{(3)}(Y) + \varepsilon^4 E^{(4)}(Y) + \dots, \quad (24)$$

Inserting these expressions in Eq. (15) and identifying the terms with the same power of

$\varepsilon$ , together with enforcing the set of "Hermiticity" conditions,  $\forall k > 0$ ,

$$\langle \psi_0 \otimes Id_{\mathbf{y}} | \phi^{(i)}(Y) \rangle_{\mathbf{x}} = \langle \phi^{(i)\dagger}(Y) | \psi_0 \otimes Id_{\mathbf{y}} \rangle_{\mathbf{x}}, \quad (25)$$

and the set of normalization conditions,  $\forall k > 0$ ,

$$\left\langle \sum_{i=0}^k \varepsilon^i \phi^{(i)\dagger}(Y) \middle| \sum_{i=0}^k \varepsilon^i \phi^{(i)}(Y) \right\rangle_{\mathbf{x}} = Id_{\mathbf{y}} + o(\varepsilon^k, Y). \quad (26)$$

where  $\phi^{(0)}(Y) = \psi_0 \otimes Id_{\mathbf{y}}$  and the notation  $o(\varepsilon^k, Y)$  means that  $\lim_{\varepsilon \rightarrow 0} \varepsilon^{-k} o(\varepsilon^k, Y) = 0_{\mathbf{y}}$ , the null operator on  $V_{\mathbf{y}}$ , one can determine unambiguously eigensolutions to any order [12].

So the perturbative solution to Eq.(17) is actually unique for a given  $H$ , within the normalization and Hermiticity constraints. Of course, if  $H$  is transformed by a unitary mapping, the effective wave operator and effective Hamiltonian will be transformed accordingly.

### 2.2.1 Effective rotational Hamiltonian

Making use of the condensed notation,

$$H_1(Y)_{i,j} := \langle \psi_i \otimes Id_{\mathbf{y}} | H_1(X, Y) | \psi_j \otimes Id_{\mathbf{y}} \rangle_{\mathbf{x}}, \quad (27)$$

the following expressions have been obtained [12] for the effective Hamiltonian corrective terms up to order 4,

$$E^{(1)}(Y) = H_1(Y)_{0,0}, \quad (28)$$

$$E^{(2)}(Y) = \sum_{k \neq 0} \frac{H_1(Y)_{0,k} H_1(Y)_{k,0}}{\nu_0 - \nu_k}, \quad (29)$$

$$\begin{aligned}
E^{(3)}(Y) &= \langle \phi^{(0)\dagger}(Y) | H_1(X, Y) | \phi^{(2)}(Y) \rangle_{\mathbf{x}} - \langle \phi^{(0)\dagger}(Y) | \phi^{(2)}(Y) \rangle_{\mathbf{x}} E^{(1)}(Y) \\
&= \sum_{k_1, k_2 \neq 0} \frac{H_1(Y)_{0, k_1} H_1(Y)_{k_1, k_2} H_1(Y)_{k_2, 0}}{(\nu_0 - \nu_{k_1})(\nu_0 - \nu_{k_2})} \\
&\quad - \frac{1}{2} \sum_{k_1 \neq 0} \frac{H_1(Y)_{0, k_1} H_1(Y)_{k_1, 0} H_1(Y)_{0, 0} + H_1(Y)_{0, 0} H_1(Y)_{0, k_1} H_1(Y)_{k_1, 0}}{(\nu_0 - \nu_{k_1})^2},
\end{aligned} \tag{30}$$

$$\begin{aligned}
E^{(4)}(Y) &= \sum_{k_1, k_2, k_3 \neq \phi_0} \frac{H_1(Y)_{0, k_1} H_1(Y)_{k_1, k_2} H_1(Y)_{k_2, k_3} H_1(Y)_{k_3, 0}}{(\nu_0 - \nu_{k_1})(\nu_0 - \nu_{k_2})(\nu_0 - \nu_{k_3})} \\
&\quad - \frac{1}{2} \sum_{k_1, k_2 \neq \phi_0} \frac{H_1(Y)_{0, 0} H_1(Y)_{0, k_1} H_1(Y)_{k_1, k_2} H_1(Y)_{k_2, 0} + H_1(Y)_{0, k_1} H_1(Y)_{k_1, k_2} H_1(Y)_{k_2, 0} H_1(Y)_{0, 0}}{(\nu_0 - \nu_{k_1})(\nu_0 - \nu_{k_2})} \left( \frac{1}{\nu_0 - \nu_{k_1}} + \frac{1}{\nu_0 - \nu_{k_2}} \right) \\
&\quad - \frac{1}{2} \left( \sum_{k_1 \neq 0} \frac{H_1(Y)_{0, k_1} H_1(Y)_{k_1, 0}}{(\nu_0 - \nu_{k_1})} \right) \left( \sum_{k_1 \neq 0} \frac{H_1(Y)_{0, k_1} H_1(Y)_{k_1, 0}}{(\nu_0 - \nu_{k_1})^2} \right) \\
&\quad - \frac{1}{2} \left( \sum_{k_1 \neq 0} \frac{H_1(Y)_{0, k_1} H_1(Y)_{k_1, 0}}{(\nu_0 - \nu_{k_1})^2} \right) \left( \sum_{k_1 \neq 0} \frac{H_1(Y)_{0, k_1} H_1(Y)_{k_1, 0}}{(\nu_0 - \nu_{k_1})} \right) \\
&\quad + \frac{1}{2} \sum_{k_1 \neq \phi_0} \frac{H_1(Y)_{0, 0}^2 H_1(Y)_{0, k_1} H_1(Y)_{k_1, 0} + H_1(Y)_{0, k_1} H_1(Y)_{k_1, 0} H_1(Y)_{0, 0}^2}{(\nu_0 - \nu_{k_1})^3}.
\end{aligned} \tag{31}$$

Equivalent formulas for the effective Hamiltonian up to order five [33,35] or six [31] have been obtained through different formalisms. However, as far as we are aware, no such explicit formulas are available for the effective dipole moment.

### 2.2.2 Effective electric dipole moment

Within the perturbational treatment, the effective dipole moment,  $D(Y)$ , as defined in Eq.(19), can be expanded as a series in  $\varepsilon$ ,

$$D(Y) = D^{(0)}(Y) + \varepsilon D^{(1)}(Y) + \varepsilon^2 D^{(2)}(Y) + \dots + \varepsilon^n D^{(n)}(Y) + \dots, \tag{32}$$

where the  $n^{\text{th}}$ -order term has the following expression,

$$D^{(n)}(Y) = \sum_{k=0}^n \langle \phi^{(k)\dagger}(Y) | D(X, Y) | \phi^{(n-k)}(Y) \rangle_{\mathbf{x}}. \tag{33}$$

The electric dipole moment operator along the  $f$ -axis in the laboratory frame,  $D_f(X, Y)$ ,

is the sum of tensor products of dipole moment components in the Eckart frame,  $D_\alpha(X)$ , by direction cosine operators,  $\lambda_{f\alpha}(Y)$ ,

$$D_f(X, Y) = \sum_{\alpha=x,y,z} D_\alpha(X) \otimes \lambda_{f\alpha}(Y). \quad (34)$$

The following perturbative formulas have been obtained [12] for the  $n^{\text{th}}$ -order terms of this effective operator up to  $n = 2$ ,

$$D_f^{(0)}(Y) = \sum_{\alpha=x,y,z} \langle \psi_0 | D_\alpha(X) | \psi_0 \rangle_{\mathbf{x}} \lambda_{f\alpha}(Y) \quad (35)$$

$$D_f^{(1)}(Y) = \sum_{\alpha=x,y,z} \sum_{k_1 \neq 0} \frac{\langle \psi_{k_1} | D_\alpha(X) | \psi_0 \rangle_{\mathbf{x}} H_1(Y)_{0,k_1} \lambda_{f\alpha}(Y) + \frac{\langle \psi_0 | D_\alpha(X) | \psi_{k_1} \rangle_{\mathbf{x}} \lambda_{f\alpha}(Y) H_1(Y)_{k_1,0}}{\nu_0 - \nu_{k_1}}}{\nu_0 - \nu_{k_1}} \quad (36)$$

$$D_f^{(2)}(Y) = \sum_{\alpha=x,y,z} \left( \sum_{k_1, k_2 \neq 0} \frac{1}{(\nu_0 - \nu_{k_1})(\nu_0 - \nu_{k_2})} (\langle \psi_{k_1} | D_\alpha(X) | \psi_{k_2} \rangle_{\mathbf{x}} H_1(Y)_{0,k_1} \lambda_{f\alpha}(Y) H_1(Y)_{k_2,0} + \langle \psi_0 | D_\alpha(X) | \psi_{k_1} \rangle_{\mathbf{x}} \lambda_{f\alpha}(Y) H_1(Y)_{k_1,k_2} H_1(Y)_{k_2,0} + \langle \psi_{k_1} | D_\alpha(X) | \psi_0 \rangle_{\mathbf{x}} H_1(Y)_{0,k_2} H_1(Y)_{k_2,k_1} \lambda_{f\alpha}(Y)) - \sum_{k_1 \neq 0} \frac{\langle \psi_0 | D_\alpha(X) | \psi_{k_1} \rangle_{\mathbf{x}}}{(\nu_0 - \nu_{k_1})^2} (\lambda_{f\alpha}(Y) H_1(Y)_{k_1,0} H_1(Y)_{0,0} + H_1(Y)_{0,0} H_1(Y)_{0,k_1} \lambda_{f\alpha}(Y)) - \frac{\langle \psi_0 | D_\alpha(X) | \psi_0 \rangle_{\mathbf{x}}}{2} \sum_{k_1 \neq 0} \frac{1}{(\nu_0 - \nu_{k_1})^2} (\lambda_{f\alpha}(Y) H_1(Y)_{0,k_1} H_1(Y)_{k_1,0} + H_1(Y)_{0,k_1} H_1(Y)_{k_1,0} \lambda_{f\alpha}(Y)) \right). \quad (37)$$

### 3 APPLICATION TO THE R-BRANCH OF METHANE VIBRATIONAL GROUND STATE

The implementation of the formulas of the previous section to calculate the R-branch of methane main isotopologue in its vibrational ground state requires several steps summarized below.

### 3.1 Electronic calculations

This work is performed within the Born-Oppenheimer approximation [40]. We consider a molecular wave function that is the product of an electronic wave function by a nuclear one. The sensitivity of our results to the electronic wave function will be assessed by comparing two pairs of potential energy surface (PES) and dipole moment surface (DMS). Each pair is made of an already published PES and a DMS computed in this work by means of the MOLPRO program suite [41] running on the HP-XC4000 cluster of the ULB/VUB computing center.

The PES of the first pair is the Lee, Martin and Taylor (LMT) PES [42] calculated with the CCSD(T) method (coupled clusters including single and double excitations [43] and a perturbative treatment of connected triples [44]) within the frozen core approximation. It was calculated by a combination of the correlation consistent polarized valence triple and quadruple zeta basis sets (cc-pVTZ and cc-pVQZ, or VTZ and VQZ in short) [45]. More precisely, CCSD(T)/VQZ was used for the harmonic part and CCSD(T)/VTZ for cubic and quartic constants. A core correlation correction was added to the CCSD(T)/VQZ equilibrium geometry and the value,  $r_e = 1.0862 \pm 0.0005 \text{ \AA}$ , was retained. The PES of the second pair is the Nikitin, Rey and Tuyterev (NRT) PES [46], also calculated at the CCSD(T) level of theory, but with all electrons correlated and using a combination of the correlation consistent, polarized, core, valence quadruple zeta (cc-pCVQZ or CVQZ in short) and augmented correlation consistent, polarized, core, valence quintuple zeta (aug-cc-pCV5Z or ACV5Z in short) basis sets. The latter basis set contains diffuse functions [47] and both basis sets possess core flexibility designed to take into account core and core-valence correlation [48]. This PES has been derived from a large grid of CCSD(T)/CVQZ points corrected for ACV5Z contributions. Its global minimum is located at the exact ACV5Z equilibrium geometry,  $r_e = 1.08601 \pm 0.00004 \text{ \AA}$ , which is close to the value derived in [1],  $r_e = 1.08606 \text{ \AA}$ . The accuracy of  $r_e$  is crucial for the prediction of the rotational spectra of the molecule, and differences between previous *ab initio* calculations and results derived from experiment have been traced back to errors in  $r_e$  [1]. Note that

the NRT PES includes also empirical quadratic constant corrections.

Both PES have been transformed using symbolic algebra softwares from internal valence coordinates to mass-weighted, Cartesian, normal coordinates. The LMT PES, which is a quartic PES, has been re-expanded to fourth order in normal coordinates [1,9]. The NRT PES, which is originally a sextic PES for stretching DOF and octic for angular DOF, has been re-expanded to tenth order in normal coordinates [8].

Each DMS have been calculated with the largest basis set that was used in the corresponding PES and with the same number of correlated electrons: VQZ/valence correlation and ACV5Z/full correlation for the LMT and NRT PES respectively. The multi-reference configuration interaction with single and internally contracted double excitations method [49,50] was preferred to the CCSD(T) method for calculating the DMS because analytical dipole moments are available at this level of theory in the MOLPRO computer package. Also, in view of deriving a global surface in the future, the MRCI method is more appropriate, since different reference configurations may have significant weights away from the equilibrium geometry. Note that the number of contracted configuration state functions in the larger MRCI calculations at DMS points of C1 symmetry amount to 2.6 and 14.2 millions for VQZ and ACV5Z basis sets, respectively.

The DMS have been represented as third order Taylor expansions, by fitting a grid of 100 nuclear configurations. We use the self-explanatory notation D(VQZ) and D(ACV5Z) to designate the two DMS expansions. The third order expansion of the z-component, electric, dipole moment contains 24 coefficients in front of symmetry adapted polynomials. The results of the least square fit of the MRCI/VQZ and MRCI/ACV5Z grid points can be found in Appendix A. The expansion of the x- and y-components are obtained by symmetry. The grid point coordinates together with the values of the z-component, electric, dipole moment are provided as supplementary material to this article. The nuclear configurations are parametrized in terms of displacements with respect to the MRCI/VQZ frozen core (respectively MRCI/ACV5Z ) equilibrium geometry for D(VQZ) (respectively D(ACV5Z) ) and along the mass-weighted, Cartesian, normal coordinates

corresponding to the related PES.

Remarkably, the mass-weighted Cartesian normal coordinates of the LMT PES, can be chosen to be the same as those of VQZ/MRCI (frozen core) and ACV<sub>n</sub>Z/MRCI calculations for n=Q,5,6, with Davidson correction (denoted by "+Q") [51,52], also to ACV6Z/MRCI calculations without Davidson correction and ACV5Z/CCSD(T) to within insignificant differences. Of course the A1 normal coordinate is fixed by symmetry to within a sign factor, and the E normal coordinates to within a unitary transformation in the degenerate vector space they span. However, the normal coordinates of mode  $\nu_3$  and  $\nu_4$  carrying the same F2 irreducible representations (irreps) could in principle vary with the level of calculation. This is not the case. For example, the projection of each of the ACV6Z/MRCI+Q normal coordinates  $q_{3x}, \dots, q_{4z}$  on their VQZ/CCSD(T) counterparts, has been found equal to .9999990 corresponding to a rotation of .00141035 radian or .0808071 degrees.

The equilibrium distances and the DMS(VQZ) and DMS(ACV5Z) expansion coefficients up to second order are compared in Tab. 1 with those available in the literature. The geometry optimizations to determine the equilibrium distances,  $r_e$ , have been performed with very tight convergence parameters to insure the precision of the tabulated numbers. The difference between the two calculated equilibrium geometries comes from the frozen core approximation in the VQZ calculation rather than from the smaller number of valence orbitals as shown in supplementary material (first table displaying  $r_e$  values for different approximation levels).

The DMS constants given in Appendix A and in supplementary material correspond to a dipole moment expansion in terms of mass-weighted, normal coordinates expressed in atomic units. Whereas in Tab. 1, they have been converted to adimensional normal coordinates (written with lower case  $q$ ) for the sake of comparison with other published results. In fact, the non zero, first derivatives of Tab. 1 and Appendix A are reasonably close to the ones obtained by finite difference presented for different approximation levels in Table 1 of the supplementary material.

Our results are probably more reliable than those of refs. [53,54]. We note that when the analysis of [53] fails to provide a number, that of [54] gives numbers that are very different from ours. For the other derivatives, the agreement between our results and those of [53,54] is much better for derivatives with respect to stretching modes than with respect to bending modes. In Debye.Å<sup>-1</sup> our ACV5Z first derivatives are:  $\frac{\partial D_z}{\partial Q_{3z}} = -0.7259$ ;  $\frac{\partial D_z}{\partial Q_{4z}} = +0.4771$  (where we use somewhat abusively the same capital "Q" notation as for the mass-weighted normal coordinates). They compare reasonably well with the DZP/MP2 results of Hollenstein et al. [55],  $\frac{\partial D_z}{\partial S_{3z}} = -0.767$  and  $\frac{\partial D_z}{\partial S_{4z}} = +0.5$ , respectively, given the fact that the latter are derivatives with respect to pure stretching and pure bending, symmetry-adapted coordinates. The values given in [56] seems erroneous as noted in [55].

### 3.2 Vibrational calculations

Once a PES is obtained, one can solve the eigenvalue problem for the  $H_0$  Hamiltonian and get the  $(\psi_n)_n$  basis functions needed in the generalized perturbation method. In fact, for the LMT PES, we have truncated the  $\mu$ -tensor expansion, Eq. (4), to zero order and for the NRT PES to second order in  $H_0$ . These choices follows our previous studies, ref. [1] for the LMT PES, and ref. [8] for the NRT PES, respectively. They correspond to good compromises between computational effort and accuracy.

The eigenvalue problem for each  $H_0$  has been solved by performing vibrational mean field configuration interaction (VMFCI) calculations as implemented in the computer code CONVIV [13]. The method has been described in details elsewhere [1,8,9,57,58]. The VMFCI method is a variational method that allows one to contract arbitrary groups of DOF in a hierarchical manner, while controlling the growth of the basis set size by discarding high energy product basis functions, according to a so-called "contraction-truncation scheme". It is different from the traditional contraction method [59–63], because the Hamiltonian of an active group of DOF takes into account the effect of the mean field of the spectator groups as proposed by Bowman and Gazdy [64]. However,



in contrast with [64], for a given partition of the DOF, self-consistency is achieved by iterating VCI calculations for active groups of DOF in the mean field of the spectator groups.

The contraction-truncation scheme employed in this work is the same as the one of [8]. It can be written in our notation as MSP-VSCFCI/VSCFCI( $\nu_1 - \nu_3$ ; 48000)/VCI(Z), in which:

- MSP-VSCFCI stands for minimal symmetry preserving (MSP) vibrational self-consistent configuration interaction calculation (VSCFCI). It means that the DOFs pertaining to the same degenerate mode have been contracted together in the mean field of the other DOFs and that this partition has been iterated until self-consistency was achieved. For the LMT PES calculation, the maximum quantum numbers of the harmonic oscillator (HO) basis functions were respectively, 19,14,19,14 for modes  $\nu_1, \nu_2, \nu_3, \nu_4$ . For the NRT PES, the calculation was the same as in [8], so the maximum quantum numbers of the HO basis functions were respectively, 14,16,14,16. Both basis sets were large enough to converge all low lying energy levels up to the octad (and many levels beyond the octad) at the  $\text{cm}^{-1}$  accuracy.
- VSCFCI( $\nu_1 - \nu_3$ ; 48000) means that the stretching modes 1 and 3 are contracted with truncation of the product basis functions at  $48000 \text{ cm}^{-1}$  on the sum of the energies of their components, and that self-consistency was achieved for this new partition.
- VCI(Z) denotes as usual a vibrational configuration interaction (VCI) step. Different truncation thresholds on the sum of component energies, Z, were used for constructing the final product basis set:  $Z=18314 \text{ cm}^{-1}$  for LMT and  $Z=19318 \text{ cm}^{-1}$  for NRT PES, respectively. we refer the interested reader to [8] for a convergence study with respect to Z. With this energy threshold, the number of VCI basis functions for the LMT PES (respectively NRT PES) is 51314 (respectively 74978).

The energy levels up to the octad have been given in our previous articles [8,13] and are not reproduced here. The 8039 first levels (counted with their degeneracy) for the LMT calculation, and the 16864 first levels obtained for the NRT calculation, are available upon request.

### 3.3 Rotational calculations

#### 3.3.1 Rotational eigenstates

Once eigenvalues and eigenfunctions of  $H_0$  have been obtained, the derivation of effective rotational eigenstates only depends upon the actual form assumed by  $H_1$ , the generalized perturbation order and the maximum number of vibrational states used in perturbation series for each corrective terms.

$H_1$  depends crucially upon the equilibrium CH bond length,  $r_e$ , and, when the  $\mu$ -matrix of the Watson Hamiltonian is Taylor-expanded, it also depends upon the expansion order. The LMT PES equilibrium CH bond length,  $r_e = 1.0862$ , has been retained to compute all  $\mu$ -matrix dependent terms of the Watson Hamiltonian in Eqs.(2) and (3) for the calculation referred to as the "VQZ" calculation, which makes use of the LMT PES to solve  $H_0$ . Similarly, the NRT value,  $r_e = 1.08601$ , has been used for the  $\mu$ -matrix dependent terms in the calculation referred to as the "ACV5Z" calculation.

The  $\mu$ -matrix has been truncated in  $H_1$ , Eq. (3), to fourth order for the VQZ calculation and to fifth order for the ACV5Z one. The choice of these expansion orders is based on our previous computations of accurate, effective, rotational Hamiltonian for methane vibrational ground state [1,8,9]. We refer the interested readers to these articles for convergence studies of rotational energy levels.

All the results presented hereafter were obtained with fourth order generalized perturbation eigenstates. They correspond to effective rotational Hamiltonians containing up to octic centrifugal distortion terms. The perturbation series of the second and third order corrective terms,  $E^{(2)}(Y)$  and  $E^{(3)}(Y)$  have been truncated at 8038 (respectively 8281) excited vibrational eigenfunctions, that of  $E^{(4)}(Y)$  at 4021 (respectively 4160) vibrational eigenfunctions for the VQZ (respectively ACV5Z) calculation. Given the accuracy of our  $r_e$  values, it does not appear justified to go beyond this truncation threshold. Again, we refer the readers to [1,8,9] for convergence studies with respect to perturbation order and

numbers of vibrational eigenfunctions.

The effective rotational Hamiltonians have been diagonalized in a symmetric rotator basis set corresponding to a given  $J$ -value. Matrix elements of angular momentum operators have been taken from [65], (with some sign error corrected for  $P_y$  in Eqs (5e) and (5f)). The rotational energy levels of the ACV5Z calculation are tabulated up to  $J = 10$  in [8]. In this work, we use the eigenstates obtained for  $J = 7$  to  $J = 19$  to compute the rotational lines observed in the SOLEIL experiment, and up to  $J = 30$  to compare with HITRAN data.

Note that the eigenfunctions of the effective rotational Hamiltonians are, within the perturbation approximation, the  $\Psi_k$ 's of Eqs. (13) and (14). Therefore, in principle, if the perturbation series converge, they lead to exact eigenstates through Eq. (13). So, bracketing the vibrational ground state, effective, dipole moment,  $D_0(Y)$  of Eq. (19), between these  $\Psi_k$ 's gives exact transition matrix elements,

$$\begin{aligned} \langle \Psi_k | D_0(Y) | \Psi_{k'} \rangle &= \langle \Psi_k | \langle \phi_0^\dagger(Y) | D(X, Y) | \phi_0(Y) \rangle_{\mathbf{x}} | \Psi_{k'} \rangle \\ &= \langle \phi_{0,k} | D(X, Y) | \phi_{0,k'} \rangle. \end{aligned} \quad (38)$$

The next section explains how approximate  $D(Y)$  (dropping the ground state label "0") have been obtained.

### 3.3.2 Rotational dipole moment parameters

Using the Taylor expansion of the dipole moment in molecular frame,  $D_z(X)$ , given in Appendix A and the related expression for  $D_x(X)$ ,  $D_y(X)$  that can be deduced by symmetry, as well as the VMFCI eigenfunctions, we can apply the formulas of section 2.2.2 and derive an effective rotational dipole moment operators in laboratory frame along the  $f$ -direction,  $D_f(Y)$ , up to second perturbation order.

The zero order term is zero by symmetry. The convergence of the Taylor expansion of  $D(X)$  is evaluated in Tab. 2 by comparing  $D_f^1(Y)$ . This is because, at first order, for

symmetry reasons, the effective operator is determined by a single real number,  $\theta_z^{xy}$  [12],

$$D_f^1(Y) = \frac{\theta_z^{xy}}{2} [(\Pi_z\Pi_y + \Pi_y\Pi_z)\cdot\lambda_{fx}(Y) + (\Pi_x\Pi_z + \Pi_z\Pi_x)\cdot\lambda_{fy}(Y) + (\Pi_x\Pi_y + \Pi_y\Pi_x)\cdot\lambda_{fz}(Y)] \\ + \textit{hermitic conjugate.} \quad (39)$$

The variations of  $\theta_z^{xy}$  with respect to the DMS order is fairly insensitive to the calculation method. This is particularly true for order 1 and 2. Order 3 does not preserve so well the difference between the two calculation levels, probably because the third order constants obtained from our fits incorporate effects from higher order terms and are more sensitive to the choice of a limited number of grid points. The contribution of second order constants is actually smaller than that of third order constants, because the vibrational ground state is only slightly anharmonic, so even order contributions tend to average out. The contributions of third order terms are a few percent of that of the first order. It is reasonable to expect the same decrease for fifth order terms, and so to neglect them together with fourth order terms.

First order effective dipole moments of the same form as Eq.(39), have been proposed and investigated as early as 1971 by several authors [11,67,68]. Experimental values for the  $\theta_z^{xy}$  collected in [15] ranges from 22.34  $\mu\text{Debye}$  to 24.06  $\mu\text{Debye}$ . Our "Order 3" values fit in this range, but not the estimate of 30.7  $\mu\text{Debye}$  found in [30].

The second order correction to the effective dipole moment has a much more complicated expression [12]. The term, denoted by  $D_{fz}(Y)$ , of the effective dipole moment,  $D_f(Y)$ , arising from the  $D_z(X)$ -dependent term in Eq.(34), can be written up to second order as,

$$D_{fz}(Y) = \lambda_{fz}(Y) \left[ \theta_1(\Pi_x\Pi_y + \Pi_y\Pi_x) + i\theta_2\Pi_z(\Pi_x^2 - \Pi_y^2) \right. \\ \left. + \theta_3(\Pi_x^2 + \Pi_y^2)(\Pi_x\Pi_y + \Pi_y\Pi_x) + \theta_4\Pi_z^2(\Pi_x\Pi_y + \Pi_y\Pi_x) \right] \\ + \theta_5\Pi_x\lambda_{fz}(Y)\Pi_y + i\theta_6\Pi_z\lambda_{fz}(Y)(\Pi_x^2 - \Pi_y^2) \\ + i\theta_7(\Pi_x\lambda_{fz}(Y)(\Pi_z\Pi_x + \Pi_x\Pi_z) - \Pi_y\lambda_{fz}(Y)(\Pi_y\Pi_z + \Pi_z\Pi_y)) \\ + \theta_8(\Pi_x^2 + \Pi_y^2)\lambda_{fz}(Y)(\Pi_x\Pi_y + \Pi_y\Pi_x) + \theta_9\Pi_z^2\lambda_{fz}(Y)(\Pi_x\Pi_y + \Pi_y\Pi_x) \\ + \theta_{10}((\Pi_z\Pi_x + \Pi_x\Pi_z)\lambda_{fz}(Y)(\Pi_y\Pi_z + \Pi_z\Pi_y) + \textit{hermitic conjugate}). \quad (40)$$

where  $\theta_1, \dots, \theta_{10}$  are real coefficients. In particular,  $\theta_1$  is in fact  $\frac{\theta_z^{xy}}{2}$  of Tab. 2 plus a second order correction. The expressions of  $D_{fx}(Y)$  and  $D_{fy}(Y)$  required to compute  $D_f(Y) = D_{fx}(Y) + D_{fy}(Y) + D_{fz}(Y)$  up to second order, can be deduced by symmetry.

Table 3 shows the convergence of the  $\theta_i$  coefficients with respect to the maximum  $k_1, k_2$ -values used in Eq.(37), for the ACV5Z third order DMS.  $\theta_1$  is clearly well converged with only 2070 excited basis functions, given the number of digits expected to be significant in our theoretical calculation as well as in the values derived from experiment. The second order coefficients are only converged to a few percent. However, this is also sufficient, since they are small quantities.

Note that expression (40) is not unique. One could for example replace  $\Pi_z(\Pi_x^2 - \Pi_y^2)$  by  $(\Pi_x\Pi_z\Pi_x - \Pi_y\Pi_z\Pi_y)$ , then, using angular momentum commutation relations  $[\Pi_\alpha, \Pi_\beta] = -ie_{\alpha\beta\gamma}\Pi_\gamma$ , with  $e_{\alpha\beta\gamma}$  the unit antisymmetrical tensor, we see that the coefficient of  $(\Pi_x\Pi_y + \Pi_y\Pi_x)$  would be  $\theta_1 - \theta_2$ , that is to say,  $22.85 \mu\text{Debye}$  for the ACV5Z calculation.

Note also that second order term related to our  $\theta_3$  and  $\theta_4$  have been explored in [16,69,70]. The order of magnitude of  $\frac{\theta_3}{\theta_1}$  and  $\frac{\theta_4}{\theta_1}$  is slightly less than  $10^{-4}$  as anticipated in [16]. In contrast the numerical estimates of Mikhailov et al. [69] give much lower ratios.

Using the ACV5Z dipole moment parameters, the effective dipole moment matrix elements between eigenstates of the effective rotational Hamiltonian have been computed according to Eq. (38), in view of calculating transition intensities. The rotational eigenstates appearing in the latter equation, are linear combinations of symmetric rotator basis functions. Matrix elements of angular momentum operators between symmetric rotator basis functions have been taken from [65], that of direction cosine operators from [66].

### 3.3.3 Rotational transition intensities

The transition intensities at  $T$  Kelvin for the transition wave number,  $\nu_{\eta\eta'} = E_{\eta'} - E_\eta$  in  $\text{cm}^{-1}$ , are calculated for all pairs of states,  $(\eta, \eta')$ , according to (a slightly rearranged

version of) formula (A.5) given in the appendix of [72],

$$S_{\eta\eta'} = \frac{8\pi^3}{3hc} \nu_{\eta\eta'} \frac{I_a \exp(-c_2 E_\eta/T)}{Q(T)} [1 - \exp(-c_2 \nu_{\eta\eta'}/T)] \mathfrak{R}_{\eta\eta'} \times 10^{-36}, \quad (41)$$

where  $c$  is the speed of light;  $h$  the Planck constant;  $c_2 = hc/k$ ,  $k$  being the Boltzmann constant;  $I_a = 0.988274$  is the terrestrial isotopic abundance of  $^{12}\text{CH}_4$ ;  $\mathfrak{R}_{\eta\eta'}$  is the transition-moment squared (note that in [72] it was the weighted transition-moment squared, so a factor  $g_\eta$  was added in the original formula to take into account spin statistical weight and rotational degeneracy);  $Q(T)$  is the partition function.

The partition function at  $T = 296$  Kelvin has been calculated *ab initio* using the vibrational ground state levels of the NRT calculation, whereas the rotational levels of the dyad have been calculated by using the LMT PES and a quasi-degenerate version of second order generalized perturbation. We have obtained  $Q(296) = 590.439$ , where the contribution of the dyad levels is only 3.6925, which justifies the use of the simpler PES. Furthermore, the value obtained with the scaled LMT rotational levels of [1] in place of the unscaled ones derived in the NRT calculation [8] is only slightly different, 590.427. Our partition function values are to be compared with 590.4 from HITRAN [73] and 590.5 from Dijon code [74]. Note that the partition function  $\tilde{Q}$  in [75] seems to be overestimated, for example  $\tilde{Q}(298) = 603$  whereas our *ab initio* value is  $Q(298) = 596.588$ .

The transition-moments squared are calculated according to,

$$\mathfrak{R}_{\eta\eta'} = 3 \sum_{k=1}^d \sum_{k'=1}^{d'} |\langle \Psi_k^{tot} | D_f(Y) | \Psi_{k'}^{tot} \rangle|^2 \quad (42)$$

where the factor 3 accounts for the three equivalent components of the dipole moment operator in laboratory frame, (in practice we used  $f = Z$ ). The wave functions,  $\Psi_k^{tot}$ ,  $\Psi_{k'}^{tot}$ , include a nuclear spin part determined according to [76], and the sum extends over all their degenerate components (due to rotational DOFs or nuclear spin). The degenerate components of a rotational  $E$  state are treated as non degenerate in the symmetry group employed in [76], hence their nuclear spin weight factor of 1. However, in Eq. (42), the two (times  $2J+1$ ,  $J$  lower state angular momentum quantum number) energy degenerate rotational-nuclear spin product functions must be considered (omitting the translational

and non degenerate vibronic factors for simplicity).

It is noteworthy to mention that the degenerate components of all rotational  $E$ , (respectively  $F_1$  and  $F_2$ ), eigenstates have been aligned by means of unitary transformations, along given directions defined by eigenvectors of appropriate matrices. Moreover, one must pay attention to choose consistently the phase of all degenerate wave functions. All this is necessary in order to combine rotational eigenstates with nuclear spin functions and obtain orthonormal wave functions having the proper symmetry under permutation of identical particles. The dipole moment operator in Eq. (42) does not depend upon nuclear spin, so, using orthonormal, nuclear spin, basis functions, the proper transition moment value is obtained only if the rotational function associated to a given nuclear spin function in the bra has the same orientation as the function associated to the same nuclear spin function in the ket. Consider for example the case of  $F$  rotational states. Following [76], the appropriate combination giving  $A$ -irrep. is  $\frac{1}{\sqrt{3}}(F_x^{rot} F_x^{spin} + F_y^{rot} F_y^{spin} + F_z^{rot} F_z^{spin})$ . So, in Eq.(42), a pair of such states, with identical nuclear spin part, will give a contribution of the form (omitting the summation over degenerate components due to rotational DOFs),

$$\begin{aligned}
& \left| \left\langle \frac{1}{\sqrt{3}}(F_x^{rot,1} F_x^{spin} + F_y^{rot,1} F_y^{spin} + F_z^{rot,1} F_z^{spin}) \middle| D_f(Y) \middle| \frac{1}{\sqrt{3}}(F_x^{rot,2} F_x^{spin} + F_y^{rot,2} F_y^{spin} + F_z^{rot,2} F_z^{spin}) \right\rangle \right|^2 \\
&= \frac{1}{9} \left| \sum_{\alpha} \langle F_{\alpha}^{rot,1} | D_f(Y) | F_{\alpha}^{rot,2} \rangle \right|^2 \\
&= \frac{1}{9} \sum_{\alpha\beta} \langle F_{\alpha}^{rot,1} | D_f(Y) | F_{\alpha}^{rot,2} \rangle \langle F_{\beta}^{rot,2} | D_f(Y) | F_{\beta}^{rot,1} \rangle \tag{43}
\end{aligned}$$

The operator  $D_Z(Y)$  carries the  $A_2$  irrep. of the  $T_d$  symmetry group, and the selection rules for rotational integrals allow only coupling between  $F_1$  and  $F_2$  pairs, in the case of triply degenerate irreps. . More precisely, for aligned  $F_{1\alpha}$  and  $F_{2\alpha}$  components with consistently chosen phase, the non zero integrals satisfies,  $\langle F_{1x}^{rot} | D_Z(Y) | F_{2x}^{rot} \rangle = \langle F_{1y}^{rot} | D_Z(Y) | F_{2y}^{rot} \rangle = \langle F_{1z}^{rot} | D_Z(Y) | F_{2z}^{rot} \rangle$ , see Clebsch-Gordan coefficients in [78]. So, finally, Eq.(43) reduces to  $|\langle F_{\alpha}^{rot,1} | D_Z(Y) | F_{\alpha}^{rot,2} \rangle|^2$  for a given  $\alpha \in \{x, y, z\}$ .

## 4 COMPARISON WITH EXPERIMENT

Using fourth order perturbation theory, rotational eigenfunctions and energies have been obtained for methane main isotopologue, in its vibrational ground state. Then, using the expressions of Eqs. (39) and (40) with the best converged coefficients of Tables 2 and 3 respectively, first and second order effective dipole moment operators have been derived at the ACV5Z level of theory. Finally, eq. (41) has been used to compute a theoretical R-branch spectrum. The results are compared to the SOLEIL experiment results (Table A1 of [15]) in Table 4.

The third column of Table 4 shows that our theoretical transition energies are systematically underestimated but by only a small amount, since the mean average of the relative error absolute values is only about  $2.10^{-5}$ . It is worth emphasizing at this point that the entire vibrational-rotational treatment is purely *ab initio* with no adjusted parameter, (not even a global scaling factor as in our previous work [9]).

The seventh and ninth columns of Table 4 display the relative errors of our *ab initio* intensities, obtained at order 1 and 2 respectively, with respect to the observed ones. In contrast with transition wave numbers, some are larger than the experimental values while others are smaller. The second order effective moment performs slightly better than the first order one with a mean average of relative error absolute values of 6.28% for the former against 6.63% for the latter. This is a small difference as could be anticipated from the order of magnitude of second order coefficients in Table 3 with respect to the first order parameter (see Table 2). These numbers should be compared to the mean average of the absolute values of the fit relative errors (sixth column of Tab. A1 of [15]) that we have calculated to be 6.42%.

The transition italicized in Tab. 3 was considered too far out and eliminated [79] from the fit of [15]. Without this transition, the fit average relative error becomes 6.03%. Our first order relative error becomes 6.30%, that is slightly more. This is normal, since the form of the effective dipole moment for the fit was the same as our first order operator.



However, our second order error without the italicized transition is equal to 5.85% that is less than the empirical fit relative error. This suggests that spectroscopists should consider adding second order corrective terms in the expression of their effective dipole moment operator to improve the fitting of experimental data.

The sixth column lists the experimental uncertainties (in %). Even though several calculated transition intensities have relative errors outside the experimental uncertainty, most of them are within. The mean calculated relative error is much smaller than the average relative uncertainty of 10.57% with, or 10.62% without the transition eliminated from the fit. We note that the experimental uncertainty claimed for this transition is 6.0%, whereas our second order relative error of 45.6% agrees with that of Tab. A1 of [15] (42.0%). Given the consistency of our *ab initio* intensity predictions for the other transitions, this suggests an error in the experimental value. So, our *ab initio* calculation confirms that it was probably justified to take this transition out of the fitting procedure.

Mirror images of the 93 observed and calculated transitions are displayed in Fig. 1. The weakest transitions are about  $10^{-26} \text{ cm}^{-1} / (\text{molecule.cm}^{-2})$  (that is HITRAN units). The two spectra are indistinguishable to the naked eyes, even if one zoom in a given  $J$ -value region. Using an intensity cutoff of  $10^{-32} \text{ cm}^{-1} / (\text{molecule.cm}^{-2})$ , increases the number of transition lines up to 388 at 296K, in both our calculated second order spectra and the spectra obtained from HITRAN. However, the general aspect of the spectra is unchanged, see Fig. 2.

Relative errors of position and intensities are plotted in Fig. 3. As already mentioned, errors on positions are all positive, meaning that there is a bias between experimental and theoretical numbers, but this discrepancy is small numerically. The solid curve corresponding to the barycenter of relative errors for a given  $J$ -value is an increasing function of  $J$ , denoting a difference between the high-order centrifugal distortion constants of the empirical and *ab initio* effective Hamiltonians, as already noted in [8]. The relative error distribution for the intensities is fairly narrow around  $R(13)$  and tends to become wider on both sides of this value. The largest deviation at both orders of theory corresponds

to the transition withdrawn from the fit.

In fact, the complete Q-branch and R-branch transitions for  $J \leq 30$  have been computed with our second order effective dipole moment at 296K for a cutoff of  $10^{-39} \text{ cm}^{-1} / (\text{molecule.cm}^{-2})$ . Tables are provided as supplementary material and spectra are displayed in Figs. 4 and 5. Such line lists can be computed from Eq. (41) at any temperature, for any cutoff, at negligible computational cost.

## 5 CONCLUSION

In this article, starting from two PES of the literature and two home-made DMS, the complete Q and R-branches at 296 K up to  $J = 30$  has been computed for a truncation threshold on the intensities at  $10^{-39} \text{ cm}^{-1} / (\text{molecule.cm}^{-2})$ . Such a list can be computed *ab initio* at any other temperature upon request.

The influence of the quality of the electronic and vibrational calculations has been assessed. Core correlation is essential to obtain accurate equilibrium geometry and consequently accurate line positions. A third order expansion of the body-fixed dipole moment has been found necessary to obtain results converged at the level of the experimental accuracy. The ACV5Z calculation reduces the value of the main dipole moment parameters with respect to the VQZ calculation. This scales down the intensities globally and improves the agreement with experiment.

The convergence of the perturbational expansion of the effective dipole moment has been found very fast with respect to both the perturbation order (order 2 is sufficient) and the number of vibrational functions necessary to evaluate the series appearing in Eqs. (36) and (37).

The second order *ab initio* R-branch spectrum has been compared with the results of the SOLEIL experiment of Boudon et al. The calculated intensities are on average well within the experimental error bar. The average relative error, 5.85%, is even less than

that of the empirical fit, 6.03%, indicating that the functional form of the second order effective dipole moment can be useful to analyse spectroscopic data. This also suggests that the accuracy of our ACV5Z DMS is very satisfactory.

The computation with the same PES/DMS of the dyad hot band transitions seen in the SOLEIL experiment is in progress. We hope that this will lead to a better understanding of the methane spectroscopy in the near future, and of other, possibly larger, systems in the long run.

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## APPENDIX A

Dipole moment z-component expansion in Cartesian mass-weighted normal coordinates (atomic units). Note that the arbitrary phase factors in the definition of the normal coordinates are those corresponding to Gray and Robiette's conventions (Tab. 1 of Ref. [17]).

$$\begin{aligned}
D_z(VQZ) = & \\
& -3.56696 \cdot 10^{-3} Q_{3z} + 2.35346 \cdot 10^{-3} Q_{4z} - 5.13769 \cdot 10^{-5} Q_1 Q_{3z} - 5.47872 \cdot 10^{-5} Q_1 Q_{4z} \\
& \quad -2.90911 \cdot 10^{-5} Q_{2a} Q_{3z} + 1.85341 \cdot 10^{-5} Q_{2a} Q_{4z} \\
& -9.03660 \cdot 10^{-5} Q_{3x} Q_{3y} - 5.76673 \cdot 10^{-5} (Q_{3x} Q_{4y} + Q_{3y} Q_{4x}) + 6.21042 \cdot 10^{-5} Q_{4x} Q_{4y} \\
& \quad +1.01133 \cdot 10^{-7} Q_1^2 Q_{3z} + 2.72953 \cdot 10^{-7} Q_1^2 Q_{4z} \\
& \quad -1.41530 \cdot 10^{-7} Q_1 Q_{2a} Q_{3z} + 8.74675 \cdot 10^{-6} Q_1 Q_{2a} Q_{4z} \\
& -5.75600 \cdot 10^{-8} Q_1 Q_{3x} Q_{3y} - 1.74394 \cdot 10^{-7} Q_1 (Q_{3x} Q_{4y} + Q_{3y} Q_{4x}) - 5.23875 \cdot 10^{-7} Q_1 Q_{4x} Q_{4y} \\
& \quad +1.33809 \cdot 10^{-7} Q_{3z} (Q_{2a}^2 + Q_{2b}^2) + 9.51762 \cdot 10^{-7} Q_{4z} (Q_{2a}^2 + Q_{2b}^2) \\
& +2.47001 \cdot 10^{-7} Q_{3z} (Q_{3x}^2 + Q_{3y}^2 + Q_{3z}^2) - 5.58876 \cdot 10^{-7} Q_{4z} (Q_{3x}^2 + Q_{3y}^2 + Q_{3z}^2) \\
& \quad +7.14234 \cdot 10^{-8} Q_{3z} (Q_{3x} Q_{4x} + Q_{3y} Q_{4y} + Q_{3z} Q_{4z}) \\
& \quad -6.19512 \cdot 10^{-7} Q_{4z} (Q_{3x} Q_{4x} + Q_{3y} Q_{4y} + Q_{3z} Q_{4z}) \\
& +4.11906 \cdot 10^{-7} Q_{3z} (Q_{4x}^2 + Q_{4y}^2 + Q_{4z}^2) + 1.19679 \cdot 10^{-7} Q_{4z} (Q_{4x}^2 + Q_{4y}^2 + Q_{4z}^2)
\end{aligned}$$

$$\begin{aligned}
D_z(ACV5Z) = & \\
& -3.54232 \cdot 10^{-3} Q_{3z} + 2.32698 \cdot 10^{-3} Q_{4z} - 5.09773 \cdot 10^{-5} Q_1 Q_{3z} - 5.44507 \cdot 10^{-5} Q_1 Q_{4z} \\
& \quad -3.05546 \cdot 10^{-5} Q_{2a} Q_{3z} + 1.75830 \cdot 10^{-5} Q_{2a} Q_{4z} \\
& -9.13824 \cdot 10^{-5} Q_{3x} Q_{3y} - 5.76193 \cdot 10^{-5} (Q_{3x} Q_{4y} + Q_{3y} Q_{4x}) + 6.15378 \cdot 10^{-5} Q_{4x} Q_{4y} \\
& \quad +9.71246 \cdot 10^{-8} Q_1^2 Q_{3z} + 2.91293 \cdot 10^{-7} Q_1^2 Q_{4z} \\
& \quad -1.08833 \cdot 10^{-7} Q_1 Q_{2a} Q_{3z} + 8.69156 \cdot 10^{-6} Q_1 Q_{2a} Q_{4z} \\
& -1.12720 \cdot 10^{-7} Q_1 Q_{3x} Q_{3y} - 1.72212 \cdot 10^{-7} Q_1 (Q_{3x} Q_{4y} + Q_{3y} Q_{4x}) - 5.27870 \cdot 10^{-7} Q_1 Q_{4x} Q_{4y} \\
& \quad +8.67445 \cdot 10^{-8} Q_{3z} (Q_{2a}^2 + Q_{2b}^2) + 9.81313 \cdot 10^{-7} Q_{4z} (Q_{2a}^2 + Q_{2b}^2) \\
& +2.46369 \cdot 10^{-7} Q_{3z} (Q_{3x}^2 + Q_{3y}^2 + Q_{3z}^2) - 5.50070 \cdot 10^{-7} Q_{4z} (Q_{3x}^2 + Q_{3y}^2 + Q_{3z}^2) \\
& \quad +5.30391 \cdot 10^{-8} Q_{3z} (Q_{3x} Q_{4x} + Q_{3y} Q_{4y} + Q_{3z} Q_{4z}) \\
& \quad -6.00613 \cdot 10^{-7} Q_{4z} (Q_{3x} Q_{4x} + Q_{3y} Q_{4y} + Q_{3z} Q_{4z}) \\
& +4.00729 \cdot 10^{-7} Q_{3z} (Q_{4x}^2 + Q_{4y}^2 + Q_{4z}^2) + 1.30009 \cdot 10^{-7} Q_{4z} (Q_{4x}^2 + Q_{4y}^2 + Q_{4z}^2)
\end{aligned}$$

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## TABLES

	VQZ	ACV5Z	[53]	[54]
$r_e$ (in Å)	1.08827	1.08628	1.08826	1.089(02)
$\frac{\partial D_z}{\partial q_{3z}}$	-0.075583	-0.075010	-0.07561(4)	-0.0754(17)
$\frac{\partial D_z}{\partial q_{4z}}$	+0.076407	+0.075529	+0.07950(8)	+0.0808(16)
$\frac{\partial^2 D_z}{\partial q_1 \partial q_{3z}}$	-0.009256	-0.009172	N/A	-0.0009(01)
$\frac{\partial^2 D_z}{\partial q_1 \partial q_{4z}}$	-0.015802	-0.015698	-0.01657	-0.0145(12)
$\frac{\partial^2 D_z}{\partial q_{2a} \partial q_{3z}}$	-0.007698	-0.008041	-0.00800	-0.0080(03)
$\frac{\partial^2 D_z}{\partial q_{2a} \partial q_{4z}}$	+0.007256	+0.006798	+0.01286	+0.0060(09)
$\frac{\partial^2 D_z}{\partial q_{3x} \partial q_{3y}}$	-0.015962	-0.016115	N/A	-0.0310(15)
$\frac{\partial^2 D_z}{\partial q_{3x} \partial q_{4y}}$	-0.015609	-0.015670	-0.01611	-0.0163(06)
$\frac{\partial^2 D_z}{\partial q_{4x} \partial q_{4y}}$	+0.025743	+0.025520	+0.02736	+0.0337(09)

Table 1

Equilibrium CH distance (in Å) and electric dipole moment  $z$ -component first and second derivatives of  $^{12}\text{CH}_4$  (in Debye) for adimensional normal coordinates. Internally contracted MRCI calculations with frozen core (FC) for the VQZ basis set and full core excitations for the ACV5Z basis sets. The sign convention for the normal coordinates is that of Gray and Robiette [17], so the signs of the derivatives including  $q_{2a}$  and  $q_{2b}$  of Loete [53] have been changed accordingly, (see also Tab. 4 of Mourbat et al. [54]).

Calculation	DMS Taylor expansion order		
	1	2	3
VQZ	22.867	22.406	23.195
ACV5Z	22.639	22.182	23.070

Table 2

Convergence of  $\theta_z^{xy}$  (in  $\mu\text{Debye}$ ) with respect to DMS Taylor expansion order for  $^{12}\text{CH}_4$

Coefficients	number of vibrational functions		
	2070	4141	8281
$\theta_1$	$+4.52262 * 10^{-6}$	$+4.52245 * 10^{-6}$	$+4.52238 * 10^{-6}$
$\theta_2$	$+2.71041 * 10^{-8}$	$+2.71023 * 10^{-8}$	$+2.71024 * 10^{-8}$
$\theta_3$	$-3.30689 * 10^{-10}$	$-3.30668 * 10^{-10}$	$-3.30678 * 10^{-10}$
$\theta_4$	$+1.35661 * 10^{-10}$	$+1.35642 * 10^{-10}$	$+1.35631 * 10^{-10}$
$\theta_5$	$-1.48633 * 10^{-9}$	$-1.56091 * 10^{-9}$	$-1.58940 * 10^{-9}$
$\theta_6$	$-1.91565 * 10^{-9}$	$-1.91320 * 10^{-9}$	$-1.91270 * 10^{-9}$
$\theta_7$	$+1.42382 * 10^{-9}$	$+1.42378 * 10^{-9}$	$+1.42347 * 10^{-9}$
$\theta_8$	$-1.61201 * 10^{-10}$	$-1.61187 * 10^{-10}$	$-1.61187 * 10^{-10}$
$\theta_9$	$+5.12521 * 10^{-11}$	$+5.12559 * 10^{-11}$	$+5.12536 * 10^{-11}$
$\theta_{10}$	$+1.28183 * 10^{-10}$	$+1.28178 * 10^{-10}$	$+1.28179 * 10^{-10}$

Table 3

Convergence of effective dipole moment parameters (in atomic units) with respect to the number of excited vibrational functions used in perturbation series (ACV5Z calculation). The value  $\theta_1 = +4.52238 * 10^{-6}$  au corresponds to an effective  $\theta_z^{xy}$  of 22.989 micro Debye.

Obs <sup>1</sup>	$\nu_{\eta\eta'}$		$S_{\eta\eta'}$						$J, \text{ irrep.}$			
	Cal.	$\frac{Obs-Cal}{Obs}$	Obs [15]	Unc. %	Ord2	$\frac{Obs-Cal}{Cal}$ %	Ord1	$\frac{Obs-Cal}{Cal}$ %	$\eta$	$\eta'$		
83.56549	83.56381	2.01E-05	7.909E-26	18.0	7.965E-26	-0.7	7.958E-26	-0.6	7	E	8	E
83.56913	83.56746	2.00E-05	1.366E-25	34.0	1.364E-25	0.2	1.362E-25	0.3	7	F2	8	F1
83.57622	83.57456	1.99E-05	2.940E-25	3.3	2.992E-25	-1.7	2.989E-25	-1.6	7	A2	8	A1
93.91555	93.91360	2.08E-05	1.851E-25	6.9	1.713E-25	8.0	1.718E-25	7.7	8	F1	9	F2
93.93107	93.92913	2.06E-05	2.259E-25	16.0	2.164E-25	4.4	2.170E-25	4.1	8	F2	9	F1
104.22470	104.22244	2.17E-05	3.375E-25	13.0	3.358E-25	0.5	3.381E-25	-0.2	9	A1	10	A2
104.24737	104.24513	2.15E-05	2.187E-25	3.9	2.249E-25	-2.8	2.265E-25	-3.4	9	F1	10	F2
104.25229	104.25006	2.14E-05	1.326E-25	33.0	1.703E-25	-22.1	1.714E-25	-22.7	9	E	10	E
104.31507	104.31292	2.06E-05	2.432E-25	5.8	2.869E-25	-15.2	2.889E-25	-15.8	9	F1	10	F2
104.31924	104.31709	2.06E-05	2.579E-25	11.0	2.645E-25	-2.5	2.663E-25	-3.2	9	F2	10	F1
104.35000	104.34789	2.02E-05	5.639E-25	16.0	5.745E-25	-1.8	5.785E-25	-2.5	9	A2	10	A1
104.36479	104.36270	2.00E-05	5.884E-26	23.0	5.561E-26	5.8	5.600E-26	5.1	9	F1	10	F2
104.39473	104.39266	1.98E-05	5.951E-26	10.0	6.498E-26	-8.4	6.543E-26	-9.0	9	F2	10	F1
114.52344	114.52087	2.25E-05	2.267E-25	20.0	2.297E-25	-1.3	2.324E-25	-2.4	10	F1	11	F2
114.53532	114.53276	2.23E-05	2.576E-25	18.0	2.670E-25	-3.5	2.701E-25	-4.6	10	F2	11	F1
114.61438	114.61192	2.15E-05	1.686E-25	7.1	1.873E-25	-10.0	1.894E-25	-11.0	10	E	11	E
114.61714	114.61467	2.15E-05	2.930E-25	6.1	2.893E-25	1.3	2.926E-25	0.1	10	F1	11	F2
114.63941	114.63697	2.13E-05	7.343E-25	28.0	7.155E-25	2.6	7.238E-25	1.5	10	A1	11	A2
114.67144	114.66904	2.09E-05	3.632E-25	7.9	3.652E-25	-0.6	3.695E-25	-1.7	10	F2	11	F1
114.69262	114.69025	2.07E-05	6.598E-26	24.0	5.628E-26	17.2	5.693E-26	15.9	10	F1	11	F2
114.87932	114.87718	1.86E-05	3.423E-26	16.0	4.862E-26	-29.6	4.919E-26	-30.4	10	F2	11	F1
124.76275	124.75985	2.33E-05	1.632E-25	7.8	1.575E-25	3.6	1.602E-25	1.9	11	E	12	E
124.77117	124.76827	2.32E-05	2.414E-25	7.6	2.434E-25	-0.8	2.475E-25	-2.5	11	F2	12	F1
124.78389	124.78101	2.30E-05	4.350E-25	3.6	4.384E-25	-0.8	4.457E-25	-2.4	11	A2	12	A1
124.86687	124.86407	2.25E-05	2.760E-25	8.7	2.710E-25	1.9	2.755E-25	0.2	11	F2	12	F1
124.90983	124.90707	2.21E-05	3.801E-25	5.4	3.856E-25	-1.4	3.920E-25	-3.0	11	F1	12	F2
124.95360	124.95089	2.17E-05	2.366E-25	5.2	2.315E-25	2.2	2.353E-25	0.5	11	E	12	E
124.95887	124.95616	2.17E-05	3.365E-25	2.9	3.253E-25	3.4	3.308E-25	1.7	11	F1	12	F2
125.28147	125.27915	1.85E-05	1.230E-25	16.0	1.097E-25	12.2	1.115E-25	10.3	11	A2	12	A1
134.95865	134.95539	2.41E-05	2.026E-25	5.1	2.118E-25	-4.3	2.165E-25	-6.4	12	F1	13	F2

134.97498	134.97175	2.40E-05	2.127E-25	1.7	2.196E-25	-3.2	2.245E-25	-5.3	12	F2	13	F1
135.06476	135.06157	2.36E-05	3.871E-25	2.1	3.934E-25	-1.6	4.022E-25	-3.8	12	A2	13	A1
135.12831	135.12520	2.30E-05	2.870E-25	1.8	2.811E-25	2.1	2.873E-25	-0.1	12	F2	13	F1
135.13616	135.13306	2.30E-05	2.268E-25	4.5	2.255E-25	0.6	2.305E-25	-1.6	12	E	13	E
135.18891	135.18584	2.27E-05	2.471E-25	6.8	2.579E-25	-4.2	2.637E-25	-6.3	12	F2	13	F1
135.24148	135.23846	2.23E-05	5.208E-25	4.6	5.334E-25	-2.4	5.453E-25	-4.5	12	A1	13	A2
135.29673	135.29379	2.17E-05	8.246E-26	12.0	7.948E-26	3.8	8.125E-26	1.5	12	F2	13	F1
135.65576	135.65325	1.85E-05	3.389E-26	4.9	4.019E-26	-15.7	4.108E-26	-17.5	12	F2	13	F1
135.73905	135.73659	1.81E-05	3.190E-26	2.4	3.023E-26	5.5	3.091E-26	3.2	12	A1	13	A2
145.09922	145.09559	2.50E-05	2.920E-25	1.1	2.833E-25	3.1	2.913E-25	0.2	13	A1	14	A2
145.11543	145.11182	2.49E-05	1.761E-25	9.1	1.729E-25	1.8	1.778E-25	-1.0	13	F1	14	F2
145.12193	145.11832	2.48E-05	1.244E-25	16.0	1.173E-25	6.1	1.206E-25	3.1	13	E	14	E
145.29512	145.29162	2.41E-05	2.128E-25	5.0	2.125E-25	0.1	2.185E-25	-2.6	13	F2	14	F1
145.31437	145.31088	2.40E-05	2.656E-25	6.7	2.653E-25	0.1	2.728E-25	-2.6	13	F1	14	F2
145.38186	145.37839	2.39E-05	1.930E-25	4.4	1.956E-25	-1.3	2.012E-25	-4.1	13	F2	14	F1
145.38969	145.38624	2.38E-05	1.388E-25	11.0	1.445E-25	-3.9	1.486E-25	-6.6	13	E	14	E
145.44356	145.44016	2.33E-05	5.557E-25	2.8	5.658E-25	-1.8	5.819E-25	-4.5	13	A2	14	A1
145.45911	145.45571	2.34E-05	2.502E-25	9.6	2.519E-25	-0.7	2.590E-25	-3.4	13	F1	14	F2
145.53228	145.52900	2.26E-05	7.812E-26	11.0	7.300E-26	7.0	7.507E-26	4.1	13	F2	14	F1
155.20508	155.20108	2.58E-05	1.174E-25	13.0	1.271E-25	-7.6	1.315E-25	-10.7	14	F1	15	F2
155.21702	155.21303	2.57E-05	1.238E-25	3.7	1.295E-25	-4.4	1.340E-25	-7.6	14	F2	15	F1
155.43277	155.42886	2.52E-05	1.694E-25	14.0	1.844E-25	-8.1	1.909E-25	-11.2	14	F1	15	F2
155.46268	155.45880	2.50E-05	3.485E-25	4.5	3.499E-25	-0.4	3.621E-25	-3.8	14	A1	15	A2
155.51376	155.50982	2.53E-05	1.512E-25	6.9	1.522E-25	-0.6	1.575E-25	-4.0	14	F1	15	F2
155.60915	155.60533	2.45E-05	2.216E-25	19.0	2.419E-25	-8.4	2.504E-25	-11.5	14	F2	15	F1
155.62286	155.61899	2.49E-05	1.143E-25	22.0	1.175E-25	-2.8	1.216E-25	-6.0	14	E	15	E
155.63624	155.63239	2.47E-05	1.896E-25	11.0	1.790E-25	5.9	1.852E-25	2.4	14	F2	15	F1
156.23286	156.22982	1.95E-05	5.215E-26	6.2	6.036E-26	-13.6	6.247E-26	-16.5	14	A1	15	A2
165.24669	165.24230	2.66E-05	6.758E-26	11.0	5.817E-26	16.2	6.062E-26	11.5	15	E	16	E
165.25216	165.24778	2.65E-05	9.349E-26	9.3	8.761E-26	6.7	9.130E-26	2.4	15	F2	16	F1
165.26211	165.25775	2.64E-05	1.488E-25	6.1	1.477E-25	0.8	1.539E-25	-3.3	15	A2	16	A1
165.48246	165.47805	2.67E-05	1.189E-25	16.0	1.251E-25	-4.9	1.303E-25	-8.8	15	F2	16	F1
165.52922	165.52488	2.62E-05	1.403E-25	16.0	1.350E-25	3.9	1.407E-25	-0.3	15	F1	16	F2

165.57721	165.57272	2.71E-05	1.793E-25	9.1	1.745E-25	2.7	1.818E-25	-1.4	15	A1	16	A2
165.71246	165.70816	2.59E-05	1.466E-25	19.0	1.381E-25	6.2	1.439E-25	1.9	15	F1	16	F2
165.71962	165.71531	2.60E-05	1.055E-25	9.8	1.107E-25	-4.7	1.153E-25	-8.5	15	E	16	E
165.72524	165.72079	2.69E-05	1.011E-25	14.0	1.038E-25	-2.6	1.082E-25	-6.6	15	F1	16	F2
165.76086	165.75646	2.66E-05	1.348E-25	8.8	1.198E-25	12.5	1.249E-25	7.9	15	F2	16	F1
165.80353	165.79916	2.64E-05	2.266E-25	10.0	2.155E-25	5.2	2.245E-25	0.9	15	A2	16	A1
175.23026	175.22546	2.74E-05	6.572E-26	13.0	5.536E-26	18.7	5.812E-26	13.1	16	F1	17	F2
175.23920	175.23442	2.73E-05	5.148E-26	9.2	5.565E-26	-7.5	5.842E-26	-11.9	16	F2	17	F1
175.47690	175.47191	2.84E-05	1.414E-25	11.0	1.336E-25	5.8	1.402E-25	0.8	16	A2	17	A1
175.52873	175.52387	2.77E-05	8.728E-26	32.0	8.248E-26	5.8	8.657E-26	0.8	16	F2	17	F1
175.54531	175.54047	2.76E-05	6.748E-26	42.0	5.762E-26	17.1	6.049E-26	11.6	16	E	17	E
175.75462	175.74976	2.77E-05	8.168E-26	20.0	8.286E-26	-1.4	8.698E-26	-6.1	16	F1	17	F2
175.77014	175.76523	2.79E-05	1.052E-25	3.7	1.003E-25	4.8	1.053E-25	-0.1	16	F2	17	F1
175.77944	175.77428	2.94E-05	5.211E-26	14.0	6.232E-26	-16.4	6.541E-26	-20.3	16	F1	17	F2
175.80961	175.80452	2.89E-05	4.971E-26	21.0	4.844E-26	2.6	5.085E-26	-2.2	16	E	17	E
175.88877	175.88369	2.89E-05	8.307E-26	10.0	7.934E-26	4.7	8.328E-26	-0.3	16	F2	17	F1
175.91944	175.91453	2.79E-05	1.914E-25	7.6	1.996E-25	-4.1	2.095E-25	-8.6	16	A1	17	A2
185.14892	185.14369	2.82E-05	5.447E-26	2.2	5.432E-26	0.3	5.746E-26	-5.2	17	A1	18	A2
185.15627	185.15108	2.81E-05	2.560E-26	4.7	3.269E-26	-21.7	3.458E-26	-26.0	17	F1	18	F2
<u>185.15978</u>	<u>185.15459</u>	<u>2.80E-05</u>	<u>3.178E-26</u>	<u>6.0</u>	<u>2.183E-26</u>	<u>45.6</u>	<u>2.310E-26</u>	<u>37.6</u>	<u>17</u>	<u>E</u>	<u>18</u>	<u>E</u>
185.72296	185.71736	3.01E-05	3.828E-26	3.0	3.538E-26	8.2	3.743E-26	2.3	17	E	18	E
185.75272	185.74712	3.01E-05	5.439E-26	3.8	5.619E-26	-3.2	5.944E-26	-8.5	17	F2	18	F1
185.77760	185.77164	3.21E-05	4.182E-26	5.6	4.018E-26	4.1	4.251E-26	-1.6	17	F2	18	F1
185.81261	185.80712	2.95E-05	1.109E-25	5.7	1.125E-25	-1.4	1.191E-25	-6.8	17	A2	18	A1
185.95843	185.95276	3.05E-05	6.835E-26	16.0	6.932E-26	-1.4	7.333E-26	-6.8	17	F1	18	F2
195.36349	195.35732	3.16E-05	1.843E-26	5.1	1.842E-26	0.1	1.965E-26	-6.2	18	E	19	E
195.38122	195.37512	3.12E-05	2.301E-26	4.3	2.789E-26	-17.5	2.975E-26	-22.6	18	F1	19	F2
195.41070	195.40470	3.07E-05	4.622E-26	10.0	4.793E-26	-3.6	5.113E-26	-9.6	18	A1	19	A2
195.69065	195.68368	3.56E-05	4.795E-26	3.3	3.738E-26	28.3	3.988E-26	20.2	18	A2	19	A1
195.74041	195.73417	3.19E-05	3.295E-26	1.8 <sup>2</sup>	3.493E-26	-5.7	3.726E-26	-11.6	18	F2	19	F1
Average of absolute values		2.46E-05		10.57		6.28		6.63				
Average of absolute values minus italicized transition				10.62		5.85		6.30				

<sup>1</sup> The line position are taken from Tab.A1 of [15] but actually they were obtained with the STDS code from an effective Hamiltonian fitted on experiments

<sup>2</sup> Jean Vander Auwera, private communication

Table 4

Comparison with the SOLEIL experiment [15] of calculated transition wave numbers and intensities for the R-branch of methane vibrational ground state. Theoretical transition wave numbers,  $\nu_{\eta\eta'}$  in  $\text{cm}^{-1}$  units, were calculated at fourth order of perturbation (second column). Order 1 and 2 of perturbation theory have been used to compute effective dipole moments and derived theoretical intensities at 296 K,  $S_{\eta\eta'}$  (6th and 8th columns respectively) in  $\text{cm}^{-1} / (\text{molecule} \cdot \text{cm}^{-2})$ . The underlined transition in italics is singled out because it was withdrawn from the fit of the observed spectra, its relative error of 42% being too large.



## FIGURES

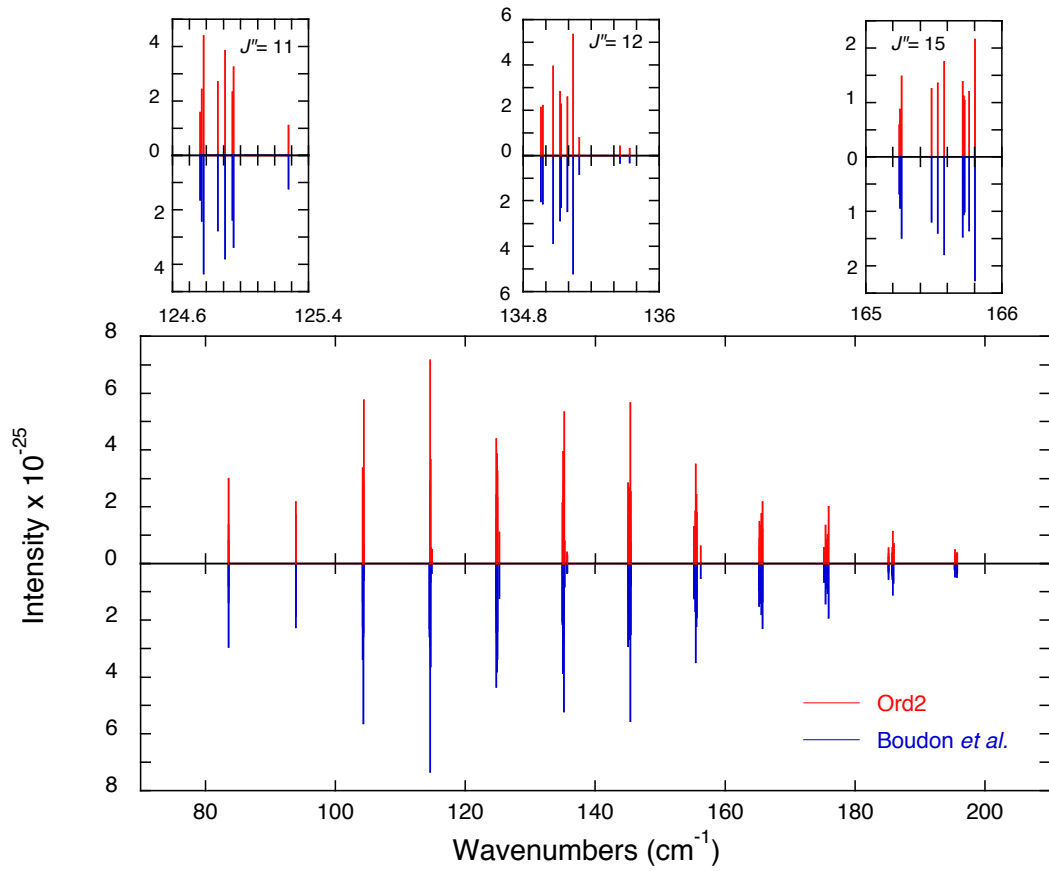


Fig. 1. Calculated R(7-18)-spectra versus observed spectra (upside-down). 93 transition lines are present in both spectra. The three panels above the main panel represent enlarged regions corresponding to a given lower level  $J$ -value.

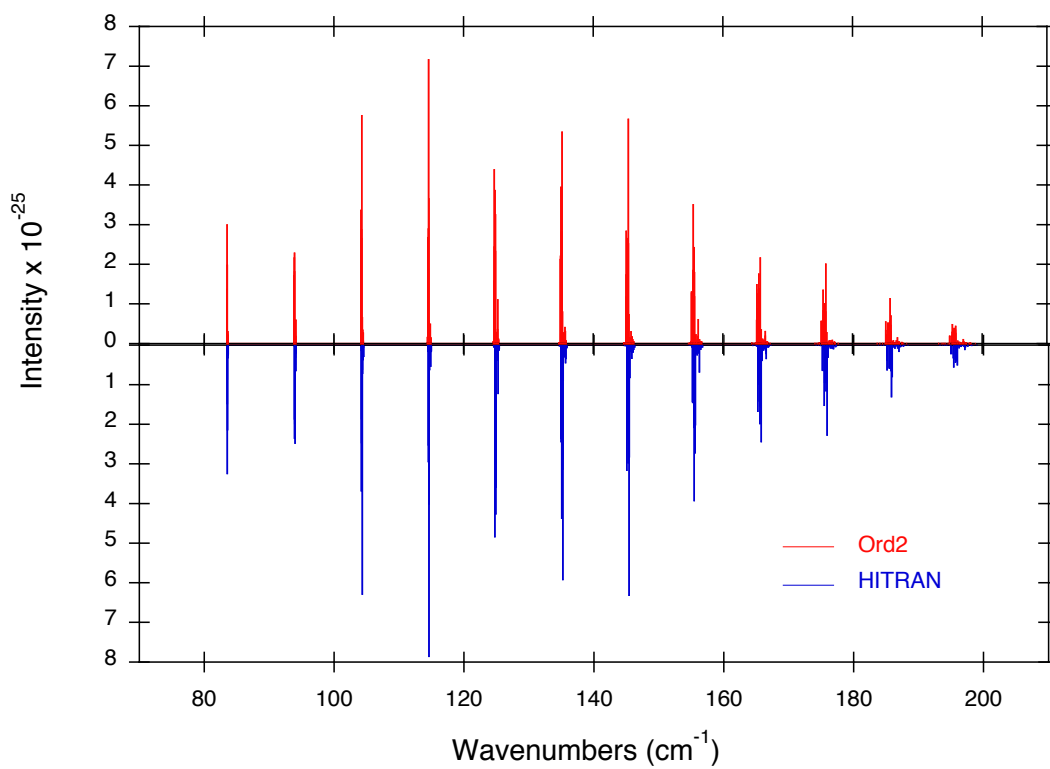


Fig. 2. Calculated R(7-18)-spectra versus spectra from HITRAN database (upside-down). 388 transition lines are present in both spectra corresponding to an intensity cutoff of  $10^{-32}$   $\text{cm}^{-1} / (\text{molecule} \cdot \text{cm}^{-2})$ .

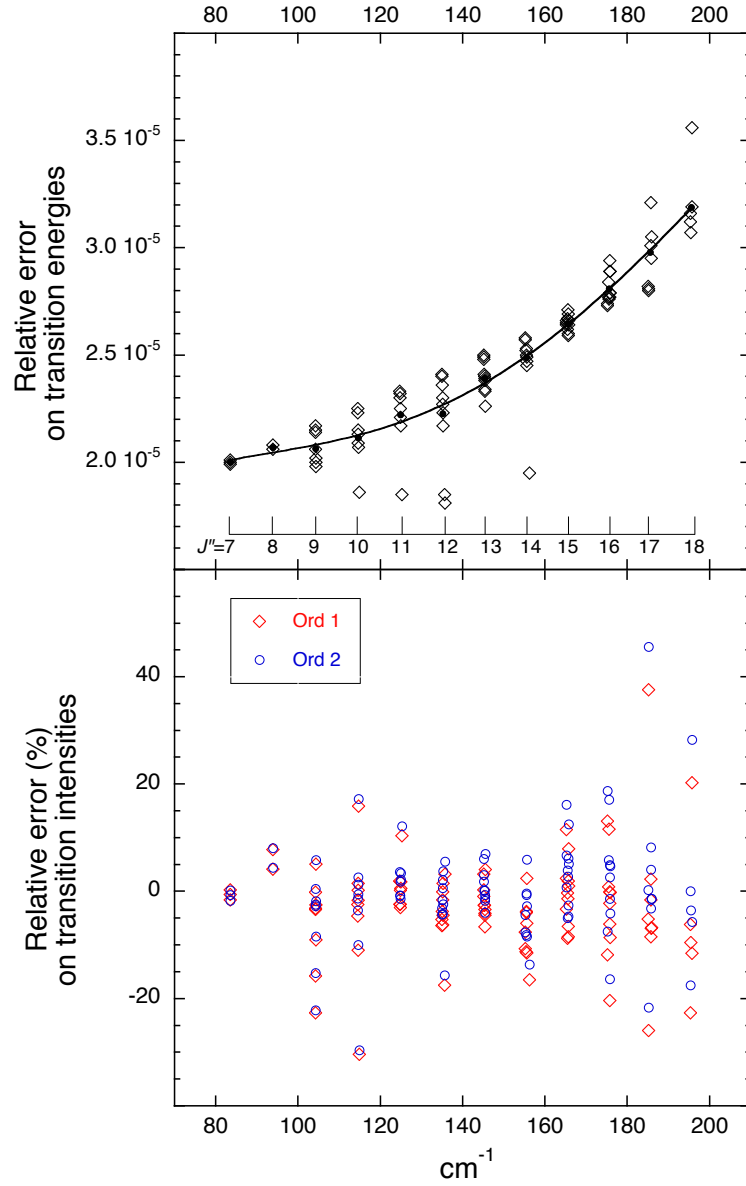


Fig. 3. Relative errors of the calculated transition wave numbers with respect to those determined by STDS [80] and of calculated intensities with respect to those obtained at SOLEIL. In the upper panel, the plotted numbers are those of column 3 of Table 4, in the lower panel, there are those of columns 7 and 9. The solid curve in the upper panel corresponds to the barycenter of relative errors for a given  $J$ -value.

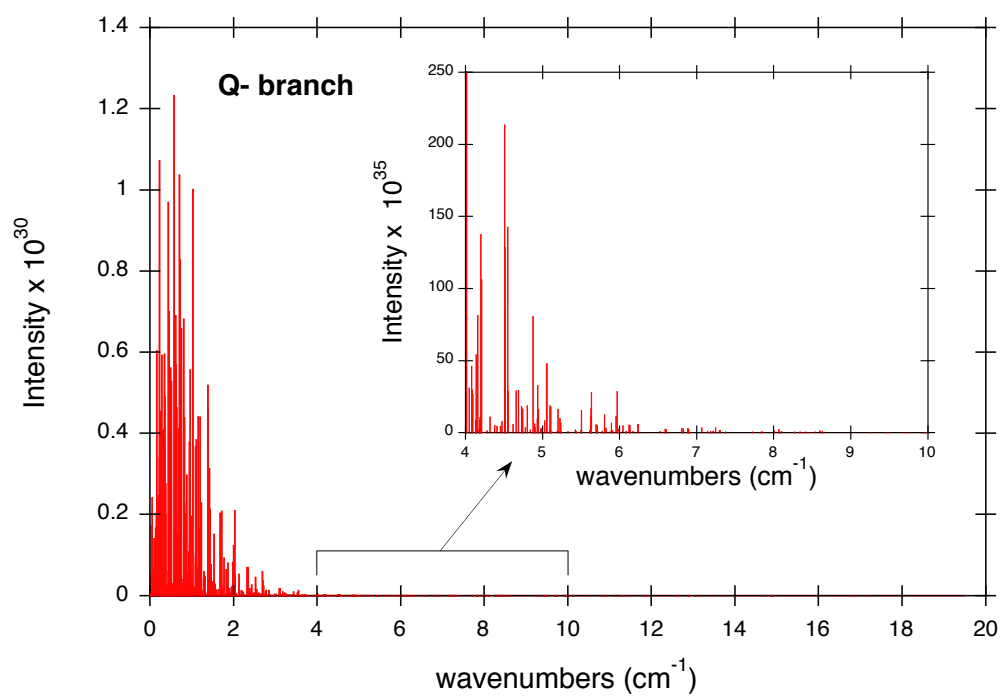


Fig. 4. *Ab initio* Q-Branch spectra for  $J \in \{1, 30\}$  corresponding to the transition wave numbers and intensities given in supplementary material.

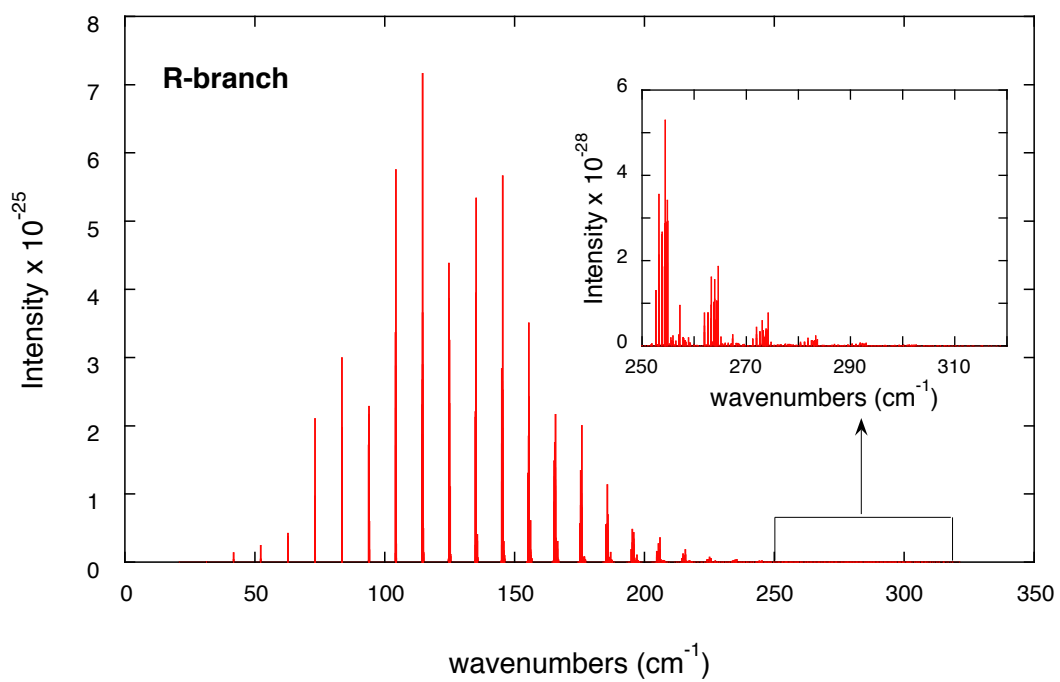


Fig. 5. *Ab initio* R-Branch spectra for  $J \in \{1, 30\}$  corresponding to the transition wave numbers and intensities given in supplementary material.

**An Alternative Perturbation Method for the  
Molecular Vibration-Rotation Problem II-  
Calculation *ab initio* of observables,  
application to the dipole moment of methane**

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**Supplementary material**

Method	$r_e$ (in Å)	$k_{33}$ (in au)	$k_{44}$ (in au)	$\frac{\partial\mu_z}{\partial Q_{3z}}$ (in au)	$\frac{\partial\mu_z}{\partial Q_{4z}}$ (in au)
MRCI/VQZ	1.08826	0.00010341	0.00001905	-0.00358(1)	+0.00233(5)
MRCI/ACVQZ	1.08690	0.00010379	0.00001924	-0.00357(65)	+0.00230(4)
MRCI/ACV5Z	1.08635	0.00010397	0.00001925	-0.00355(46)	+0.00232(0)
MRCI/ACV6Z	1.08624	0.00010404	0.00001930	-0.00354(38)	+0.00233(26)

Table 1

Convergence of the equilibrium CH distance of methane, of the quartic force constants of modes  $\nu_3$  and  $\nu_4$ , and of the non-zero first order derivatives of the electric dipole moment  $z$ -component with orbital basis set. The derivatives are with respect to the mass-weighted, Cartesian, normal coordinates of the Lee, Martin and Taylor force field [1], however, as noted in the main material, these coordinates are essentially basis set independent. The derivatives were obtained by finite difference at the equilibrium geometry with a step of 1 atomic unit. This is in contrast with the values actually used in the study, which were derived from fitting grid points extending over the range where the vibrational ground state product function has a non negligible weight at the harmonic level of approximation (typically more than or in the order of  $10^{-2}$ , that is to say  $10^{-4}$  for the square of the wave function), as this is more appropriate in view of computing expectation values. MRCI calculations were performed with frozen core for the VQZ basis set and full core excitations for the ACVnZ basis sets. The CI space for the ACV6Z calculation is spanned by about 16 Million CSFs. It is clear from this table that a full core treatment of correlation is necessary to obtain a value of the equilibrium distance to the mÅ accuracy. If the significant digits of  $\frac{\partial\mu_z}{\partial Q_{3z}}$  seem to convergence steadily with the quality of the basis set, convergence is less obvious for  $\frac{\partial\mu_z}{\partial Q_{4z}}$ , where the introduction of core correlation produces a step pattern.

$Q_1$	$Q_{2a}$	$Q_{2b}$	$Q_{3x}$	$Q_{3y}$	$Q_{3z}$	$Q_{4x}$	$Q_{4y}$	$Q_{4z}$	Dz (VQZ)	Dz (ACV5Z)
0.0	0.0	0.0	0.0	0.0	5.0	0.0	0.0	0.0	-0.01780589	-0.01769364
0.0	0.0	0.0	0.0	0.0	10.0	0.0	0.0	0.0	-0.03542519	-0.03519005
0.0	0.0	0.0	0.0	0.0	15.0	0.0	0.0	0.0	-0.05267213	-0.05231139
0.0	0.0	0.0	0.0	0.0	20.0	0.0	0.0	0.0	-0.06936261	-0.06887745
0.0	0.0	0.0	0.0	0.0	25.0	0.0	0.0	0.0	-0.08531508	-0.08470861
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	6.6	-0.01555704	-0.01537478
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	13.2	-0.03132966	-0.03099279
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	19.8	-0.04752836	-0.04708102
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	26.4	-0.06434783	-0.06384239
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	33.0	-0.08195461	-0.08144384
5.0	0.0	0.0	0.0	0.0	5.0	0.0	0.0	0.0	-0.01907791	-0.01894461
-5.0	0.0	0.0	0.0	0.0	5.0	0.0	0.0	0.0	-0.01650897	-0.01639360
5.0	0.0	0.0	0.0	0.0	10.0	0.0	0.0	0.0	-0.03796442	-0.03769769
-5.0	0.0	0.0	0.0	0.0	10.0	0.0	0.0	0.0	-0.03283425	-0.03260504
5.0	0.0	0.0	0.0	0.0	15.0	0.0	0.0	0.0	-0.05646986	-0.05606955
-5.0	0.0	0.0	0.0	0.0	15.0	0.0	0.0	0.0	-0.04879211	-0.04845200
10.0	0.0	0.0	0.0	0.0	5.0	0.0	0.0	0.0	-0.02032769	-0.02018732
-10.0	0.0	0.0	0.0	0.0	5.0	0.0	0.0	0.0	-0.01518315	-0.01508128
10.0	0.0	0.0	0.0	0.0	10.0	0.0	0.0	0.0	-0.04045761	-0.04017617
-10.0	0.0	0.0	0.0	0.0	10.0	0.0	0.0	0.0	-0.03018329	-0.02998177
-15.0	0.0	0.0	0.0	0.0	5.0	0.0	0.0	0.0	-0.01382299	-0.01373861
15.0	0.0	0.0	0.0	0.0	5.0	0.0	0.0	0.0	-0.02155671	-0.02140860
5.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	6.6	-0.01372728	-0.01356700
-5.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	6.6	-0.01747874	-0.01729402
5.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	13.2	-0.02765200	-0.02735672
-5.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	13.2	-0.03519202	-0.03484849
5.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	19.8	-0.04196824	-0.04157983
-5.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	19.8	-0.05336679	-0.05290849
10.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	6.6	-0.01198237	-0.01184378
-10.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	6.6	-0.01950177	-0.01931527
10.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	13.2	-0.02414488	-0.02389153



-10.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	13.2	-0.03925750	-0.03890980
-15.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	6.6	-0.02163790	-0.02145560
15.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	6.6	-0.01031703	-0.01020453
0.0	19.8	0.0	0.0	0.0	5.0	0.0	0.0	0.0	-0.02034093	-0.02045568
0.0	13.2	0.0	0.0	0.0	5.0	0.0	0.0	0.0	-0.01961325	-0.01962827
0.0	6.6	0.0	0.0	0.0	5.0	0.0	0.0	0.0	-0.01875741	-0.01869163
0.0	13.2	0.0	0.0	0.0	10.0	0.0	0.0	0.0	-0.03904747	-0.03907721
0.0	6.6	0.0	0.0	0.0	10.0	0.0	0.0	0.0	-0.03733145	-0.03720026
0.0	-19.8	0.0	0.0	0.0	5.0	0.0	0.0	0.0	-0.01474438	-0.01456748
0.0	-13.2	0.0	0.0	0.0	5.0	0.0	0.0	0.0	-0.01575856	-0.01558115
0.0	-6.6	0.0	0.0	0.0	5.0	0.0	0.0	0.0	-0.01679344	-0.01663132
0.0	-13.2	0.0	0.0	0.0	10.0	0.0	0.0	0.0	-0.03132955	-0.03097386
0.0	-6.6	0.0	0.0	0.0	10.0	0.0	0.0	0.0	-0.03339875	-0.03307476
0.0	6.6	0.0	0.0	0.0	0.0	0.0	0.0	6.6	-0.01666005	-0.01644861
0.0	6.6	0.0	0.0	0.0	0.0	0.0	0.0	13.2	-0.03351962	-0.03312274
0.0	6.6	0.0	0.0	0.0	0.0	0.0	0.0	19.8	-0.05077467	-0.05023466
0.0	13.2	0.0	0.0	0.0	0.0	0.0	0.0	6.6	-0.01828920	-0.01806675
0.0	13.2	0.0	0.0	0.0	0.0	0.0	0.0	13.2	-0.03676088	-0.03633552
0.0	19.8	0.0	0.0	0.0	0.0	0.0	0.0	6.6	-0.02041151	-0.02020358
0.0	-6.6	0.0	0.0	0.0	0.0	0.0	0.0	6.6	-0.01500703	-0.01488620
0.0	-6.6	0.0	0.0	0.0	0.0	0.0	0.0	13.2	-0.03024550	-0.03002398
0.0	-6.6	0.0	0.0	0.0	0.0	0.0	0.0	19.8	-0.04593582	-0.04565072
0.0	-13.2	0.0	0.0	0.0	0.0	0.0	0.0	6.6	-0.01503111	-0.01497817
0.0	-13.2	0.0	0.0	0.0	0.0	0.0	0.0	13.2	-0.03030707	-0.03021243
0.0	-19.8	0.0	0.0	0.0	0.0	0.0	0.0	6.6	-0.01564429	-0.01566284
0.0	0.0	0.0	5.0	5.0	0.0	0.0	0.0	0.0	-0.00227924	-0.00230668
0.0	0.0	0.0	5.0	10.0	0.0	0.0	0.0	0.0	-0.00453711	-0.00458983
0.0	0.0	0.0	5.0	15.0	0.0	0.0	0.0	0.0	-0.00675260	-0.00682651
0.0	0.0	0.0	10.0	10.0	0.0	0.0	0.0	0.0	-0.00903214	-0.00913343
0.0	0.0	0.0	5.0	0.0	0.0	0.0	6.6	0.0	+0.00190798	+0.00190567
0.0	0.0	0.0	5.0	0.0	0.0	0.0	13.2	0.0	+0.00380525	+0.00380258
0.0	0.0	0.0	5.0	0.0	0.0	0.0	19.8	0.0	+0.00568154	+0.00568209
0.0	0.0	0.0	10.0	0.0	0.0	0.0	6.6	0.0	+0.00381679	+0.00381170

0.0	0.0	0.0	10.0	0.0	0.0	0.0	13.2	0.0	+0.00761189	+0.00760576
0.0	0.0	0.0	15.0	0.0	0.0	0.0	6.6	0.0	+0.00572723	+0.00571858
0.0	0.0	0.0	0.0	0.0	0.0	6.6	6.6	0.0	+0.00272280	+0.00269681
0.0	0.0	0.0	0.0	0.0	0.0	6.6	13.2	0.0	+0.00542658	+0.00537597
0.0	0.0	0.0	0.0	0.0	0.0	6.6	19.8	0.0	+0.00809206	+0.00801981
0.0	0.0	0.0	0.0	0.0	0.0	13.2	13.2	0.0	+0.01081493	+0.01071640
0.0	0.0	0.0	5.0	0.0	0.0	0.0	0.0	6.6	-0.01545914	-0.01528637
0.0	0.0	0.0	5.0	0.0	0.0	0.0	0.0	13.2	-0.03113487	-0.03081504
0.0	0.0	0.0	10.0	0.0	0.0	0.0	0.0	6.6	-0.01516728	-0.01500378
0.0	0.0	0.0	0.0	0.0	5.0	6.6	0.0	0.0	-0.01769530	-0.01757348
0.0	0.0	0.0	0.0	0.0	5.0	13.2	0.0	0.0	-0.01736618	-0.01725509
0.0	0.0	0.0	0.0	0.0	10.0	6.6	0.0	0.0	-0.03520509	-0.03496197
0.0	0.0	0.0	0.0	0.0	5.0	0.0	0.0	6.6	-0.03334100	-0.03303820
0.0	0.0	0.0	0.0	0.0	5.0	0.0	0.0	13.2	-0.04920631	-0.04874985
0.0	0.0	0.0	0.0	0.0	10.0	0.0	0.0	6.6	-0.05078593	-0.05035549
0.0	0.0	0.0	0.0	0.0	5.0	0.0	0.0	-6.6	-0.00238029	-0.00243065
0.0	0.0	0.0	0.0	0.0	5.0	0.0	0.0	-13.2	+0.01315250	+0.01295399
0.0	0.0	0.0	0.0	0.0	10.0	0.0	0.0	-6.6	-0.02028316	-0.02020997
5.0	6.6	0.0	0.0	0.0	5.0	0.0	0.0	0.0	-0.02005328	-0.01997398
-5.0	6.6	0.0	0.0	0.0	5.0	0.0	0.0	0.0	-0.01743259	-0.01738289
5.0	6.6	0.0	0.0	0.0	0.0	0.0	0.0	6.6	-0.01855409	-0.01833054
-5.0	6.6	0.0	0.0	0.0	0.0	0.0	0.0	6.6	-0.01486342	-0.01467082
5.0	-6.6	0.0	0.0	0.0	5.0	0.0	0.0	0.0	-0.01804638	-0.01788099
-5.0	-6.6	0.0	0.0	0.0	5.0	0.0	0.0	0.0	-0.01551910	-0.01536173
5.0	-6.6	0.0	0.0	0.0	0.0	0.0	0.0	6.6	-0.01308892	-0.01298013
-5.0	-6.6	0.0	0.0	0.0	0.0	0.0	0.0	6.6	-0.01701842	-0.01689250
5.0	0.0	0.0	5.0	5.0	0.0	0.0	0.0	0.0	-0.00228370	-0.00231726
-5.0	0.0	0.0	5.0	5.0	0.0	0.0	0.0	0.0	-0.00226931	-0.00228908
5.0	0.0	0.0	5.0	0.0	0.0	0.0	6.6	0.0	+0.00193381	+0.00193111
-5.0	0.0	0.0	5.0	0.0	0.0	0.0	6.6	0.0	+0.00187626	+0.00187428
5.0	0.0	0.0	0.0	0.0	0.0	6.6	6.6	0.0	+0.00261414	+0.00258753
-5.0	0.0	0.0	0.0	0.0	0.0	6.6	6.6	0.0	+0.00284234	+0.00281747
0.0	0.0	0.0	5.0	0.0	5.0	6.6	0.0	0.0	-0.01766171	-0.01754207

0.0	0.0	0.0	5.0	0.0	5.0	-6.6	0.0	0.0	-0.01766927	-0.01755166
0.0	0.0	0.0	5.0	0.0	0.0	6.6	0.0	6.6	-0.01549754	-0.01532468
0.0	0.0	0.0	5.0	0.0	0.0	-6.6	0.0	-6.6	+0.01567388	+0.01550206

Table 2

z-component values of the electric dipole moment ( $D_z$ ) of CH<sub>4</sub>. Mass-weighted normal coordinates, ( $Q_1, Q_{2a}, Q_{2b}, Q_{3x}, Q_{3y}, Q_{3z}, Q_{4x}, Q_{4y}, Q_{4z}$ ), and dipole moment are in atomic units. The calculations were internally contracted MRCI with frozen core and a VQZ basis set (“VQZ” column) and full core excitations with a ACV5Z basis set (“ACV5Z” column), see main text for details. The sign convention for the normal coordinates is that of Gray Robiette [4], except for  $Q_{4x}, Q_{4y}, Q_{4z}$  whose signs are opposite in the table (but not in the main article nor in the previous table).

20.960355	1.306E-29	1.870E-12	10.4815	1	F1	2	F2
31.432812	6.201E-28	1.080E-10	31.4418	2	F2	3	F1
41.893892	1.343E-26	1.738E-09	62.8770	3	A2	4	A1
41.897084	3.359E-27	7.242E-10	62.8757	3	F2	4	F1
41.903463	2.880E-28	6.210E-11	62.8746	3	F1	4	F2
52.343336	2.386E-26	6.605E-09	104.7781	4	F2	5	F1
52.352244	3.733E-27	1.034E-09	104.7728	4	F1	5	F2
52.357936	8.191E-28	2.268E-10	104.7781	4	F2	5	F1
52.360194	4.268E-27	3.546E-09	104.7741	4	E	5	E
62.774920	4.170E-26	1.548E-08	157.1360	5	F1	6	F2
62.775060	3.722E-26	4.145E-08	157.1343	5	E	6	E
62.789521	3.543E-27	1.316E-09	157.1214	5	F1	6	F2
62.796667	1.770E-26	6.574E-09	157.1360	5	F1	6	F2
62.811268	3.748E-27	1.392E-09	157.1214	5	F1	6	F2
62.812176	6.986E-27	2.595E-09	157.1250	5	F2	6	F1
73.183842	7.001E-26	3.650E-08	219.9372	6	F1	7	F2
73.184779	9.647E-26	5.029E-08	219.9327	6	F2	7	F1
73.206525	6.996E-27	3.648E-09	219.9109	6	F2	7	F1
73.207552	2.098E-25	6.565E-08	219.9412	6	A1	7	A2
73.221913	4.202E-26	2.192E-08	219.9372	6	F1	7	F2
73.240545	5.382E-27	2.808E-09	219.9327	6	F2	7	F1
73.255322	1.016E-26	1.590E-08	219.9094	6	E	7	E
73.262291	7.205E-27	3.760E-09	219.9109	6	F2	7	F1
83.563814	7.965E-26	1.834E-07	293.1647	7	E	8	E
83.567459	1.364E-25	1.047E-07	293.1591	7	F2	8	F1
83.574556	2.992E-25	1.378E-07	293.1487	7	A2	8	A1
83.605529	7.072E-27	5.431E-09	293.1210	7	F2	8	F1
83.605554	1.967E-25	1.511E-07	293.1732	7	F1	8	F2
83.638610	2.379E-26	1.828E-08	293.1591	7	F2	8	F1
83.646000	3.452E-27	2.653E-09	293.1732	7	F1	8	F2
83.649570	2.973E-26	6.854E-08	293.1647	7	E	8	E
83.661320	2.183E-27	1.678E-09	293.1175	7	F1	8	F2

83.676681	5.457E-27	4.195E-09	293.1210	7	F2	8	F1
83.701766	2.068E-26	1.590E-08	293.1175	7	F1	8	F2
93.888687	1.870E-27	2.218E-09	376.8192	8	F2	9	F1
93.913595	1.713E-25	2.033E-07	376.7977	8	F1	9	F2
93.929134	2.164E-25	2.568E-07	376.7788	8	F2	9	F1
93.975796	1.810E-25	6.450E-07	376.8142	8	E	9	E
93.977124	2.282E-25	2.710E-07	376.8192	8	F2	9	F1
93.984746	3.392E-27	4.027E-09	376.7266	8	F1	9	F2
94.017570	1.791E-26	2.128E-08	376.7788	8	F2	9	F1
94.026906	4.494E-26	5.341E-08	376.8192	8	F2	9	F1
94.058496	2.797E-26	3.325E-08	376.7977	8	F1	9	F2
94.061552	7.029E-27	2.506E-08	376.7285	8	E	9	E
94.067352	1.955E-26	2.324E-08	376.7788	8	F2	9	F1
94.129648	1.763E-26	2.097E-08	376.7266	8	F1	9	F2
94.140804	5.898E-26	4.210E-08	376.7233	8	A1	9	A2
104.195350	1.265E-26	2.436E-08	470.8461	9	F1	10	F2
104.222435	3.358E-25	3.879E-07	470.8221	9	A1	10	A2
104.245132	2.249E-25	4.332E-07	470.7964	9	F1	10	F2
104.250055	1.703E-25	9.837E-07	470.7900	9	E	10	E
104.312916	2.869E-25	5.530E-07	470.8461	9	F1	10	F2
104.317091	2.645E-25	5.099E-07	470.8562	9	F2	10	F1
104.333568	1.627E-27	3.136E-09	470.7079	9	F1	10	F2
104.347888	5.745E-25	6.648E-07	470.8641	9	A2	10	A1
104.362698	5.561E-26	1.072E-07	470.7964	9	F1	10	F2
104.392663	6.498E-26	1.254E-07	470.8562	9	F2	10	F1
104.428397	1.445E-26	2.789E-08	470.8461	9	F1	10	F2
104.451134	2.587E-27	4.992E-09	470.7079	9	F1	10	F2
104.461992	4.614E-27	8.904E-09	470.7113	9	F2	10	F1
104.470975	3.335E-26	1.932E-07	470.7900	9	E	10	E
104.478179	1.788E-26	3.453E-08	470.7964	9	F1	10	F2
104.537565	5.040E-27	9.735E-09	470.7113	9	F2	10	F1
104.566616	2.594E-26	5.012E-08	470.7079	9	F1	10	F2
114.417282	5.441E-28	1.785E-09	575.2745	10	F2	11	F1

114.445296	1.468E-26	4.816E-08	575.2489	10	F1	11	F2
114.520868	2.297E-25	7.540E-07	575.1733	10	F1	11	F2
114.532764	2.670E-25	8.763E-07	575.1591	10	F2	11	F1
114.611917	1.873E-25	1.846E-06	575.2610	10	E	11	E
114.614673	2.893E-25	9.507E-07	575.2489	10	F1	11	F2
114.636973	7.155E-25	1.411E-06	575.2120	10	A1	11	A2
114.650329	8.567E-28	2.814E-09	575.0415	10	F2	11	F1
114.669045	3.652E-25	1.201E-06	575.2745	10	F2	11	F1
114.690246	5.628E-26	1.851E-07	575.1733	10	F1	11	F2
114.755564	2.141E-26	7.048E-08	575.2489	10	F1	11	F2
114.761698	3.728E-27	1.227E-08	575.2745	10	F2	11	F1
114.765552	3.733E-26	3.687E-07	575.2610	10	E	11	E
114.784526	7.447E-27	2.451E-08	575.1591	10	F2	11	F1
114.831137	1.636E-26	5.388E-08	575.1733	10	F1	11	F2
114.832838	3.678E-27	3.631E-08	575.0401	10	E	11	E
114.877180	4.862E-26	1.602E-07	575.1591	10	F2	11	F1
114.902092	6.024E-27	1.984E-08	575.0415	10	F2	11	F1
114.986473	1.378E-26	1.363E-07	575.0401	10	E	11	E
114.994746	1.159E-26	3.821E-08	575.0415	10	F2	11	F1
124.606213	2.552E-27	4.495E-08	690.0266	11	E	12	E
124.627383	4.286E-27	2.516E-08	690.0044	11	F2	12	F1
124.759848	1.576E-25	2.777E-06	689.8729	11	E	12	E
124.768274	2.434E-25	1.430E-06	689.8635	11	F2	12	F1
124.781015	4.384E-25	1.546E-06	689.8489	11	A2	12	A1
124.814418	3.267E-27	1.922E-08	690.0362	11	F1	12	F2
124.864066	2.710E-25	1.595E-06	690.0044	11	F2	12	F1
124.907071	3.856E-25	2.269E-06	689.9436	11	F1	12	F2
124.937651	3.653E-28	2.148E-09	689.6942	11	F2	12	F1
124.950892	2.315E-25	4.091E-06	690.0266	11	E	12	E
124.956160	3.253E-25	1.917E-06	690.0362	11	F1	12	F2
125.004957	1.876E-26	1.105E-07	689.8635	11	F2	12	F1
125.048813	1.769E-26	1.043E-07	689.9436	11	F1	12	F2
125.064116	2.762E-26	1.629E-07	690.0362	11	F1	12	F2

125.104527	2.472E-26	4.373E-07	689.8729	11	E	12	E
125.111540	2.219E-26	1.309E-07	690.0044	11	F2	12	F1
125.156770	2.139E-26	1.262E-07	689.9436	11	F1	12	F2
125.158834	5.473E-28	3.226E-09	689.6918	11	F1	12	F2
125.174334	8.160E-28	4.811E-09	689.6942	11	F2	12	F1
125.252431	3.486E-26	2.059E-07	689.8635	11	F2	12	F1
125.279148	1.097E-25	3.886E-07	689.8489	11	A2	12	A1
125.300576	8.918E-27	5.264E-08	689.6918	11	F1	12	F2
125.408532	1.098E-26	6.489E-08	689.6918	11	F1	12	F2
125.421809	7.713E-27	4.558E-08	689.6942	11	F2	12	F1
134.707919	1.240E-27	1.368E-08	815.1160	12	F1	13	F2
134.722047	1.545E-27	1.705E-08	815.1004	12	F2	13	F1
134.830004	9.676E-28	1.068E-08	814.9924	12	F2	13	F1
134.955394	2.118E-25	2.339E-06	814.8685	12	F1	13	F2
134.971746	2.196E-25	2.426E-06	814.8507	12	F2	13	F1
135.017242	2.420E-26	2.678E-07	815.1004	12	F2	13	F1
135.061569	3.935E-25	2.613E-06	815.0734	12	A2	13	A1
135.125199	2.811E-25	3.112E-06	814.9924	12	F2	13	F1
135.133055	2.255E-25	7.489E-06	814.9775	12	E	13	E
135.185838	2.579E-25	2.859E-06	815.1004	12	F2	13	F1
135.192077	1.253E-28	1.386E-09	814.6318	12	F1	13	F2
135.202292	2.824E-25	3.130E-06	815.1160	12	F1	13	F2
135.238462	5.334E-25	3.550E-06	815.1281	12	A1	13	A2
135.266941	7.673E-27	8.501E-08	814.8507	12	F2	13	F1
135.293795	7.948E-26	8.813E-07	814.9924	12	F2	13	F1
135.352901	2.570E-26	2.854E-07	815.1160	12	F1	13	F2
135.403552	9.735E-27	1.081E-07	815.1004	12	F2	13	F1
135.435537	7.690E-27	8.533E-08	814.8507	12	F2	13	F1
135.449766	1.484E-26	1.647E-07	814.8685	12	F1	13	F2
135.477734	5.782E-28	1.923E-08	814.6328	12	E	13	E
135.509124	2.668E-26	8.893E-07	814.9775	12	E	13	E
135.511509	1.049E-26	1.166E-07	814.9924	12	F2	13	F1
135.600376	6.218E-27	6.912E-08	814.8685	12	F1	13	F2

135.653251	4.019E-26	4.469E-07	814.8507	12	F2	13	F1
135.686449	4.701E-27	5.224E-08	814.6318	12	F1	13	F2
135.736595	3.023E-26	2.016E-07	814.6300	12	A1	13	A2
135.837058	6.216E-27	6.917E-08	814.6318	12	F1	13	F2
135.853803	4.252E-27	1.420E-07	814.6328	12	E	13	E
144.725510	5.484E-28	1.194E-08	950.5039	13	F1	14	F2
144.742256	7.159E-28	4.678E-08	950.4866	13	E	14	E
144.943225	1.196E-27	2.608E-08	950.2862	13	F1	14	F2
145.093169	9.216E-28	2.014E-08	950.5039	13	F1	14	F2
145.095587	2.833E-25	3.708E-06	950.1350	13	A1	14	A2
145.111821	1.729E-25	3.772E-06	950.1176	13	F1	14	F2
145.118325	1.173E-25	7.676E-06	950.1105	13	E	14	E
145.141010	2.440E-26	5.333E-07	950.4689	13	F2	14	F1
145.291620	2.125E-25	4.648E-06	950.3183	13	F2	14	F1
145.310883	2.653E-25	5.802E-06	950.2862	13	F1	14	F2
145.378387	1.956E-25	4.285E-06	950.4689	13	F2	14	F1
145.386236	1.445E-25	9.495E-06	950.4866	13	E	14	E
145.407016	4.008E-29	8.755E-10	949.8224	13	F1	14	F2
145.440164	5.658E-25	7.437E-06	950.3666	13	A2	14	A1
145.455708	2.519E-25	5.522E-06	950.5039	13	F1	14	F2
145.479479	4.955E-27	1.084E-07	950.1176	13	F1	14	F2
145.528997	7.300E-26	1.600E-06	950.3183	13	F2	14	F1
145.642516	5.312E-27	1.166E-07	950.4689	13	F2	14	F1
145.645509	1.435E-27	3.151E-08	950.5039	13	F1	14	F2
145.648796	1.387E-26	9.136E-07	950.4866	13	E	14	E
145.673422	7.768E-27	1.704E-07	950.2862	13	F1	14	F2
145.762305	9.845E-27	6.480E-07	950.1105	13	E	14	E
145.774675	1.145E-28	2.510E-09	949.8224	13	F1	14	F2
145.785992	1.401E-28	3.071E-09	949.8239	13	F2	14	F1
145.793125	1.038E-26	2.280E-07	950.3183	13	F2	14	F1
145.842018	1.020E-26	2.239E-07	950.1176	13	F1	14	F2
145.863223	2.959E-26	6.505E-07	950.2862	13	F1	14	F2
146.023369	1.054E-27	2.315E-08	949.8239	13	F2	14	F1



146.024865	1.583E-26	1.044E-06	950.1105	13	E	14	E
146.031819	1.552E-26	3.413E-07	950.1176	13	F1	14	F2
146.137213	9.360E-27	2.058E-07	949.8224	13	F1	14	F2
146.287497	4.278E-27	9.418E-08	949.8239	13	F2	14	F1
146.327014	1.531E-28	3.371E-09	949.8224	13	F1	14	F2
154.660691	4.904E-28	2.214E-08	1096.1494	14	F2	15	F1
154.699573	6.232E-29	2.814E-09	1096.1114	14	F1	15	F2
154.850492	6.154E-29	2.780E-09	1095.9596	14	F2	15	F1
154.963702	6.886E-28	3.112E-08	1095.8473	14	F1	15	F2
155.146546	3.854E-27	5.241E-07	1096.1354	14	E	15	E
155.164729	5.009E-27	2.271E-07	1096.1114	14	F1	15	F2
155.201079	1.271E-25	5.749E-06	1095.6099	14	F1	15	F2
155.213031	1.295E-25	5.857E-06	1095.5971	14	F2	15	F1
155.409106	1.166E-25	1.587E-05	1095.8728	14	E	15	E
155.415532	1.540E-27	6.997E-08	1096.1494	14	F2	15	F1
155.428857	1.844E-25	8.368E-06	1095.8473	14	F1	15	F2
155.458801	3.499E-25	9.525E-06	1095.8067	14	A1	15	A2
155.509819	1.522E-25	6.918E-06	1096.1114	14	F1	15	F2
155.580690	1.218E-29	5.517E-10	1095.2294	14	F2	15	F1
155.605333	2.419E-25	1.100E-05	1095.9596	14	F2	15	F1
155.618990	1.175E-25	1.605E-05	1096.1354	14	E	15	E
155.632392	1.790E-25	8.146E-06	1096.1494	14	F2	15	F1
155.666235	2.153E-27	9.777E-08	1095.6099	14	F1	15	F2
155.773947	1.802E-26	8.199E-07	1095.8473	14	F1	15	F2
155.822194	6.535E-27	2.977E-07	1095.9596	14	F2	15	F1
155.853255	6.030E-27	2.750E-07	1096.1494	14	F2	15	F1
155.881550	2.205E-26	3.014E-06	1095.8728	14	E	15	E
155.909932	5.581E-27	2.546E-07	1096.1114	14	F1	15	F2
155.967871	1.128E-27	5.134E-08	1095.5971	14	F2	15	F1
156.011324	2.163E-27	9.850E-08	1095.6099	14	F1	15	F2
156.043056	7.704E-27	3.516E-07	1095.9596	14	F2	15	F1
156.053085	8.421E-29	1.149E-08	1095.2288	14	E	15	E
156.174061	1.774E-26	8.100E-07	1095.8473	14	F1	15	F2

156.184732	1.419E-26	6.473E-07	1095.5971	14	F2	15	F1
156.229821	6.036E-26	1.654E-06	1095.8067	14	A1	15	A2
156.335530	4.495E-28	2.049E-08	1095.2294	14	F2	15	F1
156.405594	9.242E-27	4.224E-07	1095.5971	14	F2	15	F1
156.411438	8.354E-27	3.818E-07	1095.6099	14	F1	15	F2
156.525529	3.860E-27	5.287E-07	1095.2288	14	E	15	E
156.552391	3.810E-27	1.740E-07	1095.2294	14	F2	15	F1
156.746360	4.541E-27	1.246E-07	1095.2306	14	A2	15	A1
156.773253	6.001E-28	2.746E-08	1095.2294	14	F2	15	F1
164.486726	5.172E-28	3.048E-08	1252.0365	15	A2	16	A1
164.502575	1.247E-28	1.225E-08	1252.0213	15	F2	16	F1
164.769852	1.272E-28	3.752E-08	1251.7544	15	E	16	E
164.902689	2.029E-28	1.996E-08	1251.6212	15	F2	16	F1
165.077935	1.476E-27	1.457E-07	1252.0213	15	F2	16	F1
165.087161	1.673E-27	1.652E-07	1252.0027	15	F1	16	F2
165.242296	5.817E-26	1.719E-05	1251.2819	15	E	16	E
165.247779	8.761E-26	8.629E-06	1251.2761	15	F2	16	F1
165.257746	1.477E-25	8.727E-06	1251.2655	15	A2	16	A1
165.308024	1.011E-27	9.984E-08	1251.7818	15	F1	16	F2
165.478049	1.251E-25	1.236E-05	1251.6212	15	F2	16	F1
165.487299	1.096E-26	1.085E-06	1252.0027	15	F1	16	F2
165.524884	1.350E-25	1.335E-05	1251.5649	15	F1	16	F2
165.572716	1.745E-25	1.038E-05	1251.9769	15	A1	16	A2
165.708161	1.381E-25	1.368E-05	1251.7818	15	F1	16	F2
165.712934	3.355E-30	3.309E-10	1250.8110	15	F2	16	F1
165.715305	1.107E-25	3.291E-05	1251.7544	15	E	16	E
165.720789	1.038E-25	1.030E-05	1252.0027	15	F1	16	F2
165.756459	1.198E-25	1.190E-05	1252.0213	15	F2	16	F1
165.799155	2.155E-25	1.284E-05	1252.0365	15	A2	16	A1
165.823139	6.121E-28	6.057E-08	1251.2761	15	F2	16	F1
165.925022	6.384E-27	6.331E-07	1251.5649	15	F1	16	F2
165.941651	3.463E-26	3.438E-06	1251.7818	15	F1	16	F2
166.048755	3.773E-27	3.754E-07	1252.0213	15	F2	16	F1

166.105701	2.135E-27	2.125E-07	1252.0027	15	F1	16	F2
166.156572	1.074E-26	1.067E-06	1251.6212	15	F2	16	F1
166.158512	6.008E-27	5.969E-07	1251.5649	15	F1	16	F2
166.187749	1.366E-27	4.066E-07	1251.2819	15	E	16	E
166.279725	1.118E-29	1.108E-09	1250.8101	15	F1	16	F2
166.288294	1.235E-29	1.224E-09	1250.8110	15	F2	16	F1
166.326563	2.280E-27	2.271E-07	1251.7818	15	F1	16	F2
166.335342	7.761E-27	2.319E-06	1251.7544	15	E	16	E
166.448868	2.047E-27	2.039E-07	1251.6212	15	F2	16	F1
166.501662	6.474E-27	6.442E-07	1251.2761	15	F2	16	F1
166.543424	1.847E-26	1.841E-06	1251.5649	15	F1	16	F2
166.570174	2.988E-26	1.785E-06	1251.2655	15	A2	16	A1
166.679862	2.824E-28	2.808E-08	1250.8101	15	F1	16	F2
166.793958	4.301E-27	4.290E-07	1251.2761	15	F2	16	F1
166.807786	3.459E-27	1.035E-06	1251.2819	15	E	16	E
166.913352	3.084E-27	3.072E-07	1250.8101	15	F1	16	F2
166.966818	1.989E-27	1.983E-07	1250.8110	15	F2	16	F1
167.259114	4.234E-28	4.229E-08	1250.8110	15	F2	16	F1
167.298264	2.002E-29	2.000E-09	1250.8101	15	F1	16	F2
174.215884	8.034E-29	1.803E-08	1418.1084	16	F2	17	F1
174.254643	9.150E-30	2.054E-09	1418.0701	16	F1	17	F2
174.546939	5.342E-29	1.200E-08	1417.7778	16	F1	17	F2
174.600795	4.691E-29	1.054E-08	1417.7235	16	F2	17	F1
174.834285	4.424E-29	9.949E-09	1417.4900	16	F2	17	F1
174.905466	5.281E-28	1.192E-07	1418.1084	16	F2	17	F1
174.920430	6.341E-28	4.293E-07	1418.0897	16	E	17	E
175.225462	5.536E-26	1.246E-05	1417.0993	16	F1	17	F2
175.234423	5.565E-26	1.253E-05	1417.0898	16	F2	17	F1
175.290378	1.942E-27	4.389E-07	1417.7235	16	F2	17	F1
175.380318	4.406E-28	9.980E-08	1418.1084	16	F2	17	F1
175.457463	9.338E-27	2.116E-06	1418.0701	16	F1	17	F2
175.471915	1.336E-25	1.812E-05	1417.5496	16	A2	17	A1
175.523868	8.248E-26	1.865E-05	1417.4900	16	F2	17	F1

175.540467	5.762E-26	3.908E-05	1417.4697	16	E	17	E
175.749759	8.286E-26	1.879E-05	1417.7778	16	F1	17	F2
175.765230	1.003E-25	2.275E-05	1417.7235	16	F2	17	F1
175.774280	6.232E-26	1.416E-05	1418.0701	16	F1	17	F2
175.800822	8.396E-31	1.893E-10	1416.5239	16	F1	17	F2
175.804523	4.844E-26	3.302E-05	1418.0897	16	E	17	E
175.883688	7.934E-26	1.804E-05	1418.1084	16	F2	17	F1
175.914534	1.996E-25	2.721E-05	1417.8357	16	A1	17	A2
175.924005	1.767E-28	4.000E-08	1417.0898	16	F2	17	F1
175.998720	5.825E-27	1.322E-06	1417.4900	16	F2	17	F1
176.066576	2.678E-26	6.090E-06	1417.7778	16	F1	17	F2
176.241514	5.250E-28	1.197E-07	1418.0701	16	F1	17	F2
176.241534	2.230E-28	5.086E-08	1418.1084	16	F2	17	F1
176.244095	1.913E-27	1.308E-06	1418.0897	16	E	17	E
176.268599	3.391E-27	7.719E-07	1417.7235	16	F2	17	F1
176.398858	2.574E-28	5.848E-08	1417.0898	16	F2	17	F1
176.424561	6.309E-27	4.309E-06	1417.4697	16	E	17	E
176.428283	3.786E-28	8.605E-08	1417.0993	16	F1	17	F2
176.485920	6.514E-30	4.431E-09	1416.5242	16	E	17	E
176.502089	4.720E-27	1.075E-06	1417.4900	16	F2	17	F1
176.533810	2.249E-27	5.133E-07	1417.7778	16	F1	17	F2
176.626445	6.441E-27	1.470E-06	1417.7235	16	F2	17	F1
176.745099	1.159E-27	2.641E-07	1417.0993	16	F1	17	F2
176.859936	6.766E-27	1.546E-06	1417.4900	16	F2	17	F1
176.864133	5.545E-27	3.800E-06	1417.4697	16	E	17	E
176.902227	7.643E-27	1.743E-06	1417.0898	16	F2	17	F1
177.003643	9.481E-29	2.158E-08	1416.5239	16	F1	17	F2
177.212333	2.656E-27	6.072E-07	1417.0993	16	F1	17	F2
177.226963	3.405E-27	4.658E-07	1416.5233	16	A1	17	A2
177.260073	1.108E-28	2.533E-08	1417.0898	16	F2	17	F1
177.320459	1.466E-27	3.346E-07	1416.5239	16	F1	17	F2
177.370013	8.869E-28	6.074E-07	1416.5242	16	E	17	E
177.787693	7.255E-29	1.661E-08	1416.5239	16	F1	17	F2

177.809585	5.861E-29	4.027E-08	1416.5242	16	E	17	E
183.815008	1.461E-29	7.866E-09	1594.3499	17	F1	18	F2
183.830928	1.705E-29	2.754E-08	1594.3338	17	E	18	E
184.172855	2.186E-29	1.178E-08	1593.9921	17	F1	18	F2
184.270500	2.593E-29	4.192E-08	1593.8942	17	E	18	E
184.634756	3.766E-28	2.040E-07	1594.3499	17	F1	18	F2
184.676224	1.628E-29	8.781E-09	1593.4887	17	F1	18	F2
184.678951	4.139E-29	2.242E-08	1594.3116	17	F2	18	F1
184.992602	6.378E-29	3.458E-08	1593.9921	17	F1	18	F2
185.143693	5.432E-26	1.760E-05	1593.0216	17	A1	18	A2
185.146185	1.111E-27	6.025E-07	1593.8444	17	F2	18	F1
185.151076	3.269E-26	1.766E-05	1593.0138	17	F1	18	F2
185.154593	2.183E-26	3.538E-05	1593.0101	17	E	18	E
185.277792	1.510E-27	2.466E-06	1594.3338	17	E	18	E
185.279887	1.482E-27	8.065E-07	1594.3116	17	F2	18	F1
185.463001	4.863E-26	2.640E-05	1593.5275	17	F2	18	F1
185.495971	5.122E-26	2.780E-05	1593.4887	17	F1	18	F2
185.594914	2.819E-28	1.538E-07	1594.3499	17	F1	18	F2
185.717364	3.538E-26	5.783E-05	1593.8942	17	E	18	E
185.747121	5.619E-26	3.061E-05	1593.8444	17	F2	18	F1
185.771636	4.018E-26	2.194E-05	1594.3116	17	F2	18	F1
185.807120	1.125E-25	3.678E-05	1593.7502	17	A2	18	A1
185.840659	1.959E-31	1.060E-10	1592.3243	17	F1	18	F2
185.896210	2.883E-26	4.728E-05	1594.3338	17	E	18	E
185.923053	4.581E-26	2.505E-05	1594.3499	17	F1	18	F2
185.952760	6.932E-26	3.785E-05	1593.9921	17	F1	18	F2
185.970824	5.373E-29	2.920E-08	1593.0138	17	F1	18	F2
186.063938	2.650E-27	1.445E-06	1593.5275	17	F2	18	F1
186.238870	5.005E-27	2.737E-06	1593.8444	17	F2	18	F1
186.280899	1.149E-27	6.289E-07	1593.9921	17	F1	18	F2
186.335782	6.869E-27	1.128E-05	1593.8942	17	E	18	E
186.341191	5.670E-28	3.110E-07	1594.3499	17	F1	18	F2
186.397847	5.592E-28	3.068E-07	1594.3116	17	F2	18	F1

186.456129	6.332E-28	3.462E-07	1593.4887	17	F1	18	F2
186.555687	1.426E-27	7.801E-07	1593.5275	17	F2	18	F1
186.601458	1.902E-28	3.115E-07	1593.0101	17	E	18	E
186.660406	8.433E-31	4.592E-10	1592.3243	17	F1	18	F2
186.665822	8.822E-31	4.804E-10	1592.3247	17	F2	18	F1
186.699037	1.153E-27	6.333E-07	1593.9921	17	F1	18	F2
186.784268	6.300E-27	3.453E-06	1593.4887	17	F1	18	F2
186.865081	3.182E-27	1.748E-06	1593.8444	17	F2	18	F1
186.930981	5.233E-28	2.865E-07	1593.0138	17	F1	18	F2
186.975180	1.379E-26	4.545E-06	1593.7502	17	A2	18	A1
187.181897	3.051E-27	1.677E-06	1593.5275	17	F2	18	F1
187.202406	2.629E-27	1.446E-06	1593.4887	17	F1	18	F2
187.219875	2.546E-27	4.190E-06	1593.0101	17	E	18	E
187.259121	2.340E-27	1.284E-06	1593.0138	17	F1	18	F2
187.266758	1.930E-29	1.056E-08	1592.3247	17	F2	18	F1
187.620564	9.053E-28	4.964E-07	1592.3243	17	F1	18	F2
187.647546	2.377E-27	7.849E-07	1593.0216	17	A1	18	A2
187.677258	3.632E-28	1.999E-07	1593.0138	17	F1	18	F2
187.758507	7.411E-28	4.068E-07	1592.3247	17	F2	18	F1
187.948703	1.315E-29	7.226E-09	1592.3243	17	F1	18	F2
188.366841	2.030E-29	1.119E-08	1592.3243	17	F1	18	F2
188.384718	1.763E-29	9.720E-09	1592.3247	17	F2	18	F1
193.286196	4.632E-30	6.276E-09	1780.7094	18	F1	19	F2
193.304298	5.468E-30	7.408E-09	1780.6911	18	F2	19	F1
193.722436	1.785E-29	2.421E-08	1780.2730	18	F2	19	F1
193.912407	2.498E-30	3.390E-09	1780.0832	18	F1	19	F2
194.050575	1.488E-30	2.019E-09	1779.9448	18	F2	19	F1
194.236642	3.278E-28	2.683E-07	1780.7254	18	A1	19	A2
194.257157	7.646E-29	1.043E-07	1780.7094	18	F1	19	F2
194.404156	5.176E-30	7.031E-09	1779.5915	18	F1	19	F2
194.738903	1.401E-28	5.742E-07	1780.2300	18	E	19	E
194.883368	2.427E-28	3.316E-07	1780.0832	18	F1	19	F2
194.987891	4.581E-28	6.282E-07	1780.6911	18	F2	19	F1

195.004011	4.775E-28	6.550E-07	1780.7094	18	F1	19	F2
195.005093	1.794E-26	2.440E-05	1778.9905	18	F1	19	F2
195.010733	1.798E-26	2.446E-05	1778.9847	18	F2	19	F1
195.357321	1.842E-26	7.558E-05	1779.6116	18	E	19	E
195.375117	2.789E-26	3.815E-05	1779.5915	18	F1	19	F2
195.404702	4.793E-26	3.934E-05	1779.5573	18	A1	19	A2
195.406029	3.143E-28	4.315E-07	1780.2730	18	F2	19	F1
195.505129	1.686E-27	2.321E-06	1780.6911	18	F2	19	F1
195.630222	3.046E-26	4.184E-05	1780.0832	18	F1	19	F2
195.683676	3.738E-26	3.091E-05	1780.6691	18	A2	19	A1
195.734169	3.493E-26	4.799E-05	1779.9448	18	F2	19	F1
195.830481	4.289E-32	5.846E-11	1778.1649	18	F2	19	F1
195.837932	2.180E-26	3.007E-05	1780.6911	18	F2	19	F1
195.895729	2.445E-26	3.375E-05	1780.7094	18	F1	19	F2
195.923266	3.349E-26	4.614E-05	1780.2730	18	F2	19	F1
195.923766	2.542E-26	1.050E-04	1780.2300	18	E	19	E
195.947083	4.317E-26	3.577E-05	1780.7254	18	A1	19	A2
195.976053	1.416E-29	1.940E-08	1778.9905	18	F1	19	F2
196.121971	5.781E-28	7.951E-07	1779.5915	18	F1	19	F2
196.251406	1.622E-27	2.236E-06	1779.9448	18	F2	19	F1
196.256069	5.616E-27	7.756E-06	1780.2730	18	F2	19	F1
196.426326	2.521E-28	3.493E-07	1780.7094	18	F1	19	F2
196.480105	1.843E-28	2.554E-07	1780.6911	18	F2	19	F1
196.521939	2.567E-27	3.548E-06	1780.0832	18	F1	19	F2
196.542184	8.747E-28	3.620E-06	1779.6116	18	E	19	E
196.584209	1.728E-27	2.388E-06	1779.9448	18	F2	19	F1
196.694326	2.045E-29	2.815E-08	1778.9847	18	F2	19	F1
196.722907	2.578E-29	3.551E-08	1778.9905	18	F1	19	F2
196.804185	4.066E-31	1.674E-09	1778.1647	18	E	19	E
196.898242	2.227E-28	3.089E-07	1780.2730	18	F2	19	F1
196.923846	9.716E-28	4.044E-06	1780.2300	18	E	19	E
197.013688	2.548E-27	3.527E-06	1779.5915	18	F1	19	F2
197.052537	2.549E-28	3.537E-07	1780.0832	18	F1	19	F2

197.115143	9.762E-27	8.111E-06	1779.5573	18	A1	19	A2
197.211564	3.820E-28	5.279E-07	1778.9847	18	F2	19	F1
197.226382	3.518E-27	4.885E-06	1779.9448	18	F2	19	F1
197.514074	5.030E-30	6.938E-09	1778.1649	18	F2	19	F1
197.542263	9.597E-28	4.000E-06	1779.6116	18	E	19	E
197.544286	1.058E-27	1.470E-06	1779.5915	18	F1	19	F2
197.544366	1.528E-27	2.117E-06	1778.9847	18	F2	19	F1
197.614625	9.952E-28	1.379E-06	1778.9905	18	F1	19	F2
197.989048	2.965E-28	1.231E-06	1778.1647	18	E	19	E
198.031311	3.870E-28	5.358E-07	1778.1649	18	F2	19	F1
198.145222	2.182E-28	3.035E-07	1778.9905	18	F1	19	F2
198.186539	1.189E-29	1.654E-08	1778.9847	18	F2	19	F1
198.187530	6.108E-28	5.079E-07	1778.1653	18	A2	19	A1
198.364114	2.769E-29	3.843E-08	1778.1649	18	F2	19	F1
198.989128	5.739E-30	2.400E-08	1778.1647	18	E	19	E
199.006287	5.080E-30	7.082E-09	1778.1649	18	F2	19	F1
202.610676	1.310E-30	1.406E-08	1977.1539	19	E	20	E
202.628684	1.511E-30	5.405E-09	1977.1358	19	F2	20	F1
203.091787	1.940E-29	4.169E-08	1976.6725	19	A2	20	A1
203.159281	4.415E-30	1.581E-08	1976.6052	19	F2	20	F1
203.610755	1.408E-30	1.515E-08	1976.1538	19	E	20	E
203.726651	4.119E-29	1.485E-07	1977.1712	19	F1	20	F2
203.765637	3.915E-30	1.412E-08	1977.1358	19	F2	20	F1
204.050999	1.203E-30	4.319E-09	1975.7135	19	F2	20	F1
204.296234	4.813E-29	1.738E-07	1976.6052	19	F2	20	F1
204.368825	5.087E-29	1.837E-07	1976.5290	19	F1	20	F2
204.596807	1.394E-28	5.056E-07	1977.1712	19	F1	20	F2
204.600667	1.560E-28	1.697E-06	1977.1539	19	E	20	E
204.701627	3.988E-29	1.441E-07	1976.1962	19	F1	20	F2
204.795618	6.148E-27	6.628E-05	1974.9689	19	E	20	E
204.797853	9.227E-27	3.316E-05	1974.9666	19	F2	20	F1
204.802228	1.540E-26	3.321E-05	1974.9620	19	A2	20	A1
205.175864	8.272E-29	3.013E-07	1977.1712	19	F1	20	F2



205.187952	1.446E-26	5.231E-05	1975.7135	19	F2	20	F1
205.218865	1.466E-26	5.302E-05	1975.6790	19	F1	20	F2
205.238980	8.709E-28	3.163E-06	1976.5290	19	F1	20	F2
205.294692	1.172E-27	4.270E-06	1977.1358	19	F2	20	F1
205.445347	2.649E-26	5.776E-05	1976.3528	19	A1	20	A2
205.571783	1.653E-26	6.009E-05	1976.1962	19	F1	20	F2
205.600747	1.211E-26	1.321E-04	1976.1538	19	E	20	E
205.726795	1.085E-26	3.966E-05	1977.1358	19	F2	20	F1
205.768813	8.769E-33	3.158E-11	1973.9956	19	F2	20	F1
205.784258	8.132E-27	8.922E-05	1977.1539	19	E	20	E
205.818037	1.794E-26	6.541E-05	1976.5290	19	F1	20	F2
205.825289	1.674E-26	6.108E-05	1976.6052	19	F2	20	F1
205.870065	1.284E-26	4.700E-05	1977.1712	19	F1	20	F2
205.934806	3.218E-30	1.166E-08	1974.9666	19	F2	20	F1
205.988252	3.554E-26	7.791E-05	1976.6725	19	A2	20	A1
206.089020	1.478E-28	5.380E-07	1975.6790	19	F1	20	F2
206.150840	2.259E-27	8.246E-06	1976.1962	19	F1	20	F2
206.257392	3.457E-27	1.265E-05	1976.6052	19	F2	20	F1
206.497363	1.515E-29	5.568E-08	1977.1712	19	F1	20	F2
206.499174	2.520E-29	9.261E-08	1977.1358	19	F2	20	F1
206.499406	1.145E-28	1.262E-06	1977.1539	19	E	20	E
206.512238	6.521E-28	2.390E-06	1976.5290	19	F1	20	F2
206.668077	1.525E-28	5.572E-07	1975.6790	19	F1	20	F2
206.717007	2.652E-28	9.693E-07	1975.7135	19	F2	20	F1
206.784337	1.420E-27	1.562E-05	1976.1538	19	E	20	E
206.785609	1.211E-29	1.324E-07	1974.9689	19	E	20	E
206.845040	7.898E-28	2.896E-06	1976.1962	19	F1	20	F2
206.902458	4.332E-32	1.572E-10	1973.9954	19	F1	20	F2
206.905766	4.420E-32	1.604E-10	1973.9956	19	F2	20	F1
207.029771	2.125E-28	7.817E-07	1976.6052	19	F2	20	F1
207.139536	5.651E-28	2.080E-06	1976.5290	19	F1	20	F2
207.149109	3.433E-28	1.259E-06	1975.7135	19	F2	20	F1
207.362278	2.147E-27	7.883E-06	1975.6790	19	F1	20	F2

207.463861	1.217E-28	4.454E-07	1974.9666	19	F2	20	F1
207.472339	1.259E-27	4.638E-06	1976.1962	19	F1	20	F2
207.499486	8.396E-28	9.276E-06	1976.1538	19	E	20	E
207.698693	1.662E-27	3.657E-06	1974.9620	19	A2	20	A1
207.772613	1.473E-30	5.380E-09	1973.9954	19	F1	20	F2
207.895963	5.858E-28	2.151E-06	1974.9666	19	F2	20	F1
207.921489	5.828E-28	2.148E-06	1975.7135	19	F2	20	F1
207.969200	3.649E-28	4.021E-06	1974.9689	19	E	20	E
207.989576	2.343E-29	8.636E-08	1975.6790	19	F1	20	F2
208.351671	2.026E-28	7.426E-07	1973.9954	19	F1	20	F2
208.434821	1.736E-28	6.366E-07	1973.9956	19	F2	20	F1
208.668343	3.196E-29	1.180E-07	1974.9666	19	F2	20	F1
208.684349	2.895E-29	3.206E-07	1974.9689	19	E	20	E
208.866924	1.400E-29	5.150E-08	1973.9956	19	F2	20	F1
209.045871	6.436E-31	2.370E-09	1973.9954	19	F1	20	F2
209.639303	2.447E-31	9.050E-10	1973.9956	19	F2	20	F1
209.673169	2.741E-30	1.014E-08	1973.9954	19	F1	20	F2
211.749132	3.759E-32	3.725E-10	2183.6686	20	F2	21	F1
211.782876	6.571E-31	6.512E-09	2183.6349	20	F1	21	F2
212.376430	2.881E-30	2.859E-08	2183.0413	20	F2	21	F1
212.555256	4.599E-31	4.564E-09	2182.8626	20	F1	21	F2
212.987358	3.668E-31	3.643E-09	2182.4305	20	F1	21	F2
213.064603	6.237E-30	6.236E-08	2183.6686	20	F2	21	F1
213.070630	2.552E-31	2.535E-09	2182.3471	20	F2	21	F1
213.078547	6.829E-30	2.048E-07	2183.6533	20	E	21	E
213.649688	2.406E-31	2.392E-09	2181.7680	20	F2	21	F1
213.691901	1.535E-29	1.537E-07	2183.0413	20	F2	21	F1
213.793696	1.968E-29	5.910E-07	2182.9381	20	E	21	E
214.076829	8.289E-29	8.344E-07	2183.6686	20	F2	21	F1
214.133111	8.735E-30	8.795E-08	2183.6349	20	F1	21	F2
214.386102	1.871E-29	1.875E-07	2182.3471	20	F2	21	F1
214.516413	4.440E-27	4.423E-05	2180.9014	20	F1	21	F2
214.519843	4.444E-27	4.427E-05	2180.8979	20	F2	21	F1

214.704127	2.110E-29	2.126E-07	2183.0413	20	F2	21	F1
214.870060	1.561E-28	1.579E-06	2183.6349	20	F1	21	F2
214.902662	2.089E-28	6.343E-06	2183.6533	20	E	21	E
214.905491	4.860E-28	4.900E-06	2182.8626	20	F1	21	F2
214.937743	1.173E-26	7.058E-05	2181.7981	20	A2	21	A1
214.965159	7.086E-27	7.109E-05	2181.7680	20	F2	21	F1
214.977287	4.755E-27	1.431E-04	2181.7545	20	E	21	E
215.247437	2.379E-29	2.413E-07	2183.6686	20	F2	21	F1
215.337593	7.870E-27	7.941E-05	2182.4305	20	F1	21	F2
215.398327	8.768E-27	8.848E-05	2182.3471	20	F2	21	F1
215.574814	5.603E-27	5.696E-05	2183.6349	20	F1	21	F2
215.617811	5.486E-27	1.668E-04	2182.9381	20	E	21	E
215.642439	8.306E-27	8.416E-05	2182.8626	20	F1	21	F2
215.653366	1.678E-33	1.675E-11	2179.7645	20	F1	21	F2
215.702635	3.832E-27	1.170E-04	2183.6533	20	E	21	E
215.746016	6.117E-27	6.226E-05	2183.6686	20	F2	21	F1
215.762239	1.800E-26	1.094E-04	2182.6607	20	A1	21	A2
215.835314	6.948E-31	6.982E-09	2180.8979	20	F2	21	F1
215.874735	1.013E-26	1.029E-04	2183.0413	20	F2	21	F1
215.977385	4.874E-29	4.924E-07	2181.7680	20	F2	21	F1
216.074542	1.060E-27	1.074E-05	2182.4305	20	F1	21	F2
216.347194	4.798E-28	4.884E-06	2182.8626	20	F1	21	F2
216.373314	1.043E-28	1.063E-06	2183.0413	20	F2	21	F1
216.417784	8.465E-28	2.587E-05	2182.9381	20	E	21	E
216.475888	2.550E-29	2.608E-07	2183.6686	20	F2	21	F1
216.525124	2.568E-29	2.627E-07	2183.6349	20	F1	21	F2
216.568935	1.481E-28	1.506E-06	2182.3471	20	F2	21	F1
216.779296	3.160E-28	3.220E-06	2182.4305	20	F1	21	F2
216.801402	1.110E-28	3.381E-06	2181.7545	20	E	21	E
216.847540	1.491E-30	1.508E-08	2180.8979	20	F2	21	F1
216.866648	1.679E-30	1.699E-08	2180.9014	20	F1	21	F2
216.967278	1.789E-32	5.403E-10	2179.7645	20	E	21	E
217.067515	1.075E-27	1.097E-05	2182.3471	20	F2	21	F1

217.103187	8.160E-29	8.355E-07	2183.0413	20	F2	21	F1
217.147993	1.802E-28	1.834E-06	2181.7680	20	F2	21	F1
217.297503	2.255E-28	2.311E-06	2182.8626	20	F1	21	F2
217.513678	1.531E-27	9.415E-06	2182.6607	20	A1	21	A2
217.601375	5.759E-28	1.764E-05	2181.7545	20	E	21	E
217.603597	1.908E-29	1.939E-07	2180.9014	20	F1	21	F2
217.646572	5.338E-28	5.451E-06	2181.7680	20	F2	21	F1
217.729606	4.875E-28	4.997E-06	2182.4305	20	F1	21	F2
217.797387	3.515E-28	3.604E-06	2182.3471	20	F2	21	F1
218.003601	3.339E-31	3.385E-09	2179.7645	20	F1	21	F2
218.018148	3.530E-28	3.599E-06	2180.8979	20	F2	21	F1
218.308351	2.497E-28	2.550E-06	2180.9014	20	F1	21	F2
218.329100	4.448E-28	2.739E-06	2181.7981	20	A2	21	A1
218.376444	6.813E-29	6.992E-07	2181.7680	20	F2	21	F1
218.516727	6.361E-30	6.506E-08	2180.8979	20	F2	21	F1
218.658705	1.529E-28	9.343E-07	2179.7643	20	A1	21	A2
218.740550	8.377E-29	8.534E-07	2179.7645	20	F1	21	F2
218.791393	5.441E-29	1.664E-06	2179.7645	20	E	21	E
219.246600	8.065E-30	8.289E-08	2180.8979	20	F2	21	F1
219.258661	7.530E-30	7.740E-08	2180.9014	20	F1	21	F2
219.445304	2.195E-30	2.246E-08	2179.7645	20	F1	21	F2
219.591366	1.312E-30	4.032E-08	2179.7645	20	E	21	E
220.395614	4.085E-31	4.207E-09	2179.7645	20	F1	21	F2
220.410143	1.883E-30	1.164E-08	2179.7643	20	A1	21	A2
220.754968	7.328E-32	2.110E-09	2400.1444	21	F1	22	F2
220.772275	4.067E-31	7.026E-09	2400.1272	21	A1	22	A2
221.484840	5.147E-31	1.484E-08	2399.4146	21	F1	22	F2
221.543464	6.169E-31	5.336E-08	2399.3559	21	E	22	E
221.983420	2.143E-31	6.182E-09	2398.9160	21	F1	22	F2
222.252620	1.640E-30	4.769E-08	2400.1601	21	F2	22	F1
222.266211	1.787E-30	5.196E-08	2400.1444	21	F1	22	F2
222.343437	1.323E-31	1.146E-08	2398.5559	21	E	22	E
222.996083	1.023E-29	2.977E-07	2399.4146	21	F1	22	F2

223.154028	5.201E-32	1.503E-09	2397.7454	21	F1	22	F2
223.202929	1.436E-30	4.181E-08	2399.2098	21	F2	22	F1
223.412940	6.151E-29	1.081E-06	2400.1744	21	A2	22	A1
223.445459	1.426E-29	4.177E-07	2400.1601	21	F2	22	F1
223.494663	9.473E-31	2.760E-08	2398.9160	21	F1	22	F2
223.907684	6.082E-30	1.773E-07	2398.5050	21	F2	22	F1
224.163632	3.344E-27	5.810E-05	2396.7359	21	A1	22	A2
224.166254	2.008E-27	5.813E-05	2396.7332	21	F1	22	F2
224.167552	1.339E-27	1.163E-04	2396.7318	21	E	22	E
224.259197	4.756E-29	4.187E-06	2399.3559	21	E	22	E
224.310369	4.499E-29	1.326E-06	2400.1444	21	F1	22	F2
224.389709	5.614E-29	1.655E-06	2400.1601	21	F2	22	F1
224.395769	7.498E-29	2.200E-06	2399.2098	21	F2	22	F1
224.644632	3.227E-27	9.420E-05	2397.7681	21	F2	22	F1
224.665271	3.251E-27	9.491E-05	2397.7454	21	F1	22	F2
224.962188	1.056E-28	3.125E-06	2400.1444	21	F1	22	F2
225.040241	3.956E-29	1.167E-06	2399.4146	21	F1	22	F2
225.059170	2.533E-27	2.232E-04	2398.5559	21	E	22	E
225.100524	3.872E-27	1.138E-04	2398.5050	21	F2	22	F1
225.164379	6.873E-27	1.212E-04	2398.4230	21	A2	22	A1
225.323325	4.273E-27	7.604E-05	2400.1272	21	A1	22	A2
225.340019	3.764E-27	1.111E-04	2399.2098	21	F2	22	F1
225.465785	2.516E-27	7.469E-05	2400.1444	21	F1	22	F2
225.481725	3.025E-34	8.777E-12	2395.4177	21	F1	22	F2
225.538820	4.654E-27	1.374E-04	2398.9160	21	F1	22	F2
225.540637	2.685E-27	7.974E-05	2400.1601	21	F2	22	F1
225.600661	4.672E-27	8.330E-05	2400.1744	21	A2	22	A1
225.677497	1.439E-31	4.208E-09	2396.7332	21	F1	22	F2
225.678687	3.002E-27	2.667E-04	2399.3559	21	E	22	E
225.692060	4.253E-27	1.260E-04	2399.4146	21	F1	22	F2
225.837472	1.256E-29	3.694E-07	2397.7681	21	F2	22	F1
226.044773	1.715E-28	5.068E-06	2398.5050	21	F2	22	F1
226.190639	1.639E-28	4.859E-06	2398.9160	21	F1	22	F2

226.195658	3.794E-28	1.127E-05	2399.4146	21	F1	22	F2
226.433280	8.468E-30	2.530E-07	2400.1601	21	F2	22	F1
226.477783	7.184E-30	2.146E-07	2400.1444	21	F1	22	F2
226.478660	2.171E-28	1.931E-05	2398.5559	21	E	22	E
226.490947	2.365E-28	7.035E-06	2399.2098	21	F2	22	F1
226.694237	2.039E-28	6.065E-06	2398.9160	21	F1	22	F2
226.709428	9.335E-30	2.761E-07	2397.7454	21	F1	22	F2
226.781722	1.424E-29	4.215E-07	2397.7681	21	F2	22	F1
226.883286	6.936E-31	6.131E-08	2396.7318	21	E	22	E
226.992968	1.719E-33	5.035E-11	2395.4177	21	F1	22	F2
226.994867	1.734E-33	5.080E-11	2395.4178	21	F2	22	F1
227.195702	3.889E-28	1.158E-05	2398.5050	21	F2	22	F1
227.207656	1.073E-29	3.209E-07	2399.4146	21	F1	22	F2
227.252087	5.665E-29	5.083E-06	2399.3559	21	E	22	E
227.352099	1.381E-27	2.469E-05	2398.4230	21	A2	22	A1
227.361248	1.409E-28	4.186E-06	2397.7454	21	F1	22	F2
227.383590	1.370E-29	4.098E-07	2399.2098	21	F2	22	F1
227.706235	3.291E-28	9.851E-06	2398.9160	21	F1	22	F2
227.721654	4.792E-30	1.419E-07	2396.7332	21	F1	22	F2
227.864845	2.563E-28	7.635E-06	2397.7454	21	F1	22	F2
227.932650	1.891E-28	5.638E-06	2397.7681	21	F2	22	F1
228.052060	1.210E-28	1.087E-05	2398.5559	21	E	22	E
228.088344	1.250E-28	3.744E-06	2398.5050	21	F2	22	F1
228.187707	6.259E-32	1.848E-09	2395.4178	21	F2	22	F1
228.302776	9.621E-29	8.582E-06	2396.7318	21	E	22	E
228.373473	1.124E-28	3.343E-06	2396.7332	21	F1	22	F2
228.714682	1.736E-28	3.106E-06	2396.7359	21	A1	22	A2
228.825293	3.548E-29	1.064E-06	2397.7681	21	F2	22	F1
228.876843	2.139E-30	6.414E-08	2397.7454	21	F1	22	F2
228.877071	1.466E-29	4.375E-07	2396.7332	21	F1	22	F2
229.037125	3.595E-29	1.067E-06	2395.4177	21	F1	22	F2
229.131957	3.456E-29	1.026E-06	2395.4178	21	F2	22	F1
229.529200	1.865E-33	1.635E-10	2626.6222	22	F2	23	F1

229.558150	3.008E-32	2.638E-09	2626.5933	22	F1	23	F2
229.688944	2.593E-31	7.729E-09	2395.4177	21	F1	22	F2
229.876176	1.995E-30	1.798E-07	2396.7318	21	E	22	E
229.889069	1.864E-30	5.597E-08	2396.7332	21	F1	22	F2
230.192542	4.188E-31	1.252E-08	2395.4177	21	F1	22	F2
230.282885	3.489E-31	1.044E-08	2395.4178	21	F2	22	F1
230.450792	1.458E-31	1.280E-08	2625.7007	22	F1	23	F2
230.541199	2.183E-31	1.917E-08	2625.6102	22	F2	23	F1
231.044796	1.305E-31	1.147E-08	2625.1066	22	F2	23	F1
231.175528	1.499E-32	4.509E-10	2395.4178	21	F2	22	F1
231.204540	1.795E-31	5.402E-09	2395.4177	21	F1	22	F2
231.270326	3.889E-31	1.035E-07	2626.6080	22	E	23	E
231.284215	4.197E-31	3.722E-08	2626.5933	22	F1	23	F2
231.601720	1.165E-32	1.025E-09	2624.5498	22	F1	23	F2
231.696615	8.453E-33	7.437E-10	2624.4548	22	F2	23	F1
232.100972	8.427E-30	4.488E-07	2625.7751	22	A1	23	A2
232.176858	2.012E-30	1.786E-07	2625.7007	22	F1	23	F2
232.545970	1.069E-32	9.417E-10	2623.6055	22	F1	23	F2
232.628395	6.552E-30	5.860E-07	2626.6222	22	F2	23	F1
232.672506	5.571E-31	4.983E-08	2626.5933	22	F1	23	F2
232.843726	9.948E-31	2.652E-07	2625.0346	22	E	23	E
233.327786	1.231E-30	1.095E-07	2624.5498	22	F1	23	F2
233.565149	1.308E-29	1.172E-06	2625.7007	22	F1	23	F2
233.640393	1.495E-29	1.339E-06	2625.6102	22	F2	23	F1
233.667545	1.457E-29	3.935E-06	2626.6080	22	E	23	E
233.689075	1.332E-29	1.199E-06	2626.6222	22	F2	23	F1
233.738810	8.530E-28	7.527E-05	2622.4127	22	F1	23	F2
233.740773	8.533E-28	7.529E-05	2622.4107	22	F2	23	F1
234.143991	9.447E-30	8.467E-07	2625.1066	22	F2	23	F1
234.263216	9.245E-28	2.470E-04	2623.6151	22	E	23	E
234.272036	1.389E-27	1.237E-04	2623.6055	22	F1	23	F2
234.288693	2.327E-27	1.243E-04	2623.5874	22	A1	23	A2
234.370993	7.109E-30	6.427E-07	2626.6222	22	F2	23	F1

234.539501	5.674E-29	5.135E-06	2626.5933	22	F1	23	F2
234.701074	1.373E-28	1.238E-05	2625.6102	22	F2	23	F1
234.716077	1.665E-27	1.494E-04	2624.5498	22	F1	23	F2
234.795810	1.715E-27	1.538E-04	2624.4548	22	F2	23	F1
234.949952	2.712E-27	1.468E-04	2625.4506	22	A2	23	A1
235.172791	1.057E-27	9.600E-05	2626.5933	22	F1	23	F2
235.204671	1.735E-27	1.566E-04	2625.1066	22	F2	23	F1
235.240945	1.329E-27	3.596E-04	2625.0346	22	E	23	E
235.249344	7.478E-28	2.039E-04	2626.6080	22	E	23	E
235.252016	5.150E-35	4.554E-12	2620.8994	22	F2	23	F1
235.336466	1.154E-27	1.050E-04	2626.6222	22	F2	23	F1
235.382991	1.688E-27	1.529E-04	2625.6102	22	F2	23	F1
235.432144	1.787E-27	1.619E-04	2625.7007	22	F1	23	F2
235.464876	2.759E-32	2.461E-09	2622.4127	22	F1	23	F2
235.585106	3.417E-27	1.860E-04	2625.7751	22	A1	23	A2
235.660327	2.482E-30	2.229E-07	2623.6055	22	F1	23	F2
235.856490	3.850E-29	3.477E-06	2624.4548	22	F2	23	F1
235.886589	3.354E-28	3.039E-05	2625.1066	22	F2	23	F1
236.065434	1.761E-28	1.602E-05	2625.7007	22	F1	23	F2
236.348464	5.380E-29	4.901E-06	2625.6102	22	F2	23	F1
236.364043	4.835E-31	4.427E-08	2626.6222	22	F2	23	F1
236.365724	3.317E-30	9.110E-07	2626.6080	22	E	23	E
236.366543	6.412E-31	5.869E-08	2626.5933	22	F1	23	F2
236.538408	3.435E-29	3.115E-06	2624.4548	22	F2	23	F1
236.583072	6.378E-29	5.788E-06	2624.5498	22	F1	23	F2
236.660435	5.920E-30	1.605E-06	2623.6151	22	E	23	E
236.822744	1.338E-28	3.657E-05	2625.0346	22	E	23	E
236.839968	6.562E-32	5.903E-09	2622.4107	22	F2	23	F1
236.852062	5.487E-29	5.002E-06	2625.1066	22	F2	23	F1
236.853167	6.970E-32	6.271E-09	2622.4127	22	F1	23	F2
236.978949	6.214E-34	1.666E-10	2620.8994	22	E	23	E
237.216362	3.655E-29	3.330E-06	2624.5498	22	F1	23	F2
237.259185	9.719E-30	8.907E-07	2625.7007	22	F1	23	F2



237.376041	2.166E-29	1.985E-06	2625.6102	22	F2	23	F1
237.503881	2.656E-28	2.423E-05	2624.4548	22	F2	23	F1
237.527322	4.110E-29	3.735E-06	2623.6055	22	F1	23	F2
237.772826	3.009E-28	1.643E-05	2623.5874	22	A1	23	A2
237.879639	1.122E-28	1.029E-05	2625.1066	22	F2	23	F1
237.900648	1.580E-30	1.430E-07	2622.4107	22	F2	23	F1
237.939124	6.541E-29	1.800E-05	2625.0346	22	E	23	E
238.140338	3.033E-33	2.548E-09	2862.9737	23	E	24	E
238.154146	3.232E-33	9.051E-10	2862.9599	23	F2	24	F1
238.160612	8.082E-29	7.373E-06	2623.6055	22	F1	23	F2
238.242234	5.560E-29	1.523E-05	2623.6151	22	E	23	E
238.351211	1.201E-32	1.082E-09	2620.8994	22	F2	23	F1
238.410113	6.035E-29	5.539E-06	2624.5498	22	F1	23	F2
238.531458	1.929E-30	1.771E-07	2624.4548	22	F2	23	F1
238.582566	5.380E-29	4.892E-06	2622.4107	22	F2	23	F1
238.720161	4.088E-29	3.721E-06	2622.4127	22	F1	23	F2
239.256719	3.688E-32	3.103E-08	2861.8573	23	E	24	E
239.347897	5.453E-32	1.530E-08	2861.7661	23	F2	24	F1
239.353452	6.816E-30	6.227E-07	2622.4127	22	F1	23	F2
239.354363	4.396E-30	4.040E-07	2623.6055	22	F1	23	F2
239.358614	4.389E-30	1.210E-06	2623.6151	22	E	23	E
239.376168	9.395E-30	2.557E-06	2620.8994	22	E	23	E
239.411891	1.376E-29	1.249E-06	2620.8994	22	F2	23	F1
239.501002	2.256E-29	1.229E-06	2620.8995	22	A2	23	A1
239.548038	2.946E-31	2.694E-08	2622.4107	22	F2	23	F1
239.753806	2.203E-31	3.709E-08	2861.3602	23	A2	24	A1
239.981188	2.926E-32	8.215E-09	2861.1328	23	F2	24	F1
240.084473	1.028E-32	2.914E-09	2862.9863	23	F1	24	F2
240.093809	1.605E-31	1.462E-08	2620.8994	22	F2	23	F1
240.111984	1.628E-31	4.614E-08	2862.9599	23	F2	24	F1
240.547203	6.917E-32	6.366E-09	2622.4127	22	F1	23	F2
240.575616	8.445E-31	7.774E-08	2622.4107	22	F2	23	F1
240.838518	4.210E-33	3.549E-09	2860.2755	23	E	24	E

240.957967	1.121E-31	3.080E-08	2620.8994	22	E	23	E
241.059281	8.781E-32	8.047E-09	2620.8994	22	F2	23	F1
241.112050	1.006E-30	2.855E-07	2861.9587	23	F1	24	F2
241.305735	1.434E-31	4.072E-08	2861.7661	23	F2	24	F1
241.668916	8.570E-31	2.453E-07	2862.9863	23	F1	24	F2
241.675562	8.813E-31	7.567E-07	2862.9737	23	E	24	E
241.848183	1.920E-33	5.402E-10	2859.2659	23	F2	24	F1
241.939026	2.666E-31	7.576E-08	2861.1328	23	F2	24	F1
242.074348	2.305E-32	6.377E-09	2620.8994	22	E	23	E
242.077523	1.964E-31	5.581E-08	2860.9932	23	F1	24	F2
242.086858	2.177E-32	2.008E-09	2620.8994	22	F2	23	F1
242.696493	3.372E-30	9.662E-07	2861.9587	23	F1	24	F2
242.759440	2.060E-31	5.859E-08	2860.3113	23	F1	24	F2
242.791943	4.293E-30	3.691E-06	2861.8573	23	E	24	E
242.869391	7.028E-30	2.026E-06	2862.9863	23	F1	24	F2
242.959117	8.078E-31	2.330E-07	2862.9599	23	F2	24	F1
243.235737	2.276E-28	1.925E-04	2857.8783	23	E	24	E
243.236473	3.414E-28	9.624E-05	2857.8776	23	F2	24	F1
243.237940	5.692E-28	9.626E-05	2857.8761	23	A2	24	A1
243.661966	6.470E-30	1.856E-06	2860.9932	23	F1	24	F2
243.806020	5.600E-28	1.595E-04	2859.2659	23	F2	24	F1
243.820121	5.614E-28	1.599E-04	2859.2506	23	F1	24	F2
243.826038	6.860E-30	1.989E-06	2862.9599	23	F2	24	F1
243.896968	2.927E-30	8.450E-07	2861.9587	23	F1	24	F2
243.913701	1.168E-29	1.017E-05	2862.9737	23	E	24	E
244.152868	7.135E-29	2.061E-05	2861.7661	23	F2	24	F1
244.263786	1.022E-30	2.973E-07	2862.9863	23	F1	24	F2
244.266836	1.127E-27	1.942E-04	2860.4005	23	A1	24	A2
244.343884	6.844E-28	1.965E-04	2860.3113	23	F1	24	F2
244.373742	4.647E-28	4.003E-04	2860.2755	23	E	24	E
244.786159	6.723E-28	1.943E-04	2861.1328	23	F2	24	F1
244.851576	4.369E-28	1.275E-04	2862.9599	23	F2	24	F1
244.862441	7.872E-28	2.275E-04	2860.9932	23	F1	24	F2

244.962539	8.289E-36	2.341E-12	2856.1515	23	F2	24	F1
244.968534	2.928E-28	2.564E-04	2862.9737	23	E	24	E
245.019789	6.487E-28	1.884E-04	2861.7661	23	F2	24	F1
245.025480	4.587E-28	1.340E-04	2862.9863	23	F1	24	F2
245.030081	4.651E-28	4.053E-04	2861.8573	23	E	24	E
245.194311	4.897E-33	1.397E-09	2857.8776	23	F2	24	F1
245.257983	1.558E-27	2.712E-04	2861.3602	23	A2	24	A1
245.291363	8.053E-28	2.344E-04	2861.9587	23	F1	24	F2
245.404564	4.886E-31	1.405E-07	2859.2506	23	F1	24	F2
245.544358	1.550E-29	4.482E-06	2860.3113	23	F1	24	F2
245.653080	1.516E-28	4.405E-05	2861.1328	23	F2	24	F1
246.045327	1.789E-29	5.227E-06	2861.7661	23	F2	24	F1
246.053057	4.938E-30	1.444E-06	2861.9587	23	F1	24	F2
246.084915	4.404E-29	3.863E-05	2861.8573	23	E	24	E
246.207685	5.848E-31	1.721E-07	2862.9863	23	F1	24	F2
246.245972	5.907E-31	1.738E-07	2862.9599	23	F2	24	F1
246.256836	1.725E-29	5.027E-06	2860.9932	23	F1	24	F2
246.519601	5.734E-34	5.374E-10	3109.2059	24	F1	25	F2
246.531469	6.016E-34	5.639E-10	3109.1940	24	F2	25	F1
246.605039	6.933E-31	2.008E-07	2859.2506	23	F1	24	F2
246.611880	2.322E-29	2.027E-05	2860.2755	23	E	24	E
246.653154	8.845E-31	2.562E-07	2859.2659	23	F2	24	F1
246.678618	2.625E-29	7.673E-06	2861.1328	23	F2	24	F1
246.770961	2.583E-32	2.231E-08	2857.8783	23	E	24	E
246.919316	5.239E-35	1.497E-11	2856.1514	23	F1	24	F2
246.920377	5.260E-35	1.503E-11	2856.1515	23	F2	24	F1
246.938754	2.478E-29	7.227E-06	2860.3113	23	F1	24	F2
247.018529	7.943E-29	2.325E-05	2860.9932	23	F1	24	F2
247.235263	2.896E-30	8.530E-07	2861.9587	23	F1	24	F2
247.439723	6.797E-30	2.003E-06	2861.7661	23	F2	24	F1
247.520074	5.094E-30	1.483E-06	2859.2659	23	F2	24	F1
247.666714	5.681E-29	4.992E-05	2860.2755	23	E	24	E
247.700447	5.839E-29	1.711E-05	2860.3113	23	F1	24	F2

247.713675	6.165E-34	5.785E-10	3108.0118	24	F2	25	F1
247.857029	9.170E-29	1.622E-05	2861.3602	23	A2	24	A1
247.913996	1.716E-32	1.611E-08	3107.8115	24	F1	25	F2
247.999434	5.255E-29	1.535E-05	2859.2506	23	F1	24	F2
248.041444	3.408E-31	9.888E-08	2857.8776	23	F2	24	F1
248.073013	3.741E-29	1.103E-05	2861.1328	23	F2	24	F1
248.200735	2.561E-29	7.551E-06	2860.9932	23	F1	24	F2
248.475368	3.073E-32	2.887E-08	3107.2501	24	F2	25	F1
248.503759	2.281E-33	6.581E-10	2856.1514	23	F1	24	F2
248.545612	3.063E-29	8.974E-06	2859.2659	23	F2	24	F1
248.737552	1.658E-32	1.574E-08	3109.1940	24	F2	25	F1
248.742117	3.572E-29	6.245E-06	2857.8761	23	A2	24	A1
248.750902	8.758E-32	4.990E-08	3109.1814	24	A2	25	A1
248.761127	1.003E-30	2.944E-07	2859.2506	23	F1	24	F2
248.780933	3.932E-29	6.961E-06	2860.4005	23	A1	24	A2
248.882653	5.315E-30	1.568E-06	2860.3113	23	F1	24	F2
248.908365	1.802E-29	5.254E-06	2857.8776	23	F2	24	F1
248.939534	3.029E-33	2.847E-09	3106.7859	24	F1	25	F2
249.009099	1.145E-29	1.003E-05	2857.8783	23	E	24	E
249.704233	5.205E-30	1.513E-06	2856.1514	23	F1	24	F2
249.767510	5.070E-30	1.474E-06	2856.1515	23	F2	24	F1
249.806455	5.381E-34	5.062E-10	3105.9190	24	F1	25	F2
249.869764	4.447E-34	4.183E-10	3105.8557	24	F2	25	F1
249.919758	1.414E-31	1.344E-07	3108.0118	24	F2	25	F1
249.933903	8.359E-31	2.453E-07	2857.8776	23	F2	24	F1
249.940008	9.926E-31	2.932E-07	2859.2659	23	F2	24	F1
249.943333	9.888E-31	2.921E-07	2859.2506	23	F1	24	F2
249.988844	1.706E-31	4.868E-07	3107.9423	24	E	25	E
250.063933	5.714E-31	5.034E-07	2857.8783	23	E	24	E
250.534464	1.907E-31	1.831E-07	3109.2059	24	F1	25	F2
250.537066	1.954E-31	1.875E-07	3109.1940	24	F2	25	F1
250.634431	5.047E-32	1.475E-08	2856.1515	23	F2	24	F1
250.681451	9.538E-32	9.077E-08	3107.2501	24	F2	25	F1

251.043678	8.532E-32	2.437E-07	3106.8874	24	E	25	E
251.070238	3.174E-34	2.989E-10	3104.6552	24	F2	25	F1
251.098629	4.797E-33	1.405E-09	2856.1514	23	F1	24	F2
251.328299	1.051E-31	3.109E-08	2857.8776	23	F2	24	F1
251.341163	4.993E-31	8.864E-08	2857.8761	23	A2	24	A1
251.659969	5.610E-33	1.649E-09	2856.1515	23	F2	24	F1
251.719272	1.818E-30	1.747E-06	3108.0118	24	F2	25	F1
251.860322	4.543E-32	1.337E-08	2856.1514	23	F1	24	F2
251.889895	4.589E-30	2.665E-06	3109.2172	24	A1	25	A2
251.928859	2.342E-31	2.251E-07	3107.8115	24	F1	25	F2
251.954102	1.094E-30	1.059E-06	3109.2059	24	F1	25	F2
252.075847	4.516E-32	4.304E-08	3105.8557	24	F2	25	F1
252.480965	1.973E-31	1.898E-07	3107.2501	24	F2	25	F1
252.653588	1.288E-28	1.216E-04	3103.0719	24	F1	25	F2
252.654682	1.288E-28	1.216E-04	3103.0707	24	F2	25	F1
252.926404	1.890E-30	1.840E-06	3109.1940	24	F2	25	F1
252.954397	2.134E-30	2.054E-06	3106.7859	24	F1	25	F2
253.042528	4.895E-33	1.451E-09	2856.1514	23	F1	24	F2
253.054364	4.659E-33	1.381E-09	2856.1515	23	F2	24	F1
253.132604	2.702E-30	2.634E-06	3109.2059	24	F1	25	F2
253.247072	6.305E-30	1.834E-05	3107.9423	24	E	25	E
253.264999	3.546E-28	2.030E-04	3104.6673	24	A2	25	A1
253.276321	2.131E-28	2.034E-04	3104.6552	24	F2	25	F1
253.281816	1.422E-28	4.071E-04	3104.6493	24	E	25	E
253.348498	8.032E-30	7.787E-06	3107.8115	24	F1	25	F2
253.747357	3.107E-30	3.040E-06	3109.1940	24	F2	25	F1
253.821318	2.607E-28	2.512E-04	3105.9190	24	F1	25	F2
253.875361	2.661E-28	2.563E-04	3105.8557	24	F2	25	F1
254.108610	2.272E-30	2.215E-06	3108.0118	24	F2	25	F1
254.301905	1.847E-28	5.379E-04	3106.8874	24	E	25	E
254.374036	2.863E-28	2.778E-04	3106.7859	24	F1	25	F2
254.422248	2.760E-28	1.626E-04	3109.1814	24	A2	25	A1
254.488941	5.289E-28	3.079E-04	3106.6182	24	A1	25	A2

254.526999	2.565E-28	2.504E-04	3107.8115	24	F1	25	F2
254.541125	1.644E-28	1.615E-04	3109.1940	24	F2	25	F1
254.611426	1.264E-36	1.195E-12	3101.1140	24	F1	25	F2
254.621039	1.692E-28	1.664E-04	3109.2059	24	F1	25	F2
254.674145	1.035E-34	3.402E-10	3365.2481	25	F1	26	F2
254.684697	1.076E-34	1.061E-09	3365.2375	25	E	26	E
254.685562	2.898E-28	1.711E-04	3109.2172	24	A1	25	A2
254.860764	8.210E-34	7.848E-10	3103.0707	24	F2	25	F1
254.870303	3.414E-28	3.330E-04	3107.2501	24	F2	25	F1
254.893007	1.939E-28	5.696E-04	3107.9423	24	E	25	E
254.929563	2.924E-28	2.864E-04	3108.0118	24	F2	25	F1
255.075836	9.796E-32	9.448E-08	3104.6552	24	F2	25	F1
255.240957	4.028E-30	3.912E-06	3105.9190	24	F1	25	F2
255.552537	1.862E-29	1.819E-05	3106.7859	24	F1	25	F2
255.691256	7.992E-30	7.833E-06	3107.2501	24	F2	25	F1
255.723331	1.179E-29	1.161E-05	3108.0118	24	F2	25	F1
255.947841	2.337E-29	6.869E-05	3106.8874	24	E	25	E
256.015434	9.213E-30	9.073E-06	3107.8115	24	F1	25	F2
256.020947	1.509E-31	1.497E-07	3109.2059	24	F1	25	F2
256.054148	1.389E-31	1.378E-07	3109.1940	24	F2	25	F1
256.187169	1.083E-33	3.564E-09	3363.7351	25	F1	26	F2
256.264699	1.567E-30	1.531E-06	3105.8557	24	F2	25	F1
256.318587	8.617E-33	1.702E-08	3363.6037	25	A1	26	A2
256.419458	2.942E-30	2.877E-06	3105.9190	24	F1	25	F2
256.485024	1.062E-29	1.046E-05	3107.2501	24	F2	25	F1
256.540044	3.165E-31	9.236E-07	3104.6493	24	E	25	E
256.660279	2.326E-33	2.247E-09	3103.0707	24	F2	25	F1
256.668451	2.396E-33	2.314E-09	3103.0719	24	F1	25	F2
256.817040	1.681E-35	4.829E-11	3101.1141	24	E	25	E
256.980937	6.009E-33	1.979E-08	3362.9413	25	F1	26	F2
257.040973	2.527E-29	2.491E-05	3106.7859	24	F1	25	F2
257.085652	1.949E-29	1.913E-05	3105.8557	24	F2	25	F1
257.086982	5.887E-33	5.817E-08	3362.8353	25	E	26	E

257.146543	3.905E-34	1.302E-09	3365.2481	25	F1	26	F2
257.168454	5.887E-33	1.963E-08	3365.2268	25	F2	26	F1
257.236354	2.675E-31	2.655E-07	3108.0118	24	F2	25	F1
257.284608	9.454E-29	5.595E-05	3106.6182	24	A1	25	A2
257.295293	1.591E-30	4.739E-06	3107.9423	24	E	25	E
257.415342	3.436E-31	3.412E-07	3107.8115	24	F1	25	F2
257.465173	1.277E-30	1.249E-06	3104.6552	24	F2	25	F1
257.801890	6.571E-34	2.166E-09	3362.1204	25	F1	26	F2
257.879419	1.935E-29	1.908E-05	3105.8557	24	F2	25	F1
257.907893	1.752E-29	1.728E-05	3105.9190	24	F1	25	F2
257.998047	1.687E-29	1.676E-05	3107.2501	24	F2	25	F1
258.088090	5.315E-32	5.177E-08	3103.0719	24	F1	25	F2
258.185980	1.195E-29	3.522E-05	3104.6493	24	E	25	E
258.286126	1.248E-29	1.227E-05	3104.6552	24	F2	25	F1
258.350126	7.789E-30	2.322E-05	3106.8874	24	E	25	E
258.440880	8.067E-30	8.018E-06	3106.7859	24	F1	25	F2
258.568361	3.328E-32	1.111E-07	3363.8269	25	F2	26	F1
258.626289	3.894E-34	3.769E-10	3101.1140	24	F1	25	F2
258.659566	4.469E-32	1.492E-07	3363.7351	25	F1	26	F2
258.732918	1.662E-34	1.645E-09	3361.1893	25	E	26	E
258.936344	1.829E-29	1.083E-05	3104.6673	24	A2	25	A1
259.049616	6.798E-30	6.659E-06	3103.0707	24	F2	25	F1
259.079894	2.204E-30	2.176E-06	3104.6552	24	F2	25	F1
259.202698	3.835E-32	3.881E-07	3365.2375	25	E	26	E
259.209797	3.978E-32	1.342E-07	3365.2268	25	F2	26	F1
259.266591	6.248E-30	6.128E-06	3103.0719	24	F1	25	F2
259.307801	2.428E-30	2.415E-06	3105.9190	24	F1	25	F2
259.392443	1.596E-31	1.588E-07	3105.8557	24	F2	25	F1
259.453334	5.436E-32	1.816E-07	3362.9413	25	F1	26	F2
259.870570	8.175E-32	8.045E-08	3103.0707	24	F2	25	F1
259.993118	3.060E-30	1.791E-06	3101.1140	24	A1	25	A2
260.045927	1.804E-30	1.761E-06	3101.1140	24	F1	25	F2
260.056797	6.224E-33	2.081E-08	3362.3385	25	F2	26	F1

260.075268	1.197E-30	3.504E-06	3101.1141	24	E	25	E
260.191227	5.116E-35	1.690E-10	3359.7310	25	F1	26	F2
260.274287	4.017E-33	1.343E-08	3362.1204	25	F1	26	F2
260.526645	1.193E-30	2.418E-06	3363.9028	25	A2	26	A1
260.588265	2.181E-31	6.516E-07	3104.6493	24	E	25	E
260.592918	2.112E-31	2.104E-07	3104.6552	24	F2	25	F1
260.609704	2.864E-31	9.675E-07	3363.8269	25	F2	26	F1
260.664337	1.518E-31	1.501E-07	3103.0707	24	F2	25	F1
260.755027	1.252E-31	1.239E-07	3103.0719	24	F1	25	F2
260.799177	4.369E-31	1.488E-06	3365.2481	25	F1	26	F2
260.869067	3.492E-32	1.189E-07	3365.2268	25	F2	26	F1
261.224429	8.235E-33	8.090E-09	3101.1140	24	F1	25	F2
261.235298	9.185E-33	3.074E-08	3361.1600	25	F2	26	F1
261.604983	2.285E-31	2.318E-06	3362.8353	25	E	26	E
261.721204	5.304E-33	1.568E-08	3101.1141	24	E	25	E
261.989779	5.985E-31	6.156E-06	3365.2375	25	E	26	E
261.989933	7.649E-29	1.518E-04	3357.9323	25	A1	26	A2
261.990742	4.589E-29	1.519E-04	3357.9315	25	F1	26	F2
261.991145	3.060E-29	3.037E-04	3357.9311	25	E	26	E
262.054511	5.137E-31	1.762E-06	3365.2481	25	F1	26	F2
262.098140	3.528E-31	1.193E-06	3362.3385	25	F2	26	F1
262.154934	3.120E-33	3.111E-09	3103.0719	24	F1	25	F2
262.177361	4.008E-32	3.997E-08	3103.0707	24	F2	25	F1
262.268974	1.401E-30	4.776E-06	3363.8269	25	F2	26	F1
262.312201	1.523E-30	5.194E-06	3363.7351	25	F1	26	F2
262.595025	3.365E-35	4.060E-10	3631.0443	26	F2	27	F1
262.613923	2.572E-36	3.104E-11	3631.0254	26	F1	27	F2
262.654937	7.637E-29	2.559E-04	3359.7403	25	F2	26	F1
262.663625	7.646E-29	2.562E-04	3359.7310	25	F1	26	F2
262.712864	6.807E-33	6.745E-09	3101.1140	24	F1	25	F2
262.788785	2.885E-32	1.716E-08	3101.1140	24	A1	25	A2
262.859599	3.003E-31	1.035E-06	3365.2481	25	F1	26	F2
263.075979	1.254E-30	4.327E-06	3365.2268	25	F2	26	F1



263.105968	8.554E-31	2.919E-06	3362.9413	25	F1	26	F2
263.250919	6.318E-29	6.418E-04	3361.1893	25	E	26	E
263.276641	9.515E-29	3.222E-04	3361.1600	25	F2	26	F1
263.322311	1.607E-28	3.266E-04	3361.1071	25	A2	26	A1
263.567535	8.361E-30	2.872E-05	3363.7351	25	F1	26	F2
263.757410	1.024E-28	3.498E-04	3362.3385	25	F2	26	F1
263.919639	1.552E-28	3.203E-04	3363.6037	25	A1	26	A2
263.926921	1.087E-28	3.712E-04	3362.1204	25	F1	26	F2
264.053883	5.822E-29	2.020E-04	3365.2268	25	F2	26	F1
264.112772	9.595E-34	9.584E-10	3101.1140	24	F1	25	F2
264.123489	9.219E-34	2.763E-09	3101.1141	24	E	25	E
264.133378	3.976E-29	4.140E-04	3365.2375	25	E	26	E
264.176852	1.757E-35	2.123E-10	3629.4625	26	F2	27	F1
264.196825	1.830E-37	6.065E-13	3355.7254	25	F1	26	F2
264.214358	6.049E-29	2.100E-04	3365.2481	25	F1	26	F2
264.358644	3.723E-34	4.500E-09	3629.2807	26	F1	27	F2
264.361302	1.054E-28	3.623E-04	3362.9413	25	F1	26	F2
264.372622	9.162E-29	3.161E-04	3363.7351	25	F1	26	F2
264.392064	8.122E-29	8.371E-04	3362.8353	25	E	26	E
264.463139	1.306E-34	4.383E-10	3357.9315	25	F1	26	F2
264.475886	1.026E-28	3.542E-04	3363.8269	25	F2	26	F1
264.622953	1.855E-28	3.849E-04	3363.9028	25	A2	26	A1
264.696280	1.770E-32	6.002E-08	3359.7403	25	F2	26	F1
264.935911	6.503E-31	2.223E-06	3361.1600	25	F2	26	F1
265.166390	2.048E-29	7.070E-05	3362.9413	25	F1	26	F2
265.182255	3.694E-30	1.270E-05	3362.1204	25	F1	26	F2
265.336548	1.512E-33	1.829E-08	3628.3028	26	F1	27	F2
265.361818	5.376E-34	1.977E-08	3631.0351	26	E	27	E
265.371267	5.549E-34	6.803E-09	3631.0254	26	F1	27	F2
265.453790	4.028E-30	1.399E-05	3363.8269	25	F2	26	F1
265.531611	2.235E-33	2.704E-08	3628.1077	26	F2	27	F1
265.727381	1.899E-30	6.603E-06	3363.7351	25	F1	26	F2
265.796185	7.751E-33	2.716E-08	3365.2481	25	F1	26	F2

265.797538	4.999E-32	5.254E-07	3365.2375	25	E	26	E
265.798604	8.988E-33	3.149E-08	3365.2268	25	F2	26	F1
265.964322	5.892E-30	2.038E-05	3362.3385	25	F2	26	F1
265.987343	3.390E-30	1.171E-05	3362.1204	25	F1	26	F2
266.038000	1.109E-30	1.145E-05	3361.1893	25	E	26	E
266.316259	2.548E-32	8.716E-08	3359.7310	25	F1	26	F2
266.336699	2.142E-34	2.593E-09	3627.3026	26	F2	27	F1
266.355550	2.934E-32	1.004E-07	3359.7403	25	F2	26	F1
266.509147	7.912E-34	8.058E-09	3357.9311	25	E	26	E
266.521149	1.779E-30	6.191E-06	3362.9413	25	F1	26	F2
266.535663	5.826E-30	6.078E-05	3362.8353	25	E	26	E
266.669222	1.275E-36	4.285E-12	3355.7254	25	F1	26	F2
266.669800	1.277E-36	4.292E-12	3355.7255	25	F2	26	F1
266.942226	1.621E-30	5.637E-06	3362.3385	25	F2	26	F1
267.025978	6.971E-33	2.567E-07	3629.3709	26	E	27	E
267.115989	9.136E-33	1.122E-07	3629.2807	26	F1	27	F2
267.142823	5.100E-30	1.765E-05	3361.1600	25	F2	26	F1
267.198512	2.233E-31	7.832E-07	3363.8269	25	F2	26	F1
267.309208	3.966E-31	1.391E-06	3363.7351	25	F1	26	F2
267.342102	1.583E-29	5.511E-05	3362.1204	25	F1	26	F2
267.418620	2.580E-29	5.366E-05	3361.1071	25	A2	26	A1
267.543460	1.258E-35	1.525E-10	3626.0959	26	F1	27	F2
267.571593	4.945E-31	1.704E-06	3359.7310	25	F1	26	F2
267.592033	1.121E-35	1.359E-10	3626.0473	26	F2	27	F1
267.646281	9.009E-34	1.119E-08	3631.0443	26	F2	27	F1
267.670759	1.364E-32	1.694E-07	3631.0254	26	F1	27	F2
267.870504	5.500E-32	4.054E-07	3628.5257	26	A1	27	A2
268.093893	1.017E-32	1.249E-07	3628.3028	26	F1	27	F2
268.102976	5.246E-30	1.841E-05	3362.9413	25	F1	26	F2
268.115773	9.509E-33	3.258E-08	3357.9315	25	F1	26	F2
268.120727	5.176E-30	1.802E-05	3361.1600	25	F2	26	F1
268.181599	4.056E-30	4.237E-05	3361.1893	25	E	26	E
268.199823	2.913E-30	3.068E-05	3362.8353	25	E	26	E

268.376681	5.365E-30	1.857E-05	3359.7310	25	F1	26	F2
268.562461	3.720E-30	1.289E-05	3359.7403	25	F2	26	F1
268.686947	3.326E-30	1.168E-05	3362.3385	25	F2	26	F1
268.711143	6.092E-35	2.072E-10	3355.7255	25	F2	26	F1
268.923929	7.106E-32	2.496E-07	3362.1204	25	F1	26	F2
269.169577	2.169E-33	8.000E-08	3627.2273	26	E	27	E
269.202730	7.852E-36	9.527E-11	3624.4366	26	F1	27	F2
269.228108	1.153E-31	1.434E-06	3629.4625	26	F2	27	F1
269.296228	1.509E-30	1.561E-05	3357.9311	25	E	26	E
269.371107	2.126E-30	7.337E-06	3357.9315	25	F1	26	F2
269.415480	1.362E-32	1.694E-07	3629.2807	26	F1	27	F2
269.500241	4.930E-32	1.856E-06	3631.0351	26	E	27	E
269.510100	5.147E-32	6.460E-07	3631.0443	26	F2	27	F1
269.540366	9.051E-31	3.154E-06	3359.7403	25	F2	26	F1
269.590985	3.469E-30	7.191E-06	3357.9323	25	A1	26	A2
269.731440	4.233E-32	1.476E-07	3359.7310	25	F1	26	F2
269.845759	2.780E-31	2.932E-06	3361.1893	25	E	26	E
269.865448	2.495E-31	8.769E-07	3361.1600	25	F2	26	F1
270.176195	7.346E-32	2.546E-07	3357.9315	25	F1	26	F2
270.258518	1.458E-35	4.059E-10	3906.5514	27	A2	28	A1
270.266618	2.987E-36	1.386E-10	3906.5433	27	F2	28	F1
270.300805	1.504E-33	1.851E-08	3626.0959	26	F1	27	F2
270.321856	6.034E-31	2.071E-06	3355.7254	25	F1	26	F2
270.370413	5.987E-31	2.055E-06	3355.7255	25	F2	26	F1
270.393385	5.584E-32	6.950E-07	3628.3028	26	F1	27	F2
270.582867	4.825E-32	6.006E-07	3628.1077	26	F2	27	F1
270.878351	2.616E-31	3.308E-06	3631.0443	26	F2	27	F1
271.036318	3.662E-32	4.635E-07	3631.0254	26	F1	27	F2
271.091927	2.955E-31	3.713E-06	3629.4625	26	F2	27	F1
271.164401	3.582E-31	1.350E-05	3629.3709	26	E	27	E
271.244073	1.545E-29	1.878E-04	3622.3953	26	F1	27	F2
271.244667	1.545E-29	1.878E-04	3622.3947	26	F2	27	F1
271.285087	6.535E-33	2.299E-08	3359.7403	25	F2	26	F1

271.313267	8.207E-32	2.888E-07	3359.7310	25	F1	26	F2
271.387955	4.685E-32	5.836E-07	3627.3026	26	F2	27	F1
271.439827	3.221E-32	3.373E-07	3357.9311	25	E	26	E
271.530954	2.648E-32	9.248E-08	3357.9315	25	F1	26	F2
271.577190	1.058E-33	3.658E-09	3355.7254	25	F1	26	F2
271.956658	1.724E-29	6.375E-04	3624.4402	26	E	27	E
271.960075	2.588E-29	3.188E-04	3624.4366	26	F1	27	F2
271.966812	4.316E-29	3.191E-04	3624.4294	26	A1	27	A2
272.043789	1.387E-31	1.766E-06	3631.0254	26	F1	27	F2
272.140086	2.558E-35	3.567E-09	3904.6698	27	E	28	E
272.198437	2.897E-31	1.107E-05	3631.0351	26	E	27	E
272.245715	3.282E-35	1.526E-09	3904.5642	27	F2	28	F1
272.382278	1.107E-33	3.845E-09	3355.7254	25	F1	26	F2
272.446686	9.095E-31	1.144E-05	3628.1077	26	F2	27	F1
272.460178	1.883E-31	2.384E-06	3629.4625	26	F2	27	F1
272.535501	2.368E-32	3.023E-07	3631.0443	26	F2	27	F1
272.577325	1.270E-33	4.415E-09	3355.7255	25	F2	26	F1
272.600296	3.237E-29	4.036E-04	3626.0959	26	F1	27	F2
272.643289	3.257E-29	4.061E-04	3626.0473	26	F2	27	F1
272.781039	3.833E-30	4.858E-05	3629.2807	26	F1	27	F2
273.071829	5.837E-29	4.408E-04	3627.5233	26	A2	27	A1
273.103987	4.314E-33	4.560E-08	3357.9311	25	E	26	E
273.112781	4.192E-33	1.477E-08	3357.9315	25	F1	26	F2
273.251774	3.557E-29	4.477E-04	3627.3026	26	F2	27	F1
273.308000	2.477E-29	9.353E-04	3627.2273	26	E	27	E
273.326920	8.923E-35	4.212E-09	3906.5433	27	F2	28	F1
273.334883	9.141E-35	4.315E-09	3906.5350	27	F1	28	F2
273.538759	1.976E-29	2.537E-04	3631.0254	26	F1	27	F2
273.555229	3.148E-34	1.100E-09	3355.7255	25	F2	26	F1
273.576370	3.223E-34	4.498E-08	3903.2335	27	E	28	E
273.634721	1.318E-29	5.080E-04	3631.0351	26	E	27	E
273.696080	2.023E-29	2.599E-04	3631.0443	26	F2	27	F1
273.717064	2.520E-38	3.067E-13	3619.9223	26	F2	27	F1

273.737037	2.684E-33	9.390E-09	3355.7254	25	F1	26	F2
273.740686	5.179E-34	2.410E-08	3903.0692	27	F2	28	F1
273.758943	3.414E-29	4.330E-04	3628.3028	26	F1	27	F2
273.788510	2.962E-29	3.775E-04	3629.2807	26	F1	27	F2
273.814936	3.932E-29	4.984E-04	3628.1077	26	F2	27	F1
273.862597	2.222E-29	8.502E-04	3629.3709	26	E	27	E
274.001418	1.961E-35	2.419E-10	3622.3953	26	F1	27	F2
274.059329	1.186E-33	3.312E-08	3902.7505	27	A2	28	A1
274.117328	3.645E-29	4.659E-04	3629.4625	26	F2	27	F1
274.224818	7.646E-29	5.840E-04	3628.5257	26	A1	27	A2
274.259566	2.870E-33	3.582E-08	3624.4366	26	F1	27	F2
274.507108	1.150E-31	1.448E-06	3626.0473	26	F2	27	F1
274.620024	2.068E-30	2.622E-05	3627.3026	26	F2	27	F1
274.748157	3.725E-35	1.734E-09	3902.0617	27	F2	28	F1
274.766414	8.240E-30	1.051E-04	3628.3028	26	F1	27	F2
275.129488	1.214E-34	5.739E-09	3904.7404	27	F1	28	F2
275.277906	1.195E-31	1.537E-06	3629.4625	26	F2	27	F1
275.283481	3.018E-31	3.879E-06	3629.2807	26	F1	27	F2
275.298881	1.021E-30	3.940E-05	3629.3709	26	E	27	E
275.299950	3.223E-34	1.137E-09	3355.7255	25	F2	26	F1
275.306017	2.643E-33	1.249E-07	3904.5642	27	F2	28	F1
275.318864	2.172E-35	7.667E-11	3355.7254	25	F1	26	F2
275.472086	1.063E-30	1.359E-05	3628.1077	26	F2	27	F1
275.490685	7.155E-33	9.285E-08	3631.0443	26	F2	27	F1
275.517857	7.210E-33	9.357E-08	3631.0254	26	F1	27	F2
275.875358	1.228E-31	1.559E-06	3626.0473	26	F2	27	F1
275.904496	1.236E-33	5.918E-08	3906.5350	27	F1	28	F2
275.917295	6.398E-33	1.838E-07	3906.5265	27	A1	28	A2
275.965855	1.844E-31	2.342E-06	3626.0959	26	F1	27	F2
276.006196	1.966E-30	7.535E-05	3627.2273	26	E	27	E
276.095081	9.812E-33	3.711E-07	3624.4402	26	E	27	E
276.261385	9.204E-31	1.184E-05	3628.3028	26	F1	27	F2
276.274566	3.659E-36	5.116E-10	3900.5353	27	E	28	E

276.277174	1.487E-30	1.903E-05	3627.3026	26	F2	27	F1
276.290067	6.218E-33	2.941E-07	3903.5798	27	F1	28	F2
276.295923	6.129E-35	7.660E-10	3622.3947	26	F2	27	F1
276.300909	6.216E-35	7.769E-10	3622.3953	26	F1	27	F2
276.474659	3.668E-37	1.360E-11	3619.9222	26	E	27	E
276.632665	2.657E-30	3.421E-05	3628.1077	26	F2	27	F1
276.800988	8.438E-34	3.993E-08	3903.0692	27	F2	28	F1
276.973326	5.053E-31	6.454E-06	3626.0959	26	F1	27	F2
277.072511	5.274E-32	6.851E-07	3629.4625	26	F2	27	F1
277.262578	9.723E-32	1.263E-06	3629.2807	26	F1	27	F2
277.437753	3.319E-30	4.275E-05	3627.3026	26	F2	27	F1
277.442480	2.705E-30	1.045E-04	3627.2273	26	E	27	E
277.532508	3.829E-30	4.904E-05	3626.0473	26	F2	27	F1
277.625125	1.022E-31	1.299E-06	3624.4366	26	F1	27	F2
277.662843	8.465E-37	1.581E-10	4191.7027	28	F2	29	F1
277.677294	6.325E-38	1.182E-11	4191.6883	28	F1	29	F2
277.699101	1.315E-32	6.306E-07	3904.7404	27	F1	28	F2
277.767535	1.531E-32	2.203E-06	3904.6698	27	E	28	E
277.808459	3.181E-34	1.506E-08	3902.0617	27	F2	28	F1
277.947217	2.381E-34	1.128E-08	3901.9226	27	F1	28	F2
277.994006	9.511E-33	4.607E-07	3906.5350	27	F1	28	F2
278.017009	9.878E-33	4.786E-07	3906.5433	27	F2	28	F1
278.025629	3.189E-30	2.487E-05	3628.5257	26	A1	27	A2
278.113716	1.121E-36	5.233E-11	3898.6962	27	F2	28	F1
278.159743	1.810E-33	2.286E-08	3622.3947	26	F2	27	F1
278.240482	1.508E-30	1.960E-05	3628.3028	26	F1	27	F2
278.321126	3.297E-30	2.525E-05	3624.4294	26	A1	27	A2
278.427270	1.099E-30	1.429E-05	3628.1077	26	F2	27	F1
278.468297	1.794E-30	2.310E-05	3626.0959	26	F1	27	F2
278.632596	1.468E-30	1.877E-05	3624.4366	26	F1	27	F2
278.693087	6.629E-32	8.545E-07	3626.0473	26	F2	27	F1
278.768320	9.200E-36	1.152E-10	3619.9223	26	F2	27	F1
278.793277	9.195E-31	3.530E-05	3624.4402	26	E	27	E

278.859680	1.421E-32	6.818E-07	3903.5798	27	F1	28	F2
279.003146	1.843E-30	1.438E-05	3627.5233	26	A2	27	A1
279.203819	1.591E-32	2.291E-06	3903.2335	27	E	28	E
279.232358	1.892E-31	2.461E-06	3627.3026	26	F2	27	F1
279.315467	2.225E-34	1.055E-08	3900.5544	27	F1	28	F2
279.520239	1.560E-31	4.572E-06	3906.5514	27	A2	28	A1
279.527993	7.079E-31	9.006E-06	3622.3947	26	F2	27	F1
279.652110	3.890E-32	1.901E-06	3906.5433	27	F2	28	F1
279.666468	6.612E-31	8.418E-06	3622.3953	26	F1	27	F2
279.745262	4.062E-36	7.599E-10	4189.6203	28	F1	29	F2
279.788611	1.305E-31	6.327E-06	3904.7404	27	F1	28	F2
279.825985	4.742E-36	8.870E-10	4189.5396	28	F2	29	F1
279.996106	1.536E-32	7.450E-07	3904.5642	27	F2	28	F1
280.127567	9.257E-32	1.193E-06	3624.4366	26	F1	27	F2
280.229561	7.334E-32	2.838E-06	3624.4402	26	E	27	E
280.412989	3.281E-30	4.599E-04	3896.3969	27	E	28	E
280.413207	4.921E-30	2.299E-04	3896.3967	27	F2	28	F1
280.413643	8.202E-30	2.299E-04	3896.3962	27	A2	28	A1
280.447394	5.452E-32	7.097E-07	3626.0959	26	F1	27	F2
280.487692	4.989E-32	6.495E-07	3626.0473	26	F2	27	F1
280.516830	1.149E-32	5.519E-07	3901.9226	27	F1	28	F2
280.613083	1.267E-31	4.808E-06	3619.9222	26	E	27	E
280.632140	1.894E-31	2.396E-06	3619.9223	26	F2	27	F1
280.672880	3.143E-31	2.385E-06	3619.9223	26	A2	27	A1
280.673939	2.312E-32	2.960E-07	3622.3953	26	F1	27	F2
280.697298	3.853E-32	1.894E-06	3906.5350	27	F1	28	F2
280.949190	1.823E-32	8.844E-07	3903.5798	27	F1	28	F2
281.043975	1.406E-35	2.677E-09	4191.7027	28	F2	29	F1
281.051045	1.434E-35	8.189E-09	4191.6955	28	E	29	E
281.077192	2.589E-36	4.848E-10	4188.2884	28	F2	29	F1
281.131097	5.703E-32	2.811E-06	3906.5433	27	F2	28	F1
281.174017	8.282E-30	3.930E-04	3898.6962	27	F2	28	F1
281.179287	8.286E-30	3.932E-04	3898.6906	27	F1	28	F2

281.185143	1.463E-33	1.878E-08	3622.3947	26	F2	27	F1
281.491077	3.019E-31	1.466E-05	3903.0692	27	F2	28	F1
281.598633	3.479E-31	5.110E-05	3904.6698	27	E	28	E
281.631207	3.383E-31	1.656E-05	3904.5642	27	F2	28	F1
281.691203	1.303E-34	2.441E-08	4187.6744	28	F1	29	F2
281.753390	4.790E-32	2.368E-06	3906.5350	27	F1	28	F2
281.848612	1.736E-29	5.006E-04	3900.5952	27	A1	28	A2
281.885080	1.045E-29	5.024E-04	3900.5544	27	F1	28	F2
281.902015	6.989E-30	1.008E-03	3900.5353	27	E	28	E
282.000390	2.496E-34	3.180E-09	3619.9223	26	F2	27	F1
282.106664	8.803E-33	1.147E-07	3624.4366	26	F1	27	F2
282.121938	4.222E-32	3.301E-07	3624.4294	26	A1	27	A2
282.133284	1.561E-34	2.924E-08	4187.2323	28	F2	29	F1
282.168910	1.180E-33	1.523E-08	3622.3953	26	F1	27	F2
282.345722	1.112E-32	1.437E-07	3622.3947	26	F2	27	F1
282.491903	6.425E-32	3.162E-06	3904.7404	27	F1	28	F2
282.498548	1.137E-29	5.524E-04	3902.0617	27	F2	28	F1
282.606340	1.194E-29	5.800E-04	3901.9226	27	F1	28	F2
282.913342	1.046E-29	3.123E-04	3906.5265	27	A1	28	A2
283.004598	6.267E-30	3.120E-04	3906.5350	27	F1	28	F2
283.034917	7.766E-30	1.142E-03	3903.2335	27	E	28	E
283.077038	6.339E-30	3.157E-04	3906.5433	27	F2	28	F1
283.110194	1.016E-29	5.012E-04	3904.5642	27	F2	28	F1
283.126178	1.204E-29	5.897E-04	3903.0692	27	F2	28	F1
283.138659	1.071E-29	3.203E-04	3906.5514	27	A2	28	A1
283.170191	3.955E-36	7.414E-10	4186.1954	28	F1	29	F2
283.170552	3.306E-39	1.547E-13	3893.6393	27	F2	28	F1
283.207116	1.809E-34	3.446E-08	4189.5396	28	F2	29	F1
283.307114	1.159E-33	1.325E-07	4189.4398	28	A2	29	A1
283.311279	3.561E-34	1.371E-08	3619.9222	26	E	27	E
283.321050	2.335E-29	6.859E-04	3902.7505	27	A2	28	A1
283.473509	2.782E-36	1.322E-10	3896.3967	27	F2	28	F1
283.478097	7.255E-30	1.077E-03	3904.6698	27	E	28	E



283.547995	1.137E-29	5.627E-04	3904.7404	27	F1	28	F2
283.652482	1.429E-29	7.036E-04	3903.5798	27	F1	28	F2
283.657540	3.195E-34	4.107E-09	3619.9223	26	F2	27	F1
283.748900	4.448E-34	2.140E-08	3898.6906	27	F1	28	F2
283.902445	2.630E-35	5.084E-09	4191.7027	28	F2	29	F1
283.920143	3.821E-34	7.387E-08	4191.6883	28	F1	29	F2
283.974590	2.346E-32	1.141E-06	3900.5544	27	F1	28	F2
284.133649	5.560E-31	2.725E-05	3902.0617	27	F2	28	F1
284.140327	7.898E-34	1.030E-08	3622.3947	26	F2	27	F1
284.148007	7.714E-34	1.006E-08	3622.3953	26	F1	27	F2
284.458324	9.103E-34	1.736E-07	4188.2884	28	F2	29	F1
284.598671	9.937E-34	5.685E-07	4188.1479	28	E	29	E
284.605165	7.855E-31	3.878E-05	3903.0692	27	F2	28	F1
284.708574	2.130E-31	1.055E-05	3903.5798	27	F1	28	F2
284.747563	3.496E-34	1.356E-08	3619.9222	26	E	27	E
284.781913	6.560E-38	5.163E-11	4486.4545	29	F1	30	F2
284.788074	6.662E-38	1.573E-10	4486.4484	29	E	30	E
284.799203	1.832E-31	9.130E-06	3904.7404	27	F1	28	F2
284.805291	2.906E-37	5.453E-11	4184.5603	28	F1	29	F2
284.818119	2.987E-34	3.864E-09	3619.9223	26	F2	27	F1
284.836576	2.731E-37	5.124E-11	4184.5290	28	F2	29	F1
284.914381	1.124E-30	1.669E-04	3903.2335	27	E	28	E
285.056135	1.642E-31	8.186E-06	3904.5642	27	F2	28	F1
285.145006	1.476E-33	7.434E-08	3906.5433	27	F2	28	F1
285.167739	1.418E-33	7.142E-08	3906.5350	27	F1	28	F2
285.309632	1.180E-31	5.817E-06	3901.9226	27	F1	28	F2
285.514416	2.009E-34	3.832E-08	4187.2323	28	F2	29	F1
285.612636	2.531E-31	1.250E-05	3902.0617	27	F2	28	F1
285.733113	5.557E-32	8.181E-06	3900.5353	27	E	28	E
285.838410	8.308E-34	4.043E-08	3898.6906	27	F1	28	F2
285.864107	8.957E-34	4.359E-08	3898.6962	27	F2	28	F1
285.959782	2.654E-31	1.323E-05	3903.5798	27	F1	28	F2
285.988111	2.580E-33	4.992E-07	4189.6203	28	F1	29	F2

286.040439	1.840E-35	2.659E-09	3896.3969	27	E	28	E
286.065586	3.105E-33	6.008E-07	4189.5396	28	F2	29	F1
286.230543	2.502E-38	1.191E-12	3893.6393	27	F1	28	F2
286.230854	2.504E-38	1.192E-12	3893.6393	27	F2	28	F1
286.284626	1.707E-33	3.343E-07	4191.6883	28	F1	29	F2
286.290287	1.686E-33	9.904E-07	4191.6955	28	E	29	E
286.365724	1.169E-30	5.794E-05	3901.9226	27	F1	28	F2
286.478134	8.456E-35	4.842E-08	4186.2684	28	E	29	E
286.551106	7.235E-31	3.610E-05	3903.0692	27	F2	28	F1
286.604198	1.492E-34	1.169E-09	3619.9223	26	A2	27	A1
286.612724	2.907E-35	3.797E-10	3619.9223	26	F2	27	F1
286.677882	1.339E-31	6.604E-06	3900.5544	27	F1	28	F2
286.926086	1.511E-37	2.838E-11	4182.4395	28	F2	29	F1
286.939471	3.366E-30	1.008E-04	3902.7505	27	A2	28	A1
286.962344	3.534E-33	1.782E-07	3904.7404	27	F1	28	F2
287.025722	2.211E-32	3.344E-06	3904.6698	27	E	28	E
287.087925	6.303E-37	4.967E-10	4484.1485	29	F1	30	F2
287.124103	4.316E-33	2.176E-07	3904.5642	27	F2	28	F1
287.163089	7.228E-37	1.709E-09	4484.0733	29	E	30	E
287.316794	7.034E-33	1.362E-06	4188.2884	28	F2	29	F1
287.499207	1.255E-32	6.163E-07	3898.6962	27	F2	28	F1
287.558577	8.581E-31	4.284E-05	3902.0617	27	F2	28	F1
287.612577	7.247E-31	1.078E-04	3900.5353	27	E	28	E
287.616932	7.591E-31	3.789E-05	3901.9226	27	F1	28	F2
287.733974	7.051E-31	3.498E-05	3900.5544	27	F1	28	F2
287.934052	9.285E-34	1.798E-07	4187.6744	28	F1	29	F2
288.094072	1.386E-32	2.740E-06	4191.7027	28	F2	29	F1
288.122923	5.105E-31	2.575E-05	3903.5798	27	F1	28	F2
288.163599	2.897E-34	1.412E-08	3896.3967	27	F2	28	F1
288.217708	3.397E-35	6.491E-09	4184.5290	28	F2	29	F1
288.236337	1.063E-33	2.104E-07	4191.6883	28	F1	29	F2
288.257913	7.078E-32	8.322E-06	4189.6900	28	A1	29	A2
288.352594	1.685E-32	3.302E-06	4189.6203	28	F1	29	F2

288.372885	5.753E-34	1.115E-07	4187.2323	28	F2	29	F1
288.462006	2.758E-31	4.175E-05	3903.2335	27	E	28	E
288.502165	3.951E-36	3.172E-09	4486.4545	29	F1	30	F2
288.514816	2.928E-37	2.351E-10	4486.4420	29	F2	30	F1
288.541702	5.086E-31	2.511E-05	3898.6906	27	F1	28	F2
288.619074	3.074E-31	1.551E-05	3903.0692	27	F2	28	F1
288.800156	1.333E-36	6.433E-11	3893.6393	27	F1	28	F2
288.844659	9.298E-31	2.784E-05	3900.5952	27	A1	28	A2
288.978195	4.304E-31	2.130E-05	3898.6962	27	F2	28	F1
288.985182	1.314E-31	6.564E-06	3900.5544	27	F1	28	F2
288.985829	2.652E-36	2.091E-09	4482.2506	29	F1	30	F2
289.413039	2.360E-33	4.575E-07	4186.1954	28	F1	29	F2
289.423792	1.196E-32	7.144E-06	4191.6955	28	E	29	E
289.495380	1.484E-30	2.791E-04	4179.8702	28	F1	29	F2
289.495699	1.484E-30	2.791E-04	4179.8699	28	F2	29	F1
289.508974	5.371E-35	2.543E-08	4481.7275	29	A1	30	A2
289.547710	8.553E-33	1.704E-06	4191.7027	28	F2	29	F1
289.597794	8.399E-33	4.170E-07	3898.6906	27	F1	28	F2
289.626545	7.541E-32	3.807E-06	3902.0617	27	F2	28	F1
289.675364	3.584E-31	1.056E-05	3896.3962	27	A2	28	A1
289.780073	5.712E-33	2.884E-07	3901.9226	27	F1	28	F2
289.798699	2.058E-31	1.011E-05	3896.3967	27	F2	28	F1
289.837913	2.296E-32	1.351E-05	4188.1479	28	E	29	E
289.871537	1.357E-31	2.002E-05	3896.3969	27	E	28	E
289.986010	3.324E-35	2.623E-08	4481.2504	29	F1	30	F2
290.117115	2.558E-35	6.056E-08	4481.1193	29	E	30	E
290.257213	6.064E-32	1.200E-05	4189.5396	28	F2	29	F1
290.298534	3.758E-32	7.371E-06	4187.6744	28	F1	29	F2
290.303161	4.182E-30	4.799E-04	4182.4438	28	A2	29	A1
290.304305	6.403E-32	1.268E-05	4189.6203	28	F1	29	F2
290.307218	2.510E-30	4.800E-04	4182.4395	28	F2	29	F1
290.309232	1.674E-30	9.602E-04	4182.4373	28	E	29	E
290.547892	6.247E-33	1.251E-06	4191.7027	28	F2	29	F1

290.798416	1.458E-32	2.925E-06	4191.6883	28	F1	29	F2
290.808177	2.904E-36	2.334E-09	4484.1485	29	F1	30	F2
290.849001	1.567E-32	7.831E-07	3898.6906	27	F1	28	F2
290.889666	5.682E-32	2.772E-06	3893.6393	27	F1	28	F2
290.920943	5.658E-32	2.760E-06	3893.6393	27	F2	28	F1
290.924135	1.361E-32	6.805E-07	3898.6962	27	F2	28	F1
290.959732	5.394E-35	4.336E-08	4483.9971	29	F2	30	F1
291.048139	3.179E-30	6.167E-04	4184.5603	28	F1	29	F2
291.076177	3.191E-30	6.189E-04	4184.5290	28	F2	29	F1
291.148323	9.916E-33	5.009E-07	3900.5544	27	F1	28	F2
291.160202	1.003E-32	1.521E-06	3900.5353	27	E	28	E
291.277686	2.944E-33	1.459E-07	3896.3967	27	F2	28	F1
291.439648	5.836E-37	4.609E-10	4479.7968	29	F1	30	F2
291.508421	3.524E-32	6.978E-06	4188.2884	28	F2	29	F1
291.678373	3.113E-35	7.627E-08	4486.4484	29	E	30	E
291.683449	3.153E-35	2.574E-08	4486.4420	29	F2	30	F1
291.710852	2.114E-31	4.216E-05	4189.5396	28	F2	29	F1
291.717376	2.366E-30	1.393E-03	4186.2684	28	E	29	E
291.751000	1.742E-33	2.595E-07	3896.3969	27	E	28	E
291.777522	3.577E-30	7.021E-04	4186.1954	28	F1	29	F2
291.876334	6.152E-30	7.245E-04	4186.0716	28	A1	29	A2
292.250246	3.615E-30	7.165E-04	4187.6744	28	F1	29	F2
292.287653	5.195E-30	6.233E-04	4189.4398	28	A2	29	A1
292.308857	1.877E-30	3.794E-04	4191.6883	28	F1	29	F2
292.377819	1.262E-30	7.660E-04	4191.6955	28	E	29	E
292.445796	1.906E-30	3.856E-04	4191.7027	28	F2	29	F1
292.470174	1.906E-34	1.533E-07	4482.4867	29	F2	30	F1
292.556043	5.012E-35	2.467E-09	3893.6393	27	F2	28	F1
292.564513	4.030E-30	7.983E-04	4187.2323	28	F2	29	F1
292.706081	2.916E-34	2.346E-07	4482.2506	29	F1	30	F2
292.711033	3.030E-30	6.074E-04	4189.5396	28	F2	29	F1
292.866384	3.344E-30	6.713E-04	4189.6203	28	F1	29	F2
292.876831	3.749E-37	7.179E-11	4179.8699	28	F2	29	F1

292.962059	3.851E-30	7.685E-04	4188.2884	28	F2	29	F1
292.971417	2.849E-30	1.705E-03	4188.1479	28	E	29	E
292.992103	2.199E-34	1.112E-08	3898.6962	27	F2	28	F1
293.012143	2.929E-33	1.481E-07	3898.6906	27	F1	28	F2
293.015571	5.897E-30	7.110E-04	4189.6900	28	A1	29	A2
293.165687	6.639E-35	1.289E-08	4182.4395	28	F2	29	F1
293.223627	1.329E-33	6.650E-08	3896.3967	27	F2	28	F1
293.250620	7.630E-38	1.809E-10	4477.9858	29	E	30	E
293.293785	5.819E-33	1.748E-07	3896.3962	27	A2	28	A1
293.412622	4.059E-33	7.974E-07	4184.5603	28	F1	29	F2
293.592958	1.249E-35	6.180E-10	3893.6393	27	F1	28	F2
293.706262	7.454E-35	5.999E-08	4481.2504	29	F1	30	F2
293.729233	6.869E-32	1.362E-05	4186.1954	28	F1	29	F2
293.962241	5.406E-31	1.085E-04	4188.2884	28	F2	29	F1
294.018151	1.441E-31	2.877E-05	4187.2323	28	F2	29	F1
294.035031	2.018E-35	1.001E-09	3893.6393	27	F2	28	F1
294.053387	4.514E-34	1.107E-06	4484.0733	29	E	30	E
294.128365	5.326E-34	4.354E-07	4483.9971	29	F2	30	F1
294.305617	3.382E-35	2.800E-08	4486.4545	29	F1	30	F2
294.338627	5.148E-34	4.263E-07	4486.4420	29	F2	30	F1
294.376825	4.655E-32	9.420E-06	4189.6203	28	F1	29	F2
294.608937	3.010E-32	6.095E-06	4189.5396	28	F2	29	F1
294.649050	1.557E-34	7.748E-09	3893.6393	27	F1	28	F2
294.751808	6.580E-35	1.348E-08	4191.7027	28	F2	29	F1
294.752833	4.095E-34	2.516E-07	4191.6955	28	E	29	E
294.753774	7.085E-35	1.451E-08	4191.6883	28	F1	29	F2
294.812325	2.258E-31	4.537E-05	4187.6744	28	F1	29	F2
294.850881	9.353E-32	5.600E-05	4186.2684	28	E	29	E
295.018333	1.543E-31	3.096E-05	4187.2323	28	F2	29	F1
295.032252	5.599E-36	4.509E-09	4479.9246	29	F2	30	F1
295.159901	4.524E-36	3.643E-09	4479.7968	29	F1	30	F2
295.267805	3.633E-33	7.206E-07	4184.5290	28	F2	29	F1
295.291595	1.350E-34	6.833E-09	3896.3967	27	F2	28	F1

295.298625	1.324E-34	2.010E-08	3896.3969	27	E	28	E
295.364333	4.793E-33	9.513E-07	4184.5603	28	F1	29	F2
295.417441	4.916E-33	2.412E-06	4482.7056	29	A2	30	A1
295.548474	2.683E-34	1.582E-07	4182.4373	28	E	29	E
295.631276	1.950E-38	1.542E-11	4475.6052	29	F1	30	F2
295.638806	1.071E-33	8.764E-07	4482.4867	29	F2	30	F1
295.735300	1.301E-36	2.528E-10	4179.8699	28	F2	29	F1
295.738229	1.310E-36	2.545E-10	4179.8702	28	F1	29	F2
295.860144	2.939E-32	5.954E-06	4188.2884	28	F2	29	F1
295.900257	6.990E-35	3.501E-09	3893.6393	27	F1	28	F2
295.925444	1.244E-31	7.562E-05	4188.1479	28	E	29	E
295.936682	6.510E-39	3.744E-12	4176.8099	28	E	29	E
295.980972	5.780E-35	2.897E-09	3893.6393	27	F2	28	F1
296.291312	2.757E-31	5.542E-05	4186.1954	28	F1	29	F2
296.322766	3.296E-32	6.675E-06	4187.6744	28	F1	29	F2
296.407324	1.349E-33	3.388E-06	4486.4484	29	E	30	E
296.450650	1.549E-33	1.297E-06	4486.4545	29	F1	30	F2
296.611629	5.653E-33	4.685E-06	4484.1485	29	F1	30	F2
296.633991	1.136E-30	1.372E-04	4186.0716	28	A1	29	A2
296.721443	6.011E-32	1.201E-05	4184.5290	28	F2	29	F1
296.783544	5.605E-34	4.646E-07	4483.9971	29	F2	30	F1
296.821742	2.620E-33	5.370E-07	4189.6203	28	F1	29	F2
296.914949	3.781E-33	7.750E-07	4189.5396	28	F2	29	F1
296.916236	4.869E-31	9.868E-05	4187.2323	28	F2	29	F1
296.983964	4.963E-36	3.999E-09	4477.9729	29	F2	30	F1
297.007414	3.449E-34	8.468E-07	4481.1193	29	E	30	E
297.357315	2.117E-33	4.202E-07	4182.4395	28	F2	29	F1
297.721625	2.527E-31	5.077E-05	4184.5290	28	F2	29	F1
297.801753	1.784E-31	3.614E-05	4186.1954	28	F1	29	F2
297.804908	1.560E-31	9.488E-05	4186.2684	28	E	29	E
297.926412	1.755E-31	3.529E-05	4184.5603	28	F1	29	F2
297.957300	4.636E-33	3.913E-06	4486.4545	29	F1	30	F2
298.048940	8.901E-36	4.509E-10	3893.6393	27	F2	28	F1

298.063398	6.144E-37	3.112E-11	3893.6393	27	F1	28	F2
298.102712	4.057E-35	7.983E-09	4179.8702	28	F1	29	F2
298.166157	1.405E-31	2.882E-05	4188.2884	28	F2	29	F1
298.200885	3.440E-34	2.816E-07	4479.9246	29	F2	30	F1
298.216598	8.268E-34	6.988E-07	4486.4420	29	F2	30	F1
298.293985	4.723E-33	3.918E-06	4482.4867	29	F2	30	F1
298.300458	7.910E-32	4.866E-05	4188.1479	28	E	29	E
298.489513	7.069E-31	3.359E-04	4472.7469	29	A1	30	A2
298.489745	4.242E-31	3.359E-04	4472.7467	29	F1	30	F2
298.489862	2.828E-31	6.718E-04	4472.7466	29	E	30	E
298.509533	4.809E-33	3.989E-06	4482.2506	29	F1	30	F2
298.681979	9.612E-32	5.763E-05	4182.4373	28	E	29	E
298.756663	1.107E-32	9.279E-06	4484.1485	29	F1	30	F2
298.767682	1.043E-31	2.140E-05	4187.6744	28	F1	29	F2
298.782339	1.277E-32	3.210E-05	4484.0733	29	E	30	E
298.798531	1.816E-37	3.533E-11	4176.8099	28	F1	29	F2
298.810953	1.256E-31	2.512E-05	4182.4395	28	F2	29	F1
299.222249	1.301E-33	2.669E-07	4187.2323	28	F2	29	F1
299.283700	2.051E-31	2.467E-05	4182.4438	28	A2	29	A1
299.348447	7.204E-31	5.810E-04	4475.6084	29	F2	30	F1
299.351528	7.205E-31	5.811E-04	4475.6052	29	F1	30	F2
299.436854	4.716E-32	9.561E-06	4184.5603	28	F1	29	F2
299.439211	1.355E-33	1.153E-06	4486.4420	29	F2	30	F1
299.509714	3.795E-33	3.148E-06	4481.2504	29	F1	30	F2
299.619528	2.497E-33	5.067E-07	4184.5290	28	F2	29	F1
299.651007	3.456E-33	8.828E-06	4486.4484	29	E	30	E
299.811135	1.006E-32	2.022E-06	4182.4395	28	F2	29	F1
299.926928	5.942E-32	1.181E-05	4179.8699	28	F2	29	F1
299.961064	3.026E-34	2.581E-07	4486.4545	29	F1	30	F2
300.054423	5.837E-32	1.160E-05	4179.8702	28	F1	29	F2
300.140919	6.116E-31	1.503E-03	4477.9858	29	E	30	E
300.152597	9.182E-31	7.523E-04	4477.9729	29	F2	30	F1
300.175098	1.534E-30	7.542E-04	4477.9479	29	A2	30	A1

300.179922	8.231E-33	5.067E-06	4186.2684	28	E	29	E
300.246670	6.395E-33	1.312E-06	4186.1954	28	F1	29	F2
300.263312	5.948E-33	5.025E-06	4484.1485	29	F1	30	F2
300.654566	5.563E-32	4.666E-05	4482.2506	29	F1	30	F2
300.661515	8.080E-32	6.835E-05	4483.9971	29	F2	30	F1
300.856064	1.034E-30	8.581E-04	4479.9246	29	F2	30	F1
300.963352	1.048E-30	8.698E-04	4479.7968	29	F1	30	F2
301.138055	2.693E-32	3.182E-06	4176.8099	28	A1	29	A2
301.163013	1.611E-32	3.173E-06	4176.8099	28	F1	29	F2
301.175923	1.073E-32	6.339E-06	4176.8099	28	E	29	E
301.291262	1.748E-30	8.802E-04	4481.7275	29	A1	30	A2
301.380566	2.873E-34	5.750E-08	4179.8699	28	F2	29	F1
301.574823	5.345E-31	4.597E-04	4486.4420	29	F2	30	F1
301.636005	2.804E-33	1.707E-06	4182.4373	28	E	29	E
301.646587	3.565E-31	9.203E-04	4486.4484	29	E	30	E
301.654748	1.069E-30	8.966E-04	4481.2504	29	F1	30	F2
301.702007	5.400E-31	4.648E-04	4486.4545	29	F1	30	F2
301.709038	2.452E-33	4.978E-07	4182.4395	28	F2	29	F1
301.736365	7.753E-31	1.951E-03	4481.1193	29	E	30	E
301.881770	2.781E-34	5.709E-08	4184.5603	28	F1	29	F2
301.884128	8.431E-31	7.177E-04	4483.9971	29	F2	30	F1
301.925541	3.374E-33	6.927E-07	4184.5290	28	F2	29	F1
302.026022	6.191E-31	1.583E-03	4484.0733	29	E	30	E
302.161216	1.124E-30	9.497E-04	4482.2506	29	F1	30	F2
302.171956	1.073E-30	9.076E-04	4482.4867	29	F2	30	F1
302.209998	4.812E-38	3.885E-11	4472.7467	29	F1	30	F2
302.267077	9.783E-31	8.350E-04	4484.1485	29	F1	30	F2
302.380748	3.724E-34	7.494E-08	4179.8699	28	F2	29	F1
302.517079	9.298E-36	7.623E-09	4475.6084	29	F2	30	F1
302.586685	2.201E-30	1.121E-03	4482.7056	29	A2	30	A1
302.616502	3.554E-34	7.159E-08	4179.8702	28	F1	29	F2
302.807775	5.852E-34	4.861E-07	4477.9729	29	F2	30	F1
303.108386	1.075E-32	9.026E-06	4479.7968	29	F1	30	F2



303.114725	7.218E-36	1.436E-09	4176.8099	28	F1	29	F2
303.161397	1.219E-31	1.031E-04	4481.2504	29	F1	30	F2
303.394569	1.801E-31	1.534E-04	4482.4867	29	F2	30	F1
304.008020	1.459E-33	1.257E-06	4484.1485	29	F1	30	F2
304.011020	2.700E-34	1.664E-07	4182.4373	28	E	29	E
304.015051	2.677E-34	5.501E-08	4182.4395	28	F2	29	F1
304.019740	2.633E-33	2.266E-06	4483.9971	29	F2	30	F1
304.021601	1.130E-32	2.919E-05	4484.0733	29	E	30	E
304.126943	4.299E-35	8.728E-09	4179.8702	28	F1	29	F2
304.164980	3.361E-32	2.870E-05	4482.2506	29	F1	30	F2
304.278651	4.385E-34	8.910E-08	4179.8699	28	F2	29	F1
304.282974	4.820E-35	4.204E-08	4486.4545	29	F1	30	F2
304.300798	4.844E-35	4.225E-08	4486.4420	29	F2	30	F1
304.309428	7.353E-36	4.416E-09	4176.8099	28	E	29	E
304.615035	9.650E-33	8.163E-06	4479.7968	29	F1	30	F2
304.734035	1.670E-32	1.414E-05	4479.9246	29	F2	30	F1
304.869870	1.429E-33	3.598E-06	4477.9858	29	E	30	E
304.980048	7.281E-32	1.863E-04	4481.1193	29	E	30	E
305.154980	1.873E-35	1.557E-08	4475.6052	29	F1	30	F2
305.165162	3.999E-32	3.416E-05	4481.2504	29	F1	30	F2
305.172258	1.949E-35	1.620E-08	4475.6084	29	F2	30	F1
305.380160	3.493E-37	8.598E-10	4472.7466	29	E	30	E
305.530181	1.546E-32	1.331E-05	4482.4867	29	F2	30	F1
305.676803	2.338E-35	4.714E-09	4176.8099	28	F1	29	F2
305.895712	1.080E-34	1.308E-08	4176.8099	28	A1	29	A2
305.905923	4.085E-32	3.520E-05	4482.2506	29	F1	30	F2
305.956648	2.075E-32	1.768E-05	4479.9246	29	F2	30	F1
306.571860	4.012E-35	8.249E-09	4179.8702	28	F1	29	F2
306.584664	2.789E-36	5.735E-10	4179.8699	28	F2	29	F1
306.588986	4.993E-34	4.357E-07	4484.1485	29	F1	30	F2
306.618800	1.472E-31	1.258E-04	4479.7968	29	F1	30	F2
306.685746	1.179E-32	9.989E-06	4477.9729	29	F2	30	F1
306.745714	7.356E-34	6.420E-07	4483.9971	29	F2	30	F1

306.906105	1.006E-31	8.670E-05	4481.2504	29	F1	30	F2
306.975628	6.799E-32	1.758E-04	4481.1193	29	E	30	E
307.187245	1.188E-35	2.415E-09	4176.8099	28	F1	29	F2
307.263455	1.008E-35	6.144E-09	4176.8099	28	E	29	E
307.300013	4.282E-34	3.598E-07	4475.6052	29	F1	30	F2
307.344342	1.552E-31	7.914E-05	4477.9479	29	A2	30	A1
307.908359	5.723E-32	4.880E-05	4477.9729	29	F2	30	F1
308.013449	5.690E-36	4.732E-09	4472.7467	29	F1	30	F2
308.042540	6.794E-32	3.559E-05	4482.7056	29	A2	30	A1
308.092260	5.627E-32	4.848E-05	4479.9246	29	F2	30	F1
308.113553	3.689E-32	9.447E-05	4477.9858	29	E	30	E
308.256156	3.514E-32	3.068E-05	4482.4867	29	F2	30	F1
308.359743	1.988E-33	1.714E-06	4479.7968	29	F1	30	F2
308.486890	2.868E-32	2.504E-05	4482.2506	29	F1	30	F2
308.759928	2.336E-38	1.918E-11	4469.3656	29	F2	30	F1
308.806663	3.807E-32	3.224E-05	4475.6052	29	F1	30	F2
309.004617	4.890E-32	2.562E-05	4481.7275	29	A1	30	A2
309.050229	3.274E-32	2.775E-05	4475.6084	29	F2	30	F1
309.487071	3.154E-33	2.754E-06	4481.2504	29	F1	30	F2
309.632161	7.350E-37	1.512E-10	4176.8099	28	F1	29	F2
309.638469	7.235E-37	4.466E-10	4176.8099	28	E	29	E
310.043971	4.123E-33	3.554E-06	4477.9729	29	F2	30	F1
310.109112	1.071E-32	2.700E-05	4472.7466	29	E	30	E
310.109132	3.718E-33	9.619E-06	4477.9858	29	E	30	E
310.158483	1.589E-32	1.336E-05	4472.7467	29	F1	30	F2
310.271801	2.626E-32	1.325E-05	4472.7469	29	A1	30	A2
310.272842	3.089E-33	2.635E-06	4475.6084	29	F2	30	F1
310.810427	1.503E-34	1.285E-07	4475.6052	29	F1	30	F2
310.818234	1.394E-33	1.218E-06	4479.9246	29	F2	30	F1
310.940710	1.148E-33	1.003E-06	4479.7968	29	F1	30	F2
311.394581	4.353E-33	3.623E-06	4469.3656	29	F1	30	F2
311.415106	4.346E-33	3.617E-06	4469.3656	29	F2	30	F1
311.665133	8.578E-35	7.268E-08	4472.7467	29	F1	30	F2

312.408454	7.864E-35	6.781E-08	4475.6084	29	F2	30	F1
312.551371	8.479E-34	7.317E-07	4475.6052	29	F1	30	F2
312.769946	3.229E-34	2.822E-07	4477.9729	29	F2	30	F1
312.800197	1.527E-33	8.006E-07	4477.9479	29	A2	30	A1
313.352795	8.648E-35	2.217E-07	4472.7466	29	E	30	E
313.539615	9.116E-37	7.670E-10	4469.3656	29	F1	30	F2
313.668897	7.015E-35	6.004E-08	4472.7467	29	F1	30	F2
315.046264	8.619E-37	7.307E-10	4469.3656	29	F1	30	F2
315.132337	4.310E-35	3.768E-08	4475.6052	29	F1	30	F2
315.134428	4.283E-35	3.744E-08	4475.6084	29	F2	30	F1
315.293077	1.208E-36	1.025E-09	4469.3656	29	F2	30	F1
315.348374	4.525E-35	1.172E-07	4472.7466	29	E	30	E
315.409840	4.054E-35	3.500E-08	4472.7467	29	F1	30	F2
316.515691	1.453E-36	1.241E-09	4469.3656	29	F2	30	F1
317.050029	9.858E-36	8.441E-09	4469.3656	29	F1	30	F2
317.985156	1.631E-35	8.558E-09	4472.7469	29	A1	30	A2
317.990807	3.221E-36	2.816E-09	4472.7467	29	F1	30	F2
318.651302	3.154E-36	2.722E-09	4469.3656	29	F2	30	F1
318.790972	1.738E-37	1.501E-10	4469.3656	29	F1	30	F2
321.371938	1.070E-37	9.364E-11	4469.3656	29	F1	30	F2
321.377277	1.058E-37	9.252E-11	4469.3656	29	F2	30	F1

Table 3

R-branch of methane main isotopomer (61 in HITRAN notation) up to  $J = 30$  with an intensity limit of  $10^{-39} \text{cm}^{-1}/(\text{molecule.cm}^{-2})$  at 296K. Simplified HITRAN format is used with HITRAN units. The entries are transition  $\nu_{\eta\eta'}$  in  $\text{cm}^{-1}$ , intensity  $S_{\eta\eta'}$  in  $\text{cm}^{-1}/(\text{molecule.cm}^{-2})$ , Einstein A-coefficient in  $\text{s}^{-1}$ , lower state energy in  $\text{cm}^{-1}$ , lower state  $J$ -value and irreps, upper state  $J$ -value and irreps.

0.001064	1.441E-36	9.183E-24	62.8746	3	F1	3	F2
0.001499	4.122E-39	7.146E-25	949.8224	13	F1	13	F2
0.002350	1.116E-37	1.006E-23	689.6918	11	F1	11	F2
0.003388	1.412E-36	7.660E-23	470.7079	9	F1	9	F2
0.003566	8.392E-36	2.560E-22	293.1175	7	F1	7	F2
0.003594	7.895E-36	1.709E-22	157.1214	5	F1	5	F2
0.004502	3.140E-34	9.777E-21	219.9327	6	F2	6	F1
0.005315	9.490E-35	2.879E-21	104.7728	4	F1	4	F2
0.005889	1.340E-38	3.748E-22	1778.9847	18	F2	18	F1
0.008290	6.623E-38	5.438E-17	3906.5350	27	F1	27	F2
0.009434	5.065E-37	4.382E-21	1417.0898	16	F2	16	F1
0.010071	4.238E-33	6.838E-19	470.8461	9	F1	9	F2
0.011007	1.345E-33	8.920E-20	157.1250	5	F2	5	F1
0.011900	3.602E-36	9.882E-17	3109.1940	24	F2	24	F1
0.012478	1.285E-38	2.481E-16	4486.4420	29	F2	29	F1
0.012816	1.268E-35	3.555E-20	1095.5971	14	F2	14	F1
0.014130	4.660E-33	5.634E-19	293.1591	7	F2	7	F1
0.014246	6.763E-34	2.319E-19	575.1591	10	F2	10	F1
0.014443	6.045E-38	3.337E-16	4191.6883	28	F1	28	F2
0.015226	2.215E-39	2.406E-20	2859.2506	23	F1	23	F2
0.015618	9.714E-35	1.270E-16	2400.1444	21	F1	21	F2
0.015626	9.872E-33	1.001E-17	815.1004	12	F2	12	F1
0.016041	9.565E-39	6.046E-16	4790.7321	30	A2	30	A1
0.017851	1.150E-34	1.331E-19	814.8507	12	F2	12	F1
0.018350	1.197E-33	1.052E-16	1780.6911	18	F2	18	F1
0.018660	5.940E-33	4.851E-17	1252.0027	15	F1	15	F2
0.018882	1.083E-36	5.506E-16	3631.0254	26	F1	26	F2
0.018927	5.542E-34	1.189E-19	376.7788	8	F2	8	F1
0.021302	4.103E-36	6.721E-16	3365.2268	25	F2	25	F1
0.021520	1.983E-32	4.837E-18	376.7977	8	F1	8	F2
0.022665	1.352E-37	2.535E-19	2397.7454	21	F1	21	F2
0.024883	9.952E-37	1.472E-15	3906.5265	27	A1	27	A2

0.025414	2.601E-32	2.743E-18	219.9158	6	A2	6	A1
0.025664	2.995E-32	1.851E-17	575.2489	10	F1	10	F2
0.026249	4.032E-33	7.319E-19	219.9109	6	F2	6	F1
0.026386	4.712E-35	9.031E-16	2862.9599	23	F2	23	F1
0.028886	1.413E-34	9.811E-16	2626.5933	22	F1	22	F2
0.031797	5.165E-32	6.308E-17	690.0044	11	F2	11	F1
0.032080	4.216E-33	1.568E-17	950.2862	13	F1	13	F2
0.033617	1.003E-33	1.034E-15	2183.6349	20	F1	20	F2
0.034470	4.289E-36	1.733E-18	1975.6790	19	F1	19	F2
0.035025	4.100E-32	1.666E-16	950.4689	13	F2	13	F1
0.035429	2.306E-33	9.648E-16	1977.1358	19	F2	19	F1
0.035772	5.438E-35	2.691E-15	3109.1814	24	A2	24	A1
0.038018	3.776E-32	3.148E-16	1096.1114	14	F1	14	F2
0.038286	1.611E-32	5.683E-16	1418.0701	16	F1	16	F2
0.038306	9.660E-33	7.574E-16	1594.3116	17	F2	17	F1
0.038859	1.065E-34	8.437E-18	1593.4887	17	F1	17	F2
0.041636	4.156E-33	1.480E-18	293.1175	7	F1	7	F2
0.042009	1.719E-31	6.944E-17	470.8221	9	A1	9	A2
0.047186	1.491E-33	3.534E-15	2400.1272	21	A1	21	A2
0.048588	4.414E-39	5.639E-18	3626.0473	26	F2	26	F1
0.052200	3.433E-32	1.533E-17	293.1210	7	F2	7	F1
0.052225	6.912E-33	4.092E-18	376.7266	8	F1	8	F2
0.054330	6.002E-33	3.001E-16	1417.7235	16	F2	16	F1
0.054673	2.402E-31	5.115E-16	815.0734	12	A2	12	A1
0.056269	6.819E-34	1.676E-17	1251.5649	15	F1	15	F2
0.056296	1.931E-32	3.125E-15	1780.6691	18	A2	18	A1
0.059603	1.090E-31	1.706E-15	1251.9769	15	A1	15	A2
0.059852	3.317E-32	3.181E-17	470.7964	9	F1	9	F2
0.060856	3.513E-33	8.210E-18	689.9436	11	F1	11	F2
0.063340	2.744E-37	3.944E-17	3105.8557	24	F2	24	F1
0.076147	2.855E-33	2.560E-15	1976.5290	19	F1	19	F2
0.080035	3.368E-32	1.035E-16	689.8635	11	F2	11	F1
0.080730	1.024E-36	3.127E-14	4189.5396	28	F2	28	F1

0.083399	1.733E-34	4.403E-16	2182.3471	20	F2	20	F1
0.085049	2.438E-32	3.321E-17	470.7113	9	F2	9	F1
0.085756	6.338E-32	1.848E-16	376.7285	8	E	8	E
0.089818	2.695E-32	5.829E-17	575.1591	10	F2	10	F1
0.090470	5.062E-34	1.096E-14	2625.6102	22	F2	22	F1
0.091815	3.513E-35	2.463E-14	3363.7351	25	F1	25	F2
0.092671	5.081E-32	5.337E-17	376.7266	8	F1	8	F2
0.094959	6.835E-36	1.545E-16	2624.4548	22	F2	22	F1
0.101236	1.399E-31	3.411E-16	575.1733	10	F1	10	F2
0.112345	4.902E-32	1.206E-15	1095.8473	14	F1	14	F2
0.123583	6.361E-32	5.101E-16	814.9924	12	F2	12	F1
0.123891	1.054E-31	8.464E-16	814.8685	12	F1	12	F2
0.127821	2.458E-39	4.708E-16	4479.7968	29	F1	29	F2
0.131811	2.915E-32	9.246E-17	575.0415	10	F2	10	F1
0.134831	1.655E-31	3.574E-16	470.7113	9	F2	9	F1
0.138417	8.414E-34	5.560E-16	1779.9448	18	F2	18	F1
0.139085	1.604E-37	2.162E-15	3901.9226	27	F1	27	F2
0.139622	7.780E-35	7.817E-15	2860.9932	23	F1	23	F2
0.139662	2.582E-37	2.338E-13	4788.0169	30	F1	30	F2
0.147694	3.065E-32	9.246E-15	1593.8444	17	F2	17	F1
0.148289	9.964E-32	2.367E-16	470.7079	9	F1	9	F2
0.151382	1.077E-36	2.492E-13	4483.9971	29	F2	29	F1
0.151783	5.218E-33	1.736E-16	1095.9596	14	F2	14	F1
0.153635	2.023E-31	3.580E-15	689.8729	11	E	11	E
0.160591	1.085E-31	7.613E-15	1251.6212	15	F2	15	F1
0.167462	6.023E-31	1.456E-15	575.0445	10	A2	10	A1
0.171728	1.281E-32	8.442E-17	689.6918	11	F1	11	F2
0.172688	1.419E-31	9.407E-16	689.8635	11	F2	11	F1
0.176202	1.601E-35	2.769E-13	3904.5642	27	F2	27	F1
0.178699	8.619E-33	4.705E-14	2182.8626	20	F1	20	F2
0.181776	4.985E-35	2.421E-13	3629.2807	26	F1	26	F2
0.182689	4.693E-32	9.945E-16	950.2862	13	F1	13	F2
0.185634	1.441E-31	3.103E-15	950.3183	13	F2	13	F1

0.189723	4.083E-32	3.702E-14	1780.0832	18	F1	18	F2
0.192560	1.019E-33	1.417E-13	2861.7661	23	F2	23	F1
0.195078	1.229E-35	6.368E-14	3628.1077	26	F2	26	F1
0.200289	4.767E-34	2.188E-13	3107.8115	24	F1	24	F2
0.200676	1.032E-31	2.401E-15	950.1176	13	F1	13	F2
0.204819	6.574E-33	1.123E-13	2399.2098	21	F2	21	F1
0.207384	2.462E-31	1.229E-15	575.0415	10	F2	10	F1
0.218100	2.980E-36	4.925E-15	3362.1204	25	F1	25	F2
0.218832	8.336E-33	1.182E-16	814.6318	12	F1	12	F2
0.220921	1.592E-31	2.539E-15	575.0401	10	E	10	E
0.231566	1.071E-30	1.725E-14	950.1350	13	A1	13	A2
0.231848	3.395E-31	5.106E-15	814.8685	12	F1	12	F2
0.236080	7.961E-37	2.851E-13	4482.2506	29	F1	29	F2
0.239522	4.330E-32	4.537E-15	1251.7818	15	F1	15	F2
0.246821	3.090E-38	4.860E-14	4784.4118	30	F2	30	F1
0.249412	4.538E-31	4.343E-15	689.6942	11	F2	11	F1
0.250193	3.532E-32	1.934E-15	1095.5971	14	F2	14	F1
0.250201	1.718E-35	9.755E-13	4189.4398	28	A2	28	A1
0.262560	1.761E-31	3.040E-14	1095.8728	14	E	14	E
0.265325	2.154E-31	3.707E-15	814.8507	12	F2	12	F1
0.286042	5.916E-31	9.341E-14	1417.5496	16	A2	16	A1
0.287820	8.309E-32	2.199E-14	1417.4900	16	F2	16	F1
0.288820	2.096E-32	2.642E-15	1251.2761	15	F2	15	F1
0.293696	7.161E-33	2.434E-16	949.8239	13	F2	13	F1
0.293760	3.260E-34	7.974E-15	2398.9160	21	F1	21	F2
0.299086	6.993E-34	9.581E-13	3363.6037	25	A1	25	A2
0.302146	1.096E-31	7.260E-15	1095.8473	14	F1	14	F2
0.312619	4.047E-31	4.856E-15	689.6918	11	F1	11	F2
0.319540	2.602E-33	1.700E-15	1593.9921	17	F1	17	F2
0.319703	1.346E-31	3.040E-13	1976.3528	19	A1	19	A2
0.324522	1.401E-32	6.529E-13	2625.4506	22	A2	22	A1
0.330582	5.787E-32	1.762E-14	1417.7778	16	F1	16	F2
0.342066	1.386E-32	1.820E-16	689.6942	11	F2	11	F1

0.344679	4.090E-31	2.741E-14	814.6328	12	E	12	E
0.346626	3.055E-32	9.752E-15	1417.7235	16	F2	16	F1
0.349722	5.943E-31	4.551E-14	1095.6099	14	F1	14	F2
0.351285	3.628E-31	1.478E-14	950.1176	13	F1	13	F2
0.353332	1.363E-32	2.297E-14	1779.5915	18	F1	18	F2
0.355675	2.570E-32	1.865E-14	1593.4887	17	F1	17	F2
0.360574	4.886E-31	1.142E-14	814.6318	12	F1	12	F2
0.376069	2.753E-31	3.601E-14	950.1105	13	E	13	E
0.380475	3.775E-33	3.139E-16	1095.2294	14	F2	14	F1
0.381453	1.992E-31	3.322E-14	1251.6212	15	F2	15	F1
0.390704	2.229E-32	7.995E-15	1417.0993	16	F1	16	F2
0.408950	2.471E-32	1.189E-13	1976.1962	19	F1	19	F2
0.410994	3.572E-33	1.220E-13	2398.5050	21	F2	21	F1
0.436488	1.221E-32	2.550E-14	1780.2730	18	F2	18	F1
0.439572	5.825E-32	1.571E-13	1593.8942	17	E	17	E
0.442089	4.403E-37	7.287E-14	4187.2323	28	F2	28	F1
0.443460	9.681E-31	1.670E-14	814.6300	12	A1	12	A2
0.456383	1.410E-31	2.814E-14	1251.5649	15	F1	15	F2
0.462292	7.001E-31	3.748E-14	949.8239	13	F2	13	F1
0.464134	4.685E-34	4.961E-13	3106.7859	24	F1	24	F2
0.464510	2.492E-31	2.363E-13	1593.5275	17	F2	17	F1
0.466020	1.343E-33	2.727E-16	1250.8101	15	F1	15	F2
0.468531	1.051E-31	3.191E-15	814.6318	12	F1	12	F2
0.472444	4.327E-31	2.677E-13	1251.2819	15	E	15	E
0.482768	1.682E-32	9.534E-14	1975.7135	19	F2	19	F1
0.495871	5.607E-31	3.220E-14	949.8224	13	F1	13	F2
0.505540	3.210E-32	3.318E-14	1593.8444	17	F2	17	F1
0.505681	4.507E-31	9.951E-14	1251.2761	15	F2	15	F1
0.510594	3.390E-35	1.688E-12	3903.0692	27	F2	27	F1
0.513711	1.145E-32	1.198E-14	1593.0138	17	F1	17	F2
0.514322	5.275E-31	5.942E-14	1095.5971	14	F2	14	F1
0.515502	7.636E-33	1.200E-13	2182.3471	20	F2	20	F1
0.534331	1.314E-36	4.511E-12	4785.8813	30	F1	30	F2



0.539523	2.942E-32	3.476E-15	1095.6099	14	F1	14	F2
0.556861	4.327E-33	5.744E-13	2624.5498	22	F1	22	F2
0.561404	4.879E-35	6.265E-14	3107.2501	24	F2	24	F1
0.565926	5.068E-34	2.627E-16	1416.5239	16	F1	16	F2
0.566026	1.049E-32	7.004E-14	1976.6052	19	F2	19	F1
0.576143	1.231E-30	9.308E-14	1095.2306	14	A2	14	A1
0.580116	1.600E-31	8.544E-14	1417.4900	16	F2	16	F1
0.593681	5.196E-34	9.440E-15	2183.0413	20	F2	20	F1
0.594068	3.372E-33	4.789E-13	2625.1066	22	F2	22	F1
0.602853	4.535E-34	2.076E-12	3362.3385	25	F2	25	F1
0.606744	8.036E-33	5.749E-14	1976.5290	19	F1	19	F2
0.606825	3.072E-33	8.868E-15	1778.9847	18	F2	18	F1
0.607860	4.482E-32	1.303E-13	1780.0832	18	F1	18	F2
0.610801	4.373E-32	8.149E-13	2182.4305	20	F1	20	F2
0.614003	2.200E-35	5.070E-12	4187.6744	28	F1	28	F2
0.617852	6.895E-31	9.315E-14	1095.2294	14	F2	14	F1
0.618418	1.562E-31	1.383E-12	1779.6116	18	E	18	E
0.620038	1.522E-31	2.605E-13	1417.4697	16	E	16	E
0.624194	5.683E-31	3.259E-13	1417.0993	16	F1	16	F2
0.643980	4.619E-31	1.952E-13	1095.2288	14	E	14	E
0.646481	1.519E-31	1.138E-14	949.8224	13	F1	13	F2
0.662456	8.288E-33	1.670E-13	2181.7680	20	F2	20	F1
0.680007	6.953E-33	5.478E-16	949.8239	13	F2	13	F1
0.681472	1.406E-31	4.573E-13	1779.5915	18	F1	18	F2
0.687957	4.103E-31	2.594E-13	1417.0898	16	F2	16	F1
0.689109	1.930E-34	2.700E-16	1592.3247	17	F2	17	F1
0.711416	1.036E-30	1.931E-13	1251.2655	15	A2	15	A1
0.712384	1.061E-33	8.848E-15	1974.9666	19	F2	19	F1
0.715149	8.328E-33	5.467E-13	2182.9381	20	E	20	E
0.726543	1.653E-31	5.246E-14	1251.2761	15	F2	15	F1
0.728662	8.268E-31	7.365E-13	1593.0216	17	A1	17	A2
0.745490	1.529E-33	9.523E-14	2399.4146	21	F1	21	F2
0.753976	6.569E-31	2.159E-13	1250.8110	15	F2	15	F1

0.759614	1.681E-33	1.058E-13	2397.7454	21	F1	21	F2
0.764627	3.872E-32	1.416E-13	1779.9448	18	F2	18	F1
0.772913	1.097E-33	6.109E-13	2860.9932	23	F1	23	F2
0.799973	2.506E-32	5.005E-12	2398.5559	21	E	21	E
0.805997	3.854E-33	9.504E-14	2182.8626	20	F1	20	F2
0.811110	6.811E-31	2.408E-13	1250.8101	15	F1	15	F2
0.815570	1.568E-31	1.502E-12	1975.7135	19	F2	19	F1
0.821540	1.921E-33	1.134E-12	2860.3113	23	F1	23	F2
0.822356	1.956E-32	3.286E-14	1593.5275	17	F2	17	F1
0.822910	2.263E-31	3.804E-13	1593.4887	17	F1	17	F2
0.825636	6.133E-35	2.401E-16	1778.1649	18	F2	18	F1
0.825850	3.665E-33	2.183E-12	2861.1328	23	F2	23	F1
0.830528	4.386E-31	7.423E-13	1593.0138	17	F1	17	F2
0.849291	5.369E-34	1.083E-13	2623.6055	22	F1	22	F2
0.862608	2.002E-31	3.154E-12	2181.7981	20	A2	20	A1
0.866599	4.311E-34	1.132E-14	2180.9014	20	F1	20	F2
0.881981	5.391E-32	1.040E-14	1095.2294	14	F2	14	F1
0.884094	2.965E-31	1.603E-12	1593.0101	17	E	17	E
0.885582	2.341E-34	1.580E-12	3362.9413	25	F1	25	F2
0.906539	3.893E-32	2.317E-14	1095.2288	14	E	14	E
0.909574	1.943E-32	1.471E-12	2398.5050	21	F2	21	F1
0.921528	8.956E-34	1.980E-13	2625.7007	22	F1	22	F2
0.926187	1.076E-31	1.171E-12	1975.6790	19	F1	19	F2
0.930261	3.247E-34	6.869E-13	3105.8557	24	F2	24	F1
0.934692	4.297E-33	3.354E-13	2399.2098	21	F2	21	F1
0.939547	2.819E-32	3.121E-13	1976.1962	19	F1	19	F2
0.945452	3.780E-31	9.830E-13	1416.5242	16	E	16	E
0.954269	3.451E-31	1.568E-12	1778.9905	18	F1	18	F2
0.959675	2.244E-32	9.292E-12	2860.4005	23	A1	23	A2
0.960402	9.618E-35	6.981E-13	3361.1600	25	F2	25	F1
0.966064	5.556E-31	4.921E-13	1416.5239	16	F1	16	F2
0.970837	1.079E-32	4.571E-15	1250.8110	15	F2	15	F1
0.971209	1.682E-35	1.904E-16	1973.9954	19	F1	19	F2

0.978119	3.808E-35	3.388E-11	4481.7275	29	A1	29	A2
0.980254	1.954E-31	1.761E-13	1417.0898	16	F2	16	F1
0.983113	8.576E-34	2.022E-13	2625.6102	22	F2	22	F1
0.984377	3.182E-36	3.066E-13	3903.5798	27	F1	27	F2
1.000079	3.606E-32	1.274E-12	1976.1538	19	E	19	E
1.000166	1.709E-34	4.534E-12	3627.3026	26	F2	26	F1
1.001191	4.527E-35	3.284E-14	2861.9587	23	F1	23	F2
1.002400	1.274E-33	2.035E-11	3627.5233	26	A2	26	A1
1.009105	1.028E-32	9.539E-15	1417.0993	16	F1	16	F2
1.026386	1.001E-30	5.652E-13	1416.5233	16	A1	16	A2
1.034891	1.295E-34	1.106E-14	2396.7332	21	F1	21	F2
1.036899	7.455E-36	2.884E-12	4186.1954	28	F1	28	F2
1.045455	2.521E-34	1.885E-13	2859.2659	23	F2	23	F1
1.054834	1.969E-33	1.424E-11	3106.8874	24	E	24	E
1.060458	1.886E-32	4.773E-12	2624.5498	22	F1	22	F2
1.094559	9.715E-32	3.238E-12	2181.7680	20	F2	20	F1
1.098574	3.663E-31	1.917E-12	1778.9847	18	F2	18	F1
1.099609	7.582E-32	3.983E-13	1779.5915	18	F1	18	F2
1.111764	3.836E-31	1.222E-12	1779.5573	18	A1	18	A2
1.116381	5.472E-34	1.328E-12	2861.8573	23	E	23	E
1.133396	4.393E-36	1.501E-16	2179.7645	20	F1	20	F2
1.146556	2.746E-35	3.058E-12	3901.9226	27	F1	27	F2
1.147943	6.651E-32	6.335E-12	2397.7681	21	F2	21	F1
1.159681	1.626E-34	5.027E-12	3628.3028	26	F1	26	F2
1.163962	4.403E-31	1.042E-12	1592.3247	17	F2	17	F1
1.172982	8.028E-35	2.508E-12	3628.1077	26	F2	26	F1
1.183591	6.921E-32	7.484E-12	2181.7545	20	E	20	E
1.184863	1.646E-31	6.856E-12	1974.9689	19	E	19	E
1.191699	2.754E-32	1.432E-14	1250.8110	15	F2	15	F1
1.194106	8.855E-35	2.431E-13	3108.0118	24	F2	24	F1
1.194866	3.047E-35	8.603E-15	2622.4107	22	F2	22	F1
1.199554	2.436E-32	2.681E-14	1416.5239	16	F1	16	F2
1.203294	4.389E-31	1.074E-12	1592.3243	17	F1	17	F2

1.206746	5.438E-35	1.731E-12	3626.0959	26	F1	26	F2
1.211224	2.275E-32	1.203E-14	1250.8101	15	F1	15	F2
1.220137	1.983E-34	1.752E-13	2861.7661	23	F2	23	F1
1.225827	1.320E-33	3.699E-12	3106.7859	24	F1	24	F2
1.229622	2.287E-31	3.296E-12	1974.9666	19	F2	19	F1
1.236262	6.965E-36	1.303E-11	4481.2504	29	F1	29	F2
1.238100	5.280E-33	1.998E-13	2182.4305	20	F1	20	F2
1.244070	5.099E-33	5.294E-13	2398.9160	21	F1	21	F2
1.245887	1.312E-32	3.902E-12	2624.4548	22	F2	22	F1
1.263815	7.297E-35	2.086E-13	3104.6552	24	F2	24	F1
1.282408	9.730E-33	5.947E-14	1778.9905	18	F1	18	F2
1.287881	4.193E-32	1.650E-12	2182.3471	20	F2	20	F1
1.297762	5.855E-32	1.550E-13	1593.0138	17	F1	17	F2
1.315344	1.085E-36	1.172E-16	2395.4178	21	F2	21	F1
1.323665	4.669E-32	3.783E-13	1593.0101	17	E	17	E
1.325817	4.822E-36	9.612E-12	4479.9246	29	F2	29	F1
1.331055	5.992E-33	1.816E-11	3105.9190	24	F1	24	F2
1.331938	8.544E-36	4.292E-12	4188.2884	28	F2	28	F1
1.373065	7.305E-36	7.131E-15	2857.8776	23	F2	23	F1
1.382495	1.882E-34	5.979E-13	3107.8115	24	F1	24	F2
1.390738	4.571E-31	4.471E-12	1974.9620	19	A2	19	A1
1.392089	5.173E-31	2.052E-12	1778.1653	18	A2	18	A1
1.396621	1.091E-33	1.159E-11	3362.3385	25	F2	25	F1
1.419490	2.694E-32	2.728E-11	2623.6151	22	E	22	E
1.421209	3.664E-35	3.991E-13	3363.8269	25	F2	25	F1
1.426573	3.126E-31	2.118E-12	1778.1649	18	F2	18	F1
1.428936	1.391E-35	1.494E-13	3359.7310	25	F1	25	F2
1.436284	7.906E-35	3.332E-11	3903.2335	27	E	27	E
1.445656	1.578E-31	6.921E-12	2180.9014	20	F1	20	F2
1.446864	2.116E-31	4.361E-12	1778.1647	18	E	18	E
1.454830	9.458E-33	9.901E-12	2860.3113	23	F1	23	F2
1.456785	7.517E-32	1.288E-12	1975.6790	19	F1	19	F2
1.457744	4.439E-33	7.616E-14	1975.7135	19	F2	19	F1

1.464368	7.253E-32	8.818E-12	2397.7454	21	F1	21	F2
1.469434	1.177E-36	1.105E-11	4784.4118	30	F2	30	F1
1.486710	2.254E-33	8.030E-13	2625.1066	22	F2	22	F1
1.491722	3.841E-35	4.390E-13	3363.7351	25	F1	25	F2
1.501110	3.380E-32	1.207E-11	2623.6055	22	F1	22	F2
1.507335	1.542E-35	2.244E-12	3900.5544	27	F1	27	F2
1.513270	2.448E-37	8.695E-17	2620.8994	22	F2	22	F1
1.518065	2.736E-34	4.040E-11	3902.0617	27	F2	27	F1
1.520110	1.885E-32	5.830E-14	1592.3243	17	F1	17	F2
1.532612	1.500E-31	6.977E-12	2180.8979	20	F2	20	F1
1.562424	2.746E-32	5.033E-13	1974.9666	19	F2	19	F1
1.562945	1.794E-36	7.524E-14	3629.4625	26	F2	26	F1
1.565490	1.446E-32	6.237E-14	1416.5242	16	E	16	E
1.573400	4.128E-33	4.667E-12	2625.0346	22	E	22	E
1.581799	7.639E-33	2.609E-11	2860.2755	23	E	23	E
1.583318	1.739E-36	6.186E-15	3103.0719	24	F1	24	F2
1.584465	1.218E-32	1.773E-14	1416.5239	16	F1	16	F2
1.601281	9.722E-38	1.005E-12	4786.4156	30	F2	30	F1
1.610682	3.057E-36	1.290E-13	3624.4366	26	F1	26	F2
1.639446	1.401E-32	1.915E-12	2398.5050	21	F2	21	F1
1.645936	2.121E-33	7.930E-11	3361.1893	25	E	25	E
1.646522	2.967E-33	4.058E-13	2397.7681	21	F2	21	F1
1.661823	3.989E-36	1.010E-11	4482.4867	29	F2	29	F1
1.664160	1.717E-35	2.300E-12	3629.3709	26	E	26	E
1.666393	2.272E-36	1.403E-12	4184.5290	28	F2	28	F1
1.667331	1.348E-33	4.575E-15	1592.3247	17	F2	17	F1
1.671173	4.556E-35	7.444E-12	3903.0692	27	F2	27	F1
1.683345	2.026E-31	3.983E-12	1973.9956	19	F2	19	F1
1.687104	1.534E-31	1.284E-11	2396.7359	21	A1	21	A2
1.700546	2.653E-32	2.152E-13	1778.9905	18	F1	18	F2
1.704252	6.474E-32	5.517E-12	2398.4230	21	A2	21	A1
1.706535	8.283E-34	1.075E-11	3362.1204	25	F1	25	F2
1.718063	2.072E-31	4.158E-12	1973.9954	19	F1	19	F2

1.724785	2.265E-32	1.864E-13	1778.9847	18	F2	18	F1
1.726130	5.084E-38	6.192E-17	2856.1514	23	F1	23	F2
1.727372	2.138E-32	2.645E-11	2859.2659	23	F2	23	F1
1.746522	2.920E-36	7.764E-12	4482.2506	29	F1	29	F2
1.753470	1.319E-36	1.469E-11	4782.9052	30	F2	30	F1
1.756944	6.567E-36	7.388E-11	4784.6586	30	F1	30	F2
1.763603	4.809E-36	2.275E-13	3629.2807	26	F1	26	F2
1.771839	9.193E-32	1.347E-11	2396.7332	21	F1	21	F2
1.781355	2.322E-33	3.133E-11	3361.1600	25	F2	25	F1
1.802895	2.443E-36	4.343E-13	3904.7404	27	F1	27	F2
1.808812	3.649E-37	4.920E-15	3357.9315	25	F1	25	F2
1.823890	4.598E-37	1.251E-12	4477.9729	29	F2	29	F1
1.824115	6.310E-32	2.855E-11	2396.7318	21	E	21	E
1.853428	6.200E-34	8.309E-13	2861.1328	23	F2	23	F1
1.858223	7.350E-37	1.308E-13	3898.6962	27	F2	27	F1
1.863199	7.924E-32	2.109E-11	2623.5874	22	A1	22	A2
1.865211	3.151E-35	2.213E-11	4187.6744	28	F1	28	F2
1.866939	2.026E-32	1.154E-12	2181.7680	20	F2	20	F1
1.879464	8.807E-35	1.857E-10	4186.2684	28	E	28	E
1.882220	1.849E-32	2.494E-11	2859.2506	23	F1	23	F2
1.898739	1.649E-32	2.865E-12	2181.7545	20	E	20	E
1.918322	5.864E-33	5.348E-14	1778.1649	18	F2	18	F1
1.950822	1.755E-32	4.656E-11	3104.6673	24	A2	24	A1
1.955799	3.447E-34	1.547E-12	3107.2501	24	F2	24	F1
1.955799	6.786E-33	3.025E-11	3105.8557	24	F2	24	F1
1.956713	9.934E-39	4.330E-17	3101.1140	24	F1	24	F2
1.964714	2.048E-32	1.222E-12	2180.8979	20	F2	20	F1
1.966664	3.686E-33	5.240E-12	2860.9932	23	F1	23	F2
1.970807	4.033E-36	7.834E-13	3904.5642	27	F2	27	F1
1.978070	4.445E-34	2.337E-11	3627.3026	26	F2	26	F1
1.987344	1.193E-33	4.830E-15	1592.3243	17	F1	17	F2
1.989991	8.161E-32	1.472E-11	2179.7645	20	E	20	E
1.995580	1.647E-36	6.363E-11	4786.0994	30	E	30	E

2.003552	1.231E-31	7.451E-12	2179.7645	20	F1	20	F2
2.004708	8.658E-33	4.133E-12	2623.6055	22	F1	22	F2
2.011834	1.384E-33	7.355E-11	3626.0959	26	F1	26	F2
2.025177	1.207E-32	4.979E-14	1592.3247	17	F2	17	F1
2.033857	2.092E-31	7.718E-12	2179.7643	20	A1	20	A2
2.041953	6.871E-38	3.642E-15	3622.3947	26	F2	26	F1
2.042131	4.959E-32	2.398E-11	2622.4127	22	F1	22	F2
2.065282	3.841E-33	1.132E-13	1778.1647	18	E	18	E
2.072456	7.490E-34	3.714E-13	2624.5498	22	F1	22	F2
2.082411	7.341E-37	5.813E-13	4189.6203	28	F1	28	F2
2.092748	4.158E-34	1.985E-12	3105.9190	24	F1	24	F2
2.092991	8.255E-35	6.462E-11	4186.1954	28	F1	28	F2
2.120803	1.446E-37	1.126E-13	4182.4395	28	F2	28	F1
2.124501	1.198E-37	1.601E-12	4780.7807	30	F1	30	F2
2.130736	1.027E-32	4.960E-11	3104.6552	24	F2	24	F1
2.138529	1.230E-32	6.290E-12	2624.4548	22	F2	22	F1
2.139116	5.207E-32	2.638E-11	2622.4107	22	F2	22	F1
2.139856	1.130E-33	7.351E-14	2180.9014	20	F1	20	F2
2.143599	4.411E-34	7.540E-11	3627.2273	26	E	26	E
2.148698	7.797E-37	6.369E-13	4189.5396	28	F2	28	F1
2.155389	9.876E-34	1.235E-10	3900.5952	27	A1	27	A2
2.184942	1.135E-32	8.741E-13	1974.9689	19	E	19	E
2.200582	1.107E-33	2.848E-14	1973.9956	19	F2	19	F1
2.204598	1.016E-32	2.630E-13	1974.9666	19	F2	19	F1
2.206051	1.828E-39	2.977E-17	3355.7255	25	F2	25	F1
2.238139	7.149E-33	1.088E-10	3104.6493	24	E	24	E
2.255500	1.080E-33	6.439E-11	3626.0473	26	F2	26	F1
2.273541	2.987E-35	2.592E-10	4783.0187	30	A2	30	A1
2.275274	7.794E-37	1.144E-11	4785.8813	30	F1	30	F2
2.285490	9.070E-35	1.585E-12	3362.9413	25	F1	25	F2
2.293535	3.336E-38	1.177E-13	4484.1485	29	F1	29	F2
2.293896	1.239E-38	2.695E-15	3896.3967	27	F2	27	F1
2.325998	4.606E-35	1.615E-10	4479.9246	29	F2	29	F1

2.327570	6.832E-32	1.308E-11	2395.4178	21	F2	21	F1
2.350362	6.899E-32	1.334E-11	2395.4177	21	F1	21	F2
2.367738	2.404E-38	8.403E-14	4475.6052	29	F1	29	F2
2.375015	2.669E-37	2.925E-12	4484.0733	29	E	29	E
2.376395	8.026E-33	1.587E-12	2397.7681	21	F2	21	F1
2.380040	4.679E-33	8.386E-11	3359.7403	25	F2	25	F1
2.388030	2.872E-35	2.580E-11	4187.2323	28	F2	28	F1
2.397219	1.684E-32	8.634E-11	2857.8783	23	E	23	E
2.402285	2.418E-34	1.332E-11	3362.8353	25	E	25	E
2.408033	1.168E-33	6.446E-12	3106.7859	24	F1	24	F2
2.414678	6.862E-33	1.379E-12	2397.7454	21	F1	21	F2
2.433746	2.538E-32	4.403E-11	2857.8776	23	F2	23	F1
2.457394	6.074E-38	2.296E-13	4483.9971	29	F2	29	F1
2.476594	4.849E-33	9.947E-13	2396.7332	21	F1	21	F2
2.496581	6.665E-33	7.571E-11	3361.1071	25	A2	25	A1
2.514806	5.519E-34	1.344E-10	3900.5544	27	F1	27	F2
2.515511	5.952E-33	1.075E-11	2859.2506	23	F1	23	F2
2.524458	4.465E-32	4.822E-11	2857.8761	23	A2	23	A1
2.533385	1.884E-33	5.586E-14	1973.9956	19	F2	19	F1
2.544533	3.234E-33	3.917E-14	1778.1649	18	F2	18	F1
2.560149	1.444E-32	1.056E-13	1778.1653	18	A2	18	A1
2.563274	5.609E-33	1.977E-11	3106.6182	24	A1	24	A2
2.569287	2.132E-39	1.989E-15	4179.8702	28	F1	28	F2
2.575122	1.051E-33	2.052E-11	3361.1600	25	F2	25	F1
2.582609	6.190E-34	4.838E-14	2179.7645	20	F1	20	F2
2.586313	3.308E-38	5.584E-13	4788.1565	30	F2	30	F1
2.607437	5.098E-33	1.002E-10	3359.7310	25	F1	25	F2
2.609781	1.856E-33	5.669E-14	1973.9954	19	F1	19	F2
2.624088	3.217E-33	2.098E-12	2396.7318	21	E	21	E
2.634646	3.991E-39	6.536E-14	4778.1255	30	F1	30	F2
2.641527	3.292E-34	8.475E-11	3901.9226	27	F1	27	F2
2.648581	3.130E-33	5.983E-12	2860.3113	23	F1	23	F2
2.671999	2.169E-34	2.153E-10	4184.5603	28	F1	28	F2



2.678644	2.980E-35	7.787E-12	3902.0617	27	F2	27	F1
2.687851	5.876E-32	2.231E-11	2620.8995	22	A2	22	A1
2.689900	3.382E-35	1.371E-10	4479.7968	29	F1	29	F2
2.692845	3.039E-34	5.877E-13	2859.2659	23	F2	23	F1
2.693950	6.384E-34	4.079E-13	2622.4127	22	F1	22	F2
2.698180	2.415E-33	1.411E-11	2860.2755	23	E	23	E
2.698196	3.927E-34	3.078E-10	3900.5353	27	E	27	E
2.706109	3.551E-32	2.262E-11	2620.8994	22	F2	22	F1
2.715734	2.379E-32	4.562E-11	2620.8994	22	E	22	E
2.720628	4.487E-38	7.963E-13	4788.0169	30	F1	30	F2
2.737094	6.848E-34	5.706E-14	2180.8979	20	F2	20	F1
2.741508	3.358E-35	2.463E-12	3628.3028	26	F1	26	F2
2.746703	1.057E-35	4.408E-11	4481.2504	29	F1	29	F2
2.767155	8.074E-33	6.803E-13	2180.9014	20	F1	20	F2
2.783793	1.187E-32	7.448E-11	3103.0719	24	F1	24	F2
2.787081	1.362E-33	2.990E-10	3624.4402	26	E	26	E
2.848258	1.208E-32	7.753E-11	3103.0707	24	F2	24	F1
2.866016	2.016E-33	1.518E-10	3624.4366	26	F1	26	F2
2.909645	5.486E-35	1.219E-12	3362.3385	25	F2	25	F1
2.917704	1.580E-34	1.233E-11	3628.1077	26	F2	26	F1
2.954027	1.401E-35	1.885E-10	4481.1193	29	E	29	E
2.963474	1.237E-35	3.606E-12	3903.5798	27	F1	27	F2
2.976083	1.536E-35	2.911E-10	4782.9052	30	F2	30	F1
2.992890	2.819E-33	6.043E-12	2623.6151	22	E	22	E
3.016706	2.633E-33	1.896E-12	2623.6055	22	F1	22	F2
3.087310	2.550E-34	6.488E-14	2395.4177	21	F1	21	F2
3.093908	3.807E-33	1.857E-10	3624.4294	26	A1	26	A2
3.099131	1.707E-32	3.744E-11	2856.1515	23	F2	23	F1
3.106443	9.905E-34	2.348E-11	3362.1204	25	F1	25	F2
3.114420	1.718E-32	3.788E-11	2856.1514	23	F1	23	F2
3.115663	4.933E-34	1.097E-12	2857.8776	23	F2	23	F1
3.133504	5.485E-35	7.714E-10	4477.9858	29	E	29	E
3.140378	2.194E-34	8.073E-15	1973.9954	19	F1	19	F2

3.145381	2.468E-34	2.888E-10	4184.5290	28	F2	28	F1
3.156274	1.138E-33	8.167E-12	3104.6552	24	F2	24	F1
3.173582	1.001E-33	2.887E-13	2179.7645	20	E	20	E
3.174765	8.576E-33	1.222E-10	3357.9323	25	A1	25	A2
3.175558	2.383E-33	8.870E-14	1973.9956	19	F2	19	F1
3.197548	1.447E-33	1.099E-12	2622.4127	22	F1	22	F2
3.200993	1.091E-34	2.635E-12	3359.7403	25	F2	25	F1
3.226474	8.168E-34	2.532E-10	3898.6962	27	F2	27	F1
3.228450	5.221E-33	1.261E-10	3357.9315	25	F1	25	F2
3.233404	6.442E-34	5.519E-11	3626.0473	26	F2	26	F1
3.243683	1.161E-35	7.198E-10	4782.8557	30	E	30	E
3.258228	3.525E-33	2.577E-10	3357.9311	25	E	25	E
3.274954	1.079E-33	8.086E-12	3105.9190	24	F1	24	F2
3.276809	8.310E-34	8.255E-14	2179.7645	20	F1	20	F2
3.277528	7.678E-35	3.766E-10	4477.9729	29	F2	29	F1
3.290044	1.264E-33	9.879E-13	2622.4107	22	F2	22	F1
3.292973	8.175E-34	1.836E-11	3104.6493	24	E	24	E
3.344198	5.787E-35	7.261E-11	4186.1954	28	F1	28	F2
3.350195	8.843E-34	6.776E-12	3105.8557	24	F2	24	F1
3.366593	3.442E-35	3.072E-12	3626.0959	26	F1	26	F2
3.368220	2.992E-34	2.267E-10	4186.0716	28	A1	28	A2
3.371155	8.266E-34	2.679E-10	3898.6906	27	F1	27	F2
3.399906	1.975E-36	2.545E-12	4188.2884	28	F2	28	F1
3.426904	1.702E-33	4.842E-13	2396.7332	21	F1	21	F2
3.438542	8.005E-33	1.371E-12	2396.7359	21	A1	21	A2
3.465778	4.534E-35	1.543E-11	3903.0692	27	F2	27	F1
3.497887	1.111E-36	2.498E-11	4784.6586	30	F1	30	F2
3.498178	5.158E-35	1.489E-14	2395.4178	21	F2	21	F1
3.535223	5.126E-33	1.216E-10	3101.1141	24	E	24	E
3.541156	7.706E-33	6.102E-11	3101.1140	24	F1	24	F2
3.547625	7.398E-36	2.983E-11	4188.1479	28	E	28	E
3.553355	1.291E-32	6.153E-11	3101.1140	24	A1	24	A2
3.605046	8.610E-36	1.994E-10	4784.4118	30	F2	30	F1

3.627827	4.998E-34	4.010E-10	4182.4438	28	A2	28	A1
3.631150	2.816E-35	6.454E-10	4780.7807	30	F1	30	F2
3.650359	6.511E-35	5.609E-14	2620.8994	22	F2	22	F1
3.652025	2.112E-33	2.010E-10	3622.3953	26	F1	26	F2
3.671104	1.192E-34	1.152E-11	3624.4366	26	F1	26	F2
3.701223	2.150E-33	2.074E-10	3622.3947	26	F2	26	F1
3.709262	1.264E-34	3.373E-13	2859.2506	23	F1	23	F2
3.715179	2.070E-34	1.737E-12	3103.0707	24	F2	24	F1
3.720422	1.711E-33	4.583E-12	2859.2659	23	F2	23	F1
3.722792	2.475E-34	2.459E-11	3627.3026	26	F2	26	F1
3.728091	8.115E-36	1.127E-11	4184.5603	28	F1	28	F2
3.755903	3.060E-34	4.237E-10	4182.4395	28	F2	28	F1
3.775928	2.685E-34	5.970E-11	3902.7505	27	A2	27	A1
3.779539	1.648E-34	5.600E-10	4477.9479	29	A2	29	A1
3.792065	9.131E-35	2.859E-14	2395.4177	21	F1	21	F2
3.807759	1.722E-34	5.248E-11	3627.2273	26	E	26	E
3.831098	2.096E-34	8.882E-10	4182.4373	28	E	28	E
3.888731	5.225E-34	1.851E-13	2179.7645	20	E	20	E
3.898504	2.726E-35	6.712E-10	4780.7601	30	F2	30	F1
3.904108	4.763E-34	5.646E-14	2179.7645	20	F1	20	F2
3.967835	8.939E-37	5.435E-12	4482.4867	29	F2	29	F1
3.979018	5.601E-34	4.784E-12	2857.8783	23	E	23	E
3.994761	3.152E-34	9.519E-12	3359.7403	25	F2	25	F1
3.996757	7.331E-34	2.420E-13	2395.4178	21	F2	21	F1
4.005566	3.241E-33	9.627E-11	3355.7255	25	F2	25	F1
4.009777	1.079E-34	4.204E-11	3900.5544	27	F1	27	F2
4.014895	3.252E-33	9.680E-11	3355.7254	25	F1	25	F2
4.028352	1.817E-36	2.769E-12	4187.6744	28	F1	28	F2
4.048221	3.073E-34	2.842E-11	3361.1893	25	E	25	E
4.081136	4.605E-34	1.345E-12	2857.8776	23	F2	23	F1
4.088146	2.954E-34	9.194E-12	3361.1600	25	F2	25	F1
4.095873	2.652E-34	8.215E-12	3359.7310	25	F1	25	F2
4.134480	8.305E-35	1.001E-10	3900.5353	27	E	27	E

4.135224	6.752E-35	1.979E-13	2620.8994	22	E	22	E
4.138424	5.385E-34	6.367E-10	3896.3969	27	E	27	E
4.157715	8.121E-34	3.216E-10	3896.3967	27	F2	27	F1
4.159811	1.276E-35	3.766E-14	2856.1515	23	F2	23	F1
4.178188	2.486E-35	2.348E-13	3103.0719	24	F1	24	F2
4.182687	8.693E-35	8.654E-14	2622.4107	22	F2	22	F1
4.188373	1.050E-34	6.522E-10	4475.6084	29	F2	29	F1
4.191438	3.275E-36	2.102E-11	4482.2506	29	F1	29	F2
4.198925	1.373E-33	3.295E-10	3896.3962	27	A2	27	A1
4.200342	3.181E-35	2.022E-10	4479.7968	29	F1	29	F2
4.209546	1.059E-33	1.061E-12	2622.4127	22	F1	22	F2
4.223902	1.810E-36	1.158E-11	4479.9246	29	F2	29	F1
4.277710	1.140E-35	7.317E-11	4477.9729	29	F2	29	F1
4.319449	1.094E-34	7.008E-10	4475.6052	29	F1	29	F2
4.327256	2.384E-37	6.704E-12	4786.4156	30	F2	30	F1
4.378626	5.042E-35	2.127E-11	3898.6906	27	F1	27	F2
4.406952	4.482E-35	1.482E-12	3357.9315	25	F1	25	F2
4.455997	4.290E-35	7.226E-11	4187.2323	28	F2	28	F1
4.473249	7.462E-35	3.270E-11	3902.0617	27	F2	27	F1
4.507143	2.133E-33	1.488E-10	3619.9223	26	A2	26	A1
4.514350	1.283E-33	1.494E-10	3619.9223	26	F2	26	F1
4.518001	8.560E-34	2.994E-10	3619.9222	26	E	26	E
4.549868	1.423E-33	8.856E-12	3104.6673	24	A2	24	A1
4.550669	2.870E-34	2.979E-12	3104.6552	24	F2	24	F1
4.620624	5.690E-35	2.575E-11	3901.9226	27	F1	27	F2
4.658797	2.894E-34	4.920E-10	4179.8702	28	F1	28	F2
4.690416	2.919E-34	4.997E-10	4179.8699	28	F2	28	F1
4.726630	1.796E-34	7.022E-14	2395.4178	21	F2	21	F1
4.728951	2.300E-35	2.039E-09	4778.1267	30	E	30	E
4.740717	3.710E-35	3.981E-13	3103.0707	24	F2	24	F1
4.741631	3.286E-36	3.494E-14	3101.1140	24	F1	24	F2
4.742375	1.645E-34	6.455E-14	2395.4177	21	F1	21	F2
4.779679	3.482E-35	1.040E-09	4778.1255	30	F1	30	F2

4.801287	1.857E-34	2.110E-13	2620.8994	22	F2	22	F1
4.841729	1.659E-35	5.711E-14	2856.1515	23	F2	23	F1
4.856240	8.081E-37	2.547E-11	4785.8813	30	F1	30	F2
4.875572	8.067E-34	5.585E-13	2620.8995	22	A2	22	A1
4.883624	3.991E-36	1.880E-12	3898.6962	27	F2	27	F1
4.895703	6.024E-35	1.106E-09	4778.1230	30	A1	30	A2
4.904164	3.553E-35	3.926E-12	3357.9311	25	E	25	E
4.907359	6.738E-36	8.642E-13	3622.3953	26	F1	26	F2
4.930680	9.504E-35	3.711E-11	3624.4402	26	E	26	E
4.939881	3.274E-34	3.663E-12	3103.0719	24	F1	24	F2
4.948419	1.585E-34	2.087E-11	3626.0959	26	F1	26	F2
4.978126	9.962E-36	1.320E-12	3626.0473	26	F2	26	F1
4.979299	2.725E-35	5.070E-11	4184.5603	28	F1	28	F2
4.981415	2.378E-35	8.426E-14	2856.1514	23	F1	23	F2
5.025863	8.082E-35	1.073E-11	3624.4366	26	F1	26	F2
5.051240	4.755E-34	2.262E-10	3893.6393	27	F2	27	F1
5.056852	4.763E-34	2.268E-10	3893.6393	27	F1	27	F2
5.091322	2.294E-35	4.365E-11	4184.5290	28	F2	28	F1
5.095399	1.865E-34	2.045E-12	2857.8783	23	E	23	E
5.108713	1.763E-34	6.460E-13	2857.8776	23	F2	23	F1
5.111695	4.965E-36	1.624E-10	4782.9052	30	F2	30	F1
5.121117	4.759E-36	1.544E-10	4780.7601	30	F2	30	F1
5.191620	1.059E-35	8.395E-11	4481.2504	29	F1	29	F2
5.201000	1.618E-34	7.400E-10	4472.7469	29	A1	29	A2
5.226207	9.769E-35	7.484E-10	4472.7467	29	F1	29	F2
5.234891	8.791E-36	1.703E-11	4182.4395	28	F2	28	F1
5.239242	6.537E-35	1.506E-09	4472.7466	29	E	29	E
5.239263	3.866E-36	3.890E-10	4782.8557	30	E	30	E
5.329041	6.596E-36	1.610E-10	4481.1193	29	E	29	E
5.427089	1.699E-35	1.043E-10	4186.2684	28	E	28	E
5.434533	8.014E-37	3.241E-14	3355.7254	25	F1	25	F2
5.439814	7.490E-36	1.584E-10	4785.2923	30	A1	30	A2
5.495780	1.169E-35	4.875E-13	3359.7310	25	F1	25	F2

5.507339	1.674E-35	3.476E-11	4186.1954	28	F1	28	F2
5.507784	1.525E-34	6.375E-12	3359.7403	25	F2	25	F1
5.525965	1.897E-36	1.002E-12	3896.3967	27	F2	27	F1
5.614705	1.635E-35	6.537E-14	2856.1514	23	F1	23	F2
5.627449	1.107E-34	6.736E-10	4176.8099	28	E	28	E
5.629588	1.662E-34	3.371E-10	4176.8099	28	F1	28	F2
5.633894	2.773E-34	3.378E-10	4176.8099	28	A1	28	A2
5.634915	2.858E-37	1.021E-11	4780.7807	30	F1	30	F2
5.642011	9.483E-37	7.961E-12	4475.6084	29	F2	29	F1
5.693930	5.482E-35	7.402E-14	2620.8994	22	F2	22	F1
5.708624	5.099E-35	2.071E-13	2620.8994	22	E	22	E
5.710562	6.118E-36	3.883E-11	4182.4373	28	E	28	E
5.712446	9.490E-36	1.420E-12	3622.3953	26	F1	26	F2
5.773362	9.311E-36	3.625E-13	3101.1141	24	E	24	E
5.803278	3.084E-35	1.104E-09	4774.9569	30	F1	30	F2
5.807202	1.231E-34	5.092E-13	2856.1515	23	F2	23	F1
5.823985	3.100E-35	1.114E-09	4774.9567	30	F2	30	F1
5.873596	4.555E-36	2.587E-12	3898.6906	27	F1	27	F2
5.895387	6.538E-35	2.902E-12	3357.9315	25	F1	25	F2
5.908134	1.161E-35	1.796E-12	3622.3947	26	F2	26	F1
5.956201	1.109E-34	3.870E-11	3900.5952	27	A1	27	A2
5.970431	2.847E-34	7.679E-12	3357.9323	25	A1	25	A2
5.988874	2.097E-35	1.226E-11	3900.5544	27	F1	27	F2
6.044203	4.639E-35	2.713E-11	3898.6962	27	F2	27	F1
6.078853	2.806E-36	1.104E-10	4784.6586	30	F1	30	F2
6.087531	6.699E-36	1.844E-10	4477.9858	29	E	29	E
6.122087	5.348E-35	7.437E-13	3103.0719	24	F1	24	F2
6.135113	5.092E-35	7.097E-13	3103.0707	24	F2	24	F1
6.136026	1.179E-35	1.628E-13	3101.1140	24	F1	24	F2
6.173620	1.557E-37	2.490E-14	3619.9223	26	F2	26	F1
6.175613	5.976E-36	5.562E-11	4477.9729	29	F2	29	F1
6.239594	5.464E-35	4.928E-10	4469.3656	29	F2	29	F1
6.242856	5.468E-35	4.934E-10	4469.3656	29	F1	29	F2

6.286329	3.320E-37	1.309E-11	4778.1255	30	F1	30	F2
6.325516	4.707E-37	1.091E-12	4179.8699	28	F2	28	F1
6.331020	2.027E-36	8.297E-11	4784.4118	30	F2	30	F1
6.394903	4.902E-37	2.338E-14	3355.7255	25	F2	25	F1
6.529914	7.434E-36	7.392E-11	4479.9246	29	F2	29	F1
6.594840	2.221E-35	1.165E-11	3624.4402	26	E	26	E
6.607689	2.132E-35	3.734E-12	3624.4366	26	F1	26	F2
6.613035	8.125E-37	4.009E-14	3355.7254	25	F1	25	F2
6.642192	1.692E-36	1.677E-11	4475.6084	29	F2	29	F1
6.645258	3.716E-37	3.758E-12	4479.7968	29	F1	29	F2
6.808457	2.753E-35	1.339E-13	2856.1514	23	F1	23	F2
6.828196	2.627E-35	1.213E-12	3101.1141	24	E	24	E
6.834779	1.763E-36	8.609E-15	2856.1515	23	F2	23	F1
6.836619	4.102E-36	8.065E-12	3896.3969	27	E	27	E
6.881528	1.719E-36	1.765E-11	4475.6052	29	F1	29	F2
6.886039	3.873E-36	7.005E-13	3622.3947	26	F2	26	F1
6.886585	2.825E-35	7.091E-10	4771.2364	30	A2	30	A1
6.889058	1.696E-35	7.097E-10	4771.2364	30	F2	30	F1
6.890299	1.131E-35	1.420E-09	4771.2364	30	E	30	E
6.897719	2.219E-35	3.450E-13	3101.1140	24	F1	24	F2
6.915060	2.667E-38	1.744E-14	3893.6393	27	F2	27	F1
7.067205	3.477E-35	6.456E-12	3622.3953	26	F1	26	F2
7.142440	9.587E-36	2.572E-11	4184.5603	28	F1	28	F2
7.159289	7.086E-37	1.905E-12	4184.5290	28	F2	28	F1
7.177918	8.240E-38	8.711E-13	4472.7467	29	F1	29	F2
7.180832	7.315E-36	1.953E-11	4182.4395	28	F2	28	F1
7.183115	4.050E-36	2.791E-12	3896.3967	27	F2	27	F1
7.215856	8.512E-36	4.589E-13	3355.7255	25	F2	25	F1
7.246248	3.291E-35	5.321E-11	4182.4438	28	A2	28	A1
7.256729	2.355E-37	1.088E-11	4780.7601	30	F2	30	F1
7.295295	1.393E-35	7.675E-13	3357.9315	25	F1	25	F2
7.305083	3.172E-37	1.806E-13	3619.9222	26	E	26	E
7.306449	1.341E-35	2.221E-12	3357.9311	25	E	25	E

7.362089	1.576E-37	4.263E-13	4179.8702	28	F1	28	F2
7.375858	2.797E-36	1.314E-10	4780.7807	30	F1	30	F2
7.719098	4.701E-39	1.314E-14	4176.8099	28	F1	28	F2
7.729396	4.371E-36	1.306E-10	4783.0187	30	A2	30	A1
7.804504	2.850E-37	8.179E-13	4179.8699	28	F2	28	F1
7.837670	7.465E-37	3.770E-11	4782.9052	30	F2	30	F1
7.838808	5.403E-36	4.115E-12	3898.6962	27	F2	27	F1
7.852694	5.221E-36	3.984E-12	3898.6906	27	F1	27	F2
7.948312	1.206E-38	5.945E-13	4774.9569	30	F1	30	F2
7.972634	5.335E-37	8.036E-11	4778.1267	30	E	30	E
8.009624	8.677E-36	5.203E-13	3355.7255	25	F2	25	F1
8.067451	1.898E-35	2.077E-13	3101.1140	24	A1	24	A2
8.079925	3.614E-36	6.602E-14	3101.1140	24	F1	24	F2
8.101470	6.606E-36	4.007E-13	3355.7254	25	F1	25	F2
8.272903	5.826E-36	1.391E-11	3896.3969	27	E	27	E
8.283310	4.143E-38	3.257E-14	3893.6393	27	F2	27	F1
8.290093	4.664E-37	2.437E-11	4778.1255	30	F1	30	F2
8.343694	5.056E-36	4.058E-12	3896.3967	27	F2	27	F1
8.372746	1.131E-37	4.196E-12	4472.7466	29	E	29	E
8.380532	1.977E-36	4.314E-13	3619.9223	26	F2	26	F1
8.391969	3.053E-37	3.837E-12	4475.6052	29	F1	29	F2
8.418180	2.548E-36	7.900E-12	4179.8702	28	F1	28	F2
8.422410	5.726E-38	4.578E-14	3893.6393	27	F1	27	F2
8.462546	1.180E-36	4.542E-11	4477.9858	29	E	29	E
8.481626	1.122E-36	1.443E-11	4477.9729	29	F2	29	F1
8.540096	3.230E-36	4.133E-11	4475.6084	29	F2	29	F1
8.603452	1.130E-35	1.520E-12	3619.9223	26	A2	26	A1
8.630760	6.135E-36	1.396E-12	3622.3947	26	F2	26	F1
8.649032	4.162E-37	9.494E-14	3622.3953	26	F1	26	F2
9.248799	1.207E-36	4.170E-12	4182.4395	28	F2	28	F1
9.258187	1.183E-36	1.228E-11	4182.4373	28	E	28	E
9.358436	2.233E-36	5.455E-13	3619.9223	26	F2	26	F1
9.429881	1.920E-37	1.723E-13	3893.6393	27	F1	27	F2



9.448681	1.738E-36	1.286E-12	3619.9222	26	E	26	E
9.454962	1.595E-38	9.387E-13	4774.9569	30	F1	30	F2
9.458547	1.783E-38	1.840E-13	4176.8099	28	E	28	E
9.501378	1.629E-36	1.163E-13	3355.7254	25	F1	25	F2
9.522648	1.087E-37	7.776E-15	3355.7255	25	F2	25	F1
9.669388	1.494E-36	5.335E-12	4179.8702	28	F1	28	F2
9.701956	2.349E-38	1.419E-12	4774.9567	30	F2	30	F1
9.739997	4.815E-37	6.950E-12	4472.7467	29	F1	29	F2
9.750445	1.254E-36	4.518E-12	4179.8699	28	F2	28	F1
9.940460	1.579E-36	1.496E-12	3893.6393	27	F2	27	F1
9.956824	2.452E-37	1.565E-11	4780.7807	30	F1	30	F2
9.958657	2.322E-36	2.057E-11	4472.7469	29	A1	29	A2
9.968214	4.288E-37	8.114E-11	4778.1267	30	E	30	E
9.982703	2.354E-37	1.506E-11	4780.7601	30	F2	30	F1
10.031036	3.875E-37	2.460E-11	4778.1255	30	F1	30	F2
10.130242	3.666E-36	2.153E-12	3896.3962	27	A2	27	A1
10.138299	7.163E-37	7.016E-13	3896.3967	27	F2	27	F1
10.422390	5.184E-38	1.970E-13	4176.8099	28	F1	28	F2
10.431221	1.081E-39	1.646E-14	4469.3656	29	F2	29	F1
10.559050	1.372E-39	2.116E-14	4469.3656	29	F1	29	F2
10.836886	4.644E-37	7.582E-12	4475.6052	29	F1	29	F2
10.846108	3.267E-38	5.340E-13	4475.6084	29	F2	29	F1
10.924569	3.548E-38	2.421E-12	4774.9567	30	F2	30	F1
10.924852	8.172E-37	8.527E-13	3893.6393	27	F1	27	F2
11.101039	3.886E-38	4.123E-14	3893.6393	27	F2	27	F1
11.103157	1.940E-37	5.648E-14	3619.9223	26	F2	26	F1
11.112841	1.882E-37	1.645E-13	3619.9222	26	E	26	E
11.250439	3.226E-37	5.399E-12	4472.7467	29	F1	29	F2
11.326773	2.771E-37	1.401E-11	4472.7466	29	E	29	E
11.338011	3.058E-37	3.800E-12	4176.8099	28	E	28	E
11.458726	2.638E-37	1.891E-11	4774.9569	30	F1	30	F2
11.478482	2.873E-37	1.205E-12	4176.8099	28	F1	28	F2
11.818412	2.792E-37	1.225E-12	4179.8699	28	F2	28	F1

11.832529	1.932E-38	8.490E-14	4179.8702	28	F1	28	F2
11.884859	2.340E-38	4.074E-13	4469.3656	29	F2	29	F1
12.609058	2.410E-37	1.161E-11	4778.1230	30	A1	30	A2
12.612003	4.784E-38	3.842E-12	4778.1255	30	F1	30	F2
12.629941	4.470E-37	1.241E-12	4176.8099	28	A1	28	A2
12.729690	7.097E-38	3.312E-13	4176.8099	28	F1	28	F2
12.885041	1.084E-37	2.053E-12	4469.3656	29	F2	29	F1
12.895644	4.011E-38	4.963E-14	3893.6393	27	F2	27	F1
12.903950	3.917E-38	4.851E-14	3893.6393	27	F1	27	F2
13.060181	1.083E-37	8.879E-12	4774.9567	30	F2	30	F1
13.121129	7.361E-38	1.419E-12	4469.3656	29	F1	29	F2
13.199669	6.093E-39	5.050E-13	4774.9569	30	F1	30	F2
13.422208	4.509E-39	3.735E-13	4771.2364	30	F2	30	F1
13.695355	2.902E-38	5.947E-13	4472.7467	29	F1	29	F2
13.701788	2.859E-38	1.758E-12	4472.7466	29	E	29	E
14.055829	6.529E-38	3.403E-12	4771.2364	30	A2	30	A1
14.631570	2.624E-38	5.663E-13	4469.3656	29	F1	29	F2
14.644821	2.496E-38	2.262E-12	4771.2364	30	F2	30	F1
14.782944	1.444E-39	3.150E-14	4469.3656	29	F2	29	F1
14.862933	1.640E-38	4.528E-12	4771.2364	30	E	30	E
14.885636	7.840E-39	1.290E-13	4176.8099	28	E	28	E
14.892831	7.695E-39	4.224E-14	4176.8099	28	F1	28	F2
15.780636	5.259E-39	5.244E-13	4774.9569	30	F1	30	F2
15.786155	5.198E-39	5.185E-13	4774.9567	30	F2	30	F1
16.780433	2.513E-39	2.623E-13	4771.2364	30	F2	30	F1
16.858512	2.196E-39	6.909E-13	4771.2364	30	E	30	E
17.088957	2.677E-39	6.787E-14	4469.3656	29	F2	29	F1
19.511684	1.247E-39	9.137E-14	4771.2364	30	A2	30	A1

Table 4

Q-branch of methane main isotopomer (61 in HITRAN notation) up to  $J = 30$  with an intensity limit of  $10^{-39} \text{cm}^{-1}/(\text{molecule.cm}^{-2})$  at 296K. Simplified HITRAN format is used with HITRAN units. The entries are transition  $\nu_{\eta\eta'}$  in  $\text{cm}^{-1}$ , intensity  $S_{\eta\eta'}$  in  $\text{cm}^{-1}/(\text{molecule.cm}^{-2})$ , Einstein A-coefficient in  $\text{s}^{-1}$ , lower state energy in  $\text{cm}^{-1}$ , lower state  $J$ -value and irreps, upper state  $J$ -value and irreps.

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