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# Calculated $^{14}N_2{}^{16}O$ line intensities using Radau coordinates and an accurate potential energy surface

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ABSTRACT

Line intensities of the $^{14}N_2{}^{16}O$ molecule are calculated using the DVR3D nuclear-motion program suite. Recently, we (Mizus *et al.*, JQSRT, **344**, 109463 (2025)) presented a potential energy surface (PES) fitted to empirical energy levels with an accuracy close to 0.002 $cm^{-1}$ and very accurate dipole moment surfaces (DMS) calculated *ab initio* using a MRCI (multi-reference configuration interactions) level of theory. However, these accurate PES and DMS did not yield uniformly accurate calculated line intensities: some transition intensities disagreed with the measured ones by orders of magnitude. Here we analyze the reasons for these inaccurately calculated line intensities and develop a spectroscopic model which gives consistently accurate intensity predictions. This improvement is based on a relative minor improvement in the accuracy of the PES, the need for which was highlighted by changing the internal coordinates used in the calculation from Jacobi to Radau. In particular, the new model predicts line intensities with close to experimental accuracy for those vibrational bands, namely ($v_1v_2\ell v_3$) equals (5000), (4200), (3200) and (0112), whose intensities have been measured with sub-percent accuracy.

## 1. Introduction

The accuracy requirements on line intensities for metrology, climate studies, planetary physics and astrophysics can go below 0.1%. The $N_2O$ molecule plays an important role in all these areas, as illustrated by its position among the top five molecules in the key HITRAN database [1]. However, neither experiment nor theory has yet been able to approach this level of accuracy for $N_2O$ line intensities.

Recently, line intensities for several vibrational bands of $^{14}N_2{}^{16}O$ have been measured with the sub-percent accuracy [2–5]. Two of these studies [2,3] used lasers for the intensity measurements, which increases somewhat the accuracy of the line intensity determination. Specifically, Adkins et al. [3] observed the (4200)←(0000) and (5000)←(0000) bands near 1.6 μm and obtained a nominal combined standard uncertainty for the intensities of 1% for most lines (for simplicity, we use throughout the paper the vibrational state notation $v_1v_2lv_3$ instead of $v_1v_2^lv_3$). Odintsova et al. [2] studied eight $^{14}N_2{}^{16}O$ transitions, mainly belonging to the (3200) and (0112) vibrational band obtaining an experimental uncertainty of about 0.4%. While Karlovets et al. [4] observed 47 bands belonging to the $^{14}N_2{}^{16}O$, $^{14}N^{15}N^{16}O$, $^{15}N^{14}N^{16}O$ and $^{14}N_2{}^{18}O$ isotopologues with intensities estimated to be accurate to 3% or better for most lines but up to 20% for the weakest or strongly blended lines. Subsequently, Karlovets et al. [5] presented measurements for a further 49 bands with the same uncertainties.

Theoretically, the $^{14}N_2{}^{16}O$ molecule has been studied extensively using the effective Hamiltonian approach [6]. Variational calculations of $^{14}N_2{}^{16}O$ line intensities have been made by the NASA Ames group [7] and ExoMol [8]. Recently we performed variational nuclear-motion calculation for $^{14}N_2{}^{16}O$ obtaining a very accurate, fitted potential energy surface (PES) [9]. Combining wavefunctions generated using this PES with high accuracy *ab initio* dipole moment surfaces (DMS) gave very mixed results. While some vibrational bands were predicted to have intensities in line with experiment, the intensities for some bands showed large differences. For example, calculated lines of the (0112) – (0000) band measured with sub-percent accuracy by Odintsova et al. [2] differed by 80%; for other bands the calculated intensities were found to differ by a factor of five or more.

We address this issue in this paper which is organized as follows. Section 2 describes the calculation of new fitted PESs, which are

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required to give accurate wavefunctions. In Section 3 we present the $^{14}N_2{}^{16}O$ intensity calculations and extensively compare these results with the experimental values, focusing on the sub-percent accurate measurements; conclusions are outlined in Section 4.

## 2. Brief review of the PES, DMS and nuclear motion program used

There are three major requirements for high accuracy *ab initio* intensity calculations: (1) an accurate program for the solution of the ro-vibrational Schrödinger equation such as DVR3D [10]; (2) an accurate potential energy surface (PES), which in practice is obtained starting from an *ab initio* PES which is then modified by fitting to experimentally-derived ro-vibrational energy levels and (3) accurate, usually purely *ab initio*, dipole moment surfaces (DMS). In this section we briefly outline the quality of all three factors used in the intensity calculations.

### 2.1. Accuracy of the molecular energy levels calculation using DVR3D program suite

Until recently the accuracy with which the vibration–rotation energy levels of a triatomic molecule could be determined by variational nuclear motion calculations using a given PES typically was found to be between 0.01 to 0.001 $cm^{-1}$. However, huge improvements in the experimental accuracy with which the line centers can be determined [11,12] has raised the question of whether it is possible to improve spectroscopic models and hence the accuracy of the solutions of the nuclear-motion Schrödinger equation. We have shown recently [13] that for diatomics the rotation-vibration energy levels for a given potential can be determined with an accuracy of $10^{-5}$ $cm^{-1}$; in work parallel to this study [14] we showed that for $CO_2$, importantly a linear molecule like $N_2O$, rotation-vibration energy levels can also be determined to better than $10^{-5}$ $cm^{-1}$ using kinetic energy operators that are exact within the Born–Oppenheimer approximation and variational procedures. Significantly for this study, this accuracy was obtained for calculations performed in both Radau and Jacobi geometrically-defined internal coordinates. However, for $CO_2$ convergence was found to be much faster for calculations in Radau coordinates; the desired convergence could be achieved in Radau coordinates using a final Hamiltonian matrix of dimension 2000, while in Jacobi coordinates a matrix of dimension 16 000 was needed in DVR3D. We note that normal coordinates give a very good representation of low-lying states of semi-rigid molecules such as $N_2O$ or $CO_2$ but become problematic for highly excited states as they can leave the true domain of the problem. Conversely, our geometrically-defined internal coordinates are rigorously defined to remain within the physical domain of the problem [15].

For the calculations presented in this paper the following DVR3D parameters have been used. Radau coordinates were used to represent the exact kinetic energy operator. For energies up to 7000 $cm^{-1}$, Morse oscillator-like basis functions for both radial coordinates were defined using $r_e = 2.99$, $D_e = 0.3$, and $\omega_e = 0.01$ in atomic units; the calculations used 30, 30, and 100 discrete variable representation (DVR) grid points for the two radial and the associated Legendre functions angular coordinates, respectively, and a final vibrational Hamiltonian matrix dimension set equal to 2000; atomic masses equal to 15.994915 Da for oxygen and 14.003074 Da for nitrogen were used.

For calculations extending above 7000 $cm^{-1}$ we used expanded basis sets with new parameters as the initial basis proved to be too compact to accurately reproduce the higher energy levels. In this case Morse oscillator-like basis functions for the radial coordinates were defined using $r_e = 2.65$, $D_e = 0.03$, and $\omega_e = 0.0012$ in atomic units. The DVR grids were extended to 90, 90, and 100 points for two radial and the angular coordinates, respectively, and a final vibrational Hamiltonian matrix dimension was set equal to 5000.

**Table 1**
Summary of our fitted and previous PESs; $\sigma$ gives the standard deviation of obs.-calc. for the $N$ empirical levels [16] used in our fits. $E_{max}$ and $J_{max}$ are the upper limits of the energies and rotational quantum numbers, $J$, used when calculating the corresponding $\sigma$ values. For our PESs the internal coordinates used in the fit are also given in parenthesis.

| PES | $\sigma$, $cm^{-1}$ | $N$ | $E_{max}$, $cm^{-1}$ | $J_{max}$ |
|---|---|---|---|---|
| Schröder *ab initio*[22] | 1.2520 | 279 | 7800 | 5 |
| Huang et al. fitted [7] | 0.038 | 279 | 7800 | 5 |
| PES60hJ (Jacobi) [9] | 0.0049 | 512 | 7000 | 15 |
| PES96G (Jacobi) [this work] | 0.0339 | 504 | 11 845 | 5 |
| PES60 (Jacobi) [9] | 0.0041 | 266 | 7000 | 5 |
| PES60hJ (Radau) [this work] | 0.0104 | 512 | 7000 | 15 |
| PES96G (Radau) [this work] | 0.0434 | 504 | 11 845 | 5 |
| PES60f (Radau) [this work] | 0.0038 | 266 | 7000 | 5 |

### 2.2. Fitted PESs and ab initio DMS used for the calculations

The typical accuracy of the majority of the empirically-determined energy levels is about $10^{-3}$ $cm^{-1}$ [16]. This accuracy for calculated rovibrational energy levels using a variational approach has so far only been achieved for diatomic molecules. For triatomic molecules the best accuracy reached is about $10^{-2}$ $cm^{-1}$ for water spectra up to 15 000 $cm^{-1}$ [17]. For triatomics comprising of heavier atoms, like ozone and carbon dioxide, the best accuracy reached until recently was about 0.03 $cm^{-1}$ [18–21]; this is approximately the accuracy of the energy levels computed by Huang et al. for $N_2O$ [7] as part of the Ames-296K line list.

Table 1 compares standard deviations for various PESs from our previous study [9] and other published works [7,22] with respect to a set of experimentally determined energy levels of $^{14}N_2{}^{16}O$ [16]; results for the PESs determined in this work are also given.

As a starting point for the intensity calculations presented here we first tested the PES60hJ potential, which was obtained by fitting, using a calculation in Jacobi coordinates, to experimental energy levels with total angular momentum $J$ up to 15 and was shown to accurately represent high-$J$ levels [9]. However, there are known issues with using Jacobi coordinates to represent linear molecules [23]; although this issue has been successfully overcome by abandoning the standard discrete variable quadrature approximation [24], an approach has been used to successfully compute intensities in states which probe linear geometries [25], we decided to test the effect of switching coordinate systems. Switching to Radau coordinates, with the nuclear-motion problem parameters given in Section 2.1, showed that calculations performed with the PES60hJ did not precisely reproduce the previous Jacobi coordinate calculations [9]; in particular, the new calculations reproduced the 512 experimental energies up to 7000 $cm^{-1}$, with $J = 0$, 2, 5, 10, and 15 with a standard deviation $\sigma = 0.01$ $cm^{-1}$ compared to 0.005 $cm^{-1}$ obtained in Jacobi coordinates. For this reason we decided to perform another fit of the potential using nuclear motion calculations in Radau coordinates and PES60hJ as the starting point.

#### 2.2.1. Fitting in Radau coordinates

In order to recover a PES with a standard deviation similar to that of PES60hJ value, we performed a new fit starting from PES60hJ and using wavefunctions computed in Radau coordinates. This fit allowed us to increase the accuracy of our predicted energy levels $J = 0, 2$ and 5 below 7000 $cm^{-1}$ by a factor of almost four; the resulting new PES60f potential (with 60 fitted parameters) gave $\sigma = 0.0038$ $cm^{-1}$. This and other PESs created in this work are given in the Supplementary Materials.

Table 2 presents a comparison of the experimental and calculated $J = 0$ levels, as well as prediction of band origins ($J = 0$ levels) between 7000 and 15 000 $cm^{-1}$. It can be seen that the deviations from experiment for PES60f are greatly reduced compared to those given by a Radau-coordinate calculation using PES60hJ both below 7000 $cm^{-1}$ and for predictions above 7000 $cm^{-1}$. PES60f also allowed us to obtain greatly improved predicted intensities, see Section 3 below.

*2.2.2. Extending the PES to higher energies*

In order to construct a global PES, we decided to use the energy-switching approach of Varandas [26], as we have done many times for the water molecule [27].

The final global PES96G consists of two independent parts, $V_l$ and $V_u$, representing the lower and upper energy regions which are then linked by a switching function. Both $V_l$ and $V_u$ are new potentials, which are similar to PES96 (see Mizus et al. [9] and Table 1) in their analytic forms, but each with an independent set of 96 linear parameters optimized in the fit. $V_l$ gives better accuracy for calculations with energies up to 7000 $cm^{-1}$, while $V_u$ allows us to obtain good accuracy in the energy range from 7000 $cm^{-1}$ to about 13 500 $cm^{-1}$. Each of the potentials was obtained using the fitting procedure proposed in [28,29], with the other potential fixed during the fit.

The final version of PES96G, the result of fitting both $V_l$ and $V_u$ potentials, was obtained using wavefunctions generated in Jacobi coordinates following the procedure described by us previously [9] for PES60hJ. A set of experimental energies up to about 12 000 $cm^{-1}$, with the values of total angular momentum quantum number $J = 0$, 2, and 5, as well as the set of *ab initio* points, which were used for fitting PES96G [9], were utilized to obtain two independent sets of 96 fitting parameters (see files "pot_low.fit" and "pot_up.fit" in Supplementary materials).

The final surfaces were stitched together smoothly using the following switching scheme analogous to the one due to Varandas [26]:

$$V_G = f_l V_l + f_u V_u, \tag{1}$$

where

$$f_{l/u} = \left(1 + \exp(\pm 2\alpha d_e)\right)^{-1}, \tag{2}$$

$$\alpha = \ln\left(\frac{100}{\delta} - 1\right)/b,$$

$$d_e = V_u - E_0.$$

In the above equations the parameters $\delta$, $b$, and $E_0$ were obtained using trial-and-error during the fitting procedure. They have a clear meaning: $\alpha$ is the parameter that controls the sharpness of the switching, $E_0$ denotes the switching point, $b$ is the width of the switching range, and $\delta$ determines how close the switching functions, $f_{l/u}$, are from their asymptotic values of zero or one at the edges of the region $E_0 \pm \frac{b}{2}$, expressed as a percentage. After a trial-and-error adjustment procedure, these parameters were set to $E_0$ = 12 850 $cm^{-1}$, $b$ = 4000 $cm^{-1}$, and $\delta = 0.1$.

The final version of our global PES96G represents 504 experimental energies used in the fitting procedure with $\sigma$ = 0.034 $cm^{-1}$. The 243 empirical levels with the energies below 7000 $cm^{-1}$, are represented by the new potential with an unprecedented average accuracy of $\sigma$ = 0.0025 $cm^{-1}$; the analogous accuracy for 261 levels with energies between 7000 $cm^{-1}$ and about 12 000 $cm^{-1}$ is 0.047 $cm^{-1}$. About 20% of the 634 available empirical energies below 12 000 $cm^{-1}$, whose inclusion reduced the accuracy, were excluded from the fit.

To overcome the issue with intensity calculations in Jacobi coordinates, we switched to using Radau coordinates in DVR3D. The sparser radial DVR grids used in the calculations with a restricted energy range are too small to provide high accuracy energy levels above 7000 $cm^{-1}$, so the larger grids were used. Switching coordinate systems, however, somewhat reduced the accuracy of the energy levels obtained using PES96G. Using Radau coordinates, calculation for PES96G reproduced 506 experimental energies with $J = 0, 2$ and 5 with $\sigma$ = 0.043 $cm^{-1}$. 248 levels from this set, with energies below 7000 $cm^{-1}$, are represented by the new potential with $\sigma$ = 0.006 $cm^{-1}$; the accuracy for 256 levels with energies between 7000 $cm^{-1}$ to about 12 000 $cm^{-1}$ is about 0.06 $cm^{-1}$.

The predicted $J = 0$ energy levels calculated using Radau coordinates for the new PES96G are given in Table 2.

An additional comparison of the calculated levels with $J = 1$ with empirical ones taken from the MARVEL study [16] for the three new potentials PES60hJ, PES96G, and PES60f is given in Table 1 of the Supplementary Materials. As none of these $J = 1$ levels were used in our fits, this comparison provides an independent evaluation for the quality of our new PESes. The standard deviation for these comparisons are

$$\sigma(\text{PES60f}, < 7000\ cm^{-1}) = 0.009\ cm^{-1},$$

$$\sigma(\text{PES60hJ}, < 7000\ cm^{-1}) = 0.017\ cm^{-1},$$

$$\sigma(\text{PES96G}, < 7000\ cm^{-1}, -19.7\%\ \text{outliers}) = 0.011\ cm^{-1},$$

$$\sigma(\text{PES96G}, > 7000\ cm^{-1}, -19.8\%\ \text{outliers}) = 0.07\ cm^{-1}.$$

## 3. Intensity calculations

The line intensities calculated in our previous paper [9] turned out to be unexpectedly erratic. DVR3D provides very accurate solutions to the rovibrational Schrödinger equation [14], the PES used was fitted to unprecedentedly high accuracy and both DMSs used proved to be very accurate when we calculated the lines of the bands with $v_3 = 0$ and $l = 0$. However, the $v_3 = 1$ and 2 bands and the $l = 1$ bands in many cases gave wild results, with some bands up to 4 500% off. Table 3 presents the results of the calculations in Jacobi coordinates for comparison. For some bands differences with HITRAN data are absurdly high. We tested several explanations for this strange behavior. For example, we tried the option for DVR3D to avoid making the quadrature approximation [23] while evaluating integrals. As can be seen from Table 3, this did not change the results significantly.

Here we demonstrate a satisfactory solution of this problem: changing the coordinate system used for intensity calculations from Jacobi, which were used to obtain excellent fits for the $N_2O$ PESs in the first place, to Radau coordinates. Use of wavefunctions expressed in Radau coordinates allowed very accurate line intensities to be obtained for all the bands considered in the calculations. These results are presented in the Tables 3, 4, 5 and 6; in all tables the differences between observed and calculated intensities are given as (Obs/Calc − 1) × 100%.

### 3.1. Intensity calculations using Radau coordinates

An option we considered to improve the intensity predictions was changing coordinate from Jacobi to Radau in the DVR3D calculations. However, doing this meant that the $^{14}N_2{}^{16}O$ energy levels calculated using the same PES were less accurate than those obtained from calculations using Jacobi coordinates in DVR3D; the problem of the erratic intensities prediction in our Jacobi coordinates remained unresolved.

However, when we refitted the PES parameters using Radau coordinates in the DVR3D we were able to both compute energy levels with a similar accuracy to the fits obtained using Jacobi coordinates and to find a solution to our problematic intensities. With these parameters we calculated the line intensities of $^{14}N_2{}^{16}O$ with fully satisfactory results.

Let us first consider the results for the accurately measured intensities in the (3200) and (0112) bands [2] given in Table 4 and (4200) and (5000) bands [3] in Tables 5 and 6. As shown by Table 4, a high discrepancy of about 80% was found using Jacobi coordinates for lines in the (0112) and (3200) bands. The present Radau coordinate calculations reduced this difference to about one percent for 6 lines of these bands and to about 4% for the other two lines. We consider the agreement with experiment of our final result, given in last column, to be excellent.

The best previous calculation results are presented in the column Ames and taken from the Ames-296K line list [7]. Six lines out of eight from the column Ames of the Table 4 show discrepancies between 1.5% and 8%, and only the two remaining lines have sub-percent accuracy

**Table 2**
Comparison $J = 0$ levels with the empirical ones, in $cm^{-1}$, for PES60hJ, PES96G, and PES60f for calculations in Radau coordinates. The empirical levels are taken from the MARVEL study [16] and the HITRAN database [1]. The levels not used for calculating the corresponding standard deviations ($\sigma$) are marked by a star; for PES60hJ and PES60f the starred levels essentially represent predictions for band origins above 7000 $cm^{-1}$.

| exp. | vib. | PES96G | exp. - PES96G | PES60hJ | exp. - PES60hJ | PES60f | exp.−PES60f |
|---|---|---|---|---|---|---|---|
| 1168.1324 | 0 2 0 0 | 1168.1316 | 0.001 | 1168.1292 | 0.003 | 1168.1324 | −0.000 |
| 1284.9033 | 1 0 0 0 | 1284.9056 | −0.002 | 1284.9091 | −0.006 | 1284.9050 | −0.002 |
| 2223.7567 | 0 0 0 1 | 2223.7522 | 0.004 | 2223.7579 | −0.001 | 2223.7587 | −0.002 |
| 2322.5732 | 0 4 0 0 | 2322.5742 | −0.001 | 2322.5706 | 0.003 | 2322.5751 | −0.002 |
| 2461.9965 | 1 2 0 0 | 2461.9977 | −0.001 | 2462.0006 | −0.004 | 2462.0034 | −0.007 |
| 2563.3403 | 2 0 0 0 | 2563.3352 | 0.005 | 2563.3419 | −0.002 | 2563.3405 | −0.000 |
| 3363.9780 | 0 2 0 1 | 3363.9753 | 0.003 | 3363.9780 | 0.000 | 3363.9822 | −0.004 |
| 3466.6002 | 0 6 0 0 | 3466.5975 | 0.003 | 3466.5989 | 0.001 | 3466.5988 | 0.001 |
| 3480.8193 | 1 0 0 1 | 3480.8072 | 0.012 | 3480.8151 | 0.004 | 3480.8207 | −0.001 |
| 3620.9430 | 1 4 0 0 | 3620.9433 | −0.000 | 3620.9422 | 0.001 | 3620.9463 | −0.003 |
| 3748.2521 | 2 2 0 0 | 3748.2527 | −0.001 | 3748.2601 | −0.008 | 3748.2586 | −0.007 |
| 3836.3710 | 3 0 0 0 | 3836.3598 | 0.011 | 3836.3699 | 0.001 | 3836.3711 | −0.000 |
| 4417.3778 | 0 0 0 2 | 4417.3602 | 0.018 | 4417.3729 | 0.005 | 4417.3745 | 0.003 |
| 4491.5421 | 0 4 0 1 | 4491.5369 | 0.005 | 4491.5392 | 0.003 | 4491.5438 | −0.002 |
| 4630.1613 | 1 2 0 1 | 4630.1550 | 0.006 | 4630.1635 | −0.002 | 4630.1641 | −0.003 |
| 4730.8251 | 2 0 0 1 | 4730.8065 | 0.019 | 4730.8252 | −0.000 | 4730.8284 | −0.003 |
| 4767.1421 | 1 6 0 0 | 4767.1398 | 0.002 | 4767.1394 | 0.003 | 4767.1364 | 0.006 |
| 4910.9955 | 2 4 0 0 | 4911.0001 | −0.005 | 4911.0045 | −0.009 | 4911.0004 | −0.005 |
| 5026.3030 | 3 2 0 0 | 5026.3035 | −0.001 | 5026.3164 | −0.013 | 5026.3068 | −0.004 |
| 5105.6769 | 4 0 0 0 | 5105.6619 | 0.015 | 5105.6772 | −0.000 | 5105.6773 | −0.000 |
| 5529.6950 | 0 2 0 2 | 5529.6703* | 0.025* | 5529.6930 | 0.002 | 5529.6934 | 0.002 |
| 5646.7402 | 1 0 0 2 | 5646.6861* | 0.054* | 5646.7296 | 0.011 | 5646.7351 | 0.005 |
| 5762.3720 | 1 4 0 1 | 5762.3664 | 0.006 | 5762.3822 | −0.010 | 5762.3715 | 0.001 |
| 5888.1059 | 2 2 0 1 | 5888.0922 | 0.014 | 5888.1259 | −0.020 | 5888.1106 | −0.005 |
| 5974.8450 | 3 0 0 1 | 5974.7868* | 0.058* | 5974.8512 | −0.006 | 5974.8416 | 0.003 |
| 6058.6678 | 2 6 0 0 | 6058.6665 | 0.001 | 6058.6850 | −0.017 | 6058.6704 | −0.003 |
| 6192.2702 | 3 4 0 0 | 6192.2733 | −0.003 | 6192.2922 | −0.022 | 6192.2804 | −0.010 |
| 6295.4476 | 4 2 0 0 | 6295.4424 | 0.005 | 6295.4647 | −0.017 | 6295.4456 | 0.002 |
| 6373.3080 | 5 0 0 0 | 6373.2936 | 0.014 | 6373.3191 | −0.011 | 6373.3128 | −0.005 |
| 6580.8535 | 0 0 0 3 | 6580.8113* | 0.042* | 6580.8308 | 0.023 | 6580.8533 | 0.000 |
| 6768.5018 | 1 2 0 2 | 6768.4505* | 0.051* | 6768.5344 | −0.033 | 6768.4962 | 0.005 |
| 6868.5498 | 2 0 0 2 | 6868.4237* | 0.126* | 6868.5748 | −0.025 | 6868.5519 | −0.002 |
| 7137.1271 | 3 2 0 1 | 7137.0947 | 0.033 | 7137.1840* | −0.057* | 7137.1511* | −0.024* |
| 7214.6797 | 4 0 0 1 | 7214.5774 | 0.102 | 7214.7411* | −0.061* | 7214.6835* | −0.004* |
| 7463.9850 | 4 4 0 0 | 7463.9524 | 0.033 | 7464.0223* | −0.037* | 7464.0033* | −0.018* |
| 7556.1361 | 5 2 0 0 | 7556.0968 | 0.039 | 7556.1560* | −0.020* | 7556.1367* | −0.001* |
| 7640.4737 | 6 0 0 0 | 7640.4431 | 0.031 | 7640.5152* | −0.042* | 7640.4855* | −0.012* |
| 7665.2728 | 0 2 0 3 | 7665.2158 | 0.057 | 7665.3376* | −0.065* | 7665.3036* | −0.031* |
| 7782.6615 | 1 0 0 3 | 7782.5196* | 0.142* | 7782.7226* | −0.061* | 7782.6905* | −0.029* |
| 7874.1557 | 1 4 0 2 | 7874.0984 | 0.057 | 7874.2412* | −0.086* | 7874.1405* | 0.015* |
| 7998.5891 | 2 2 0 2 | 7998.5067 | 0.082 | 7998.7515* | −0.162* | 7998.6176* | −0.029* |
| 8083.9526 | 3 0 0 2 | 8083.7798* | 0.173* | 8084.1188* | −0.166* | 8084.0434* | −0.091* |
| 8276.3257 | 3 0 0 2 | 8276.2984 | 0.027 | 8276.5043* | −0.178* | 8276.4418* | −0.116* |
| 8376.3502 | 4 2 0 1 | 8376.2246* | 0.126* | 8376.5839* | −0.234* | 8376.4837* | −0.134* |
| 8452.6357 | 5 0 0 1 | 8452.5114* | 0.124* | 8452.8904* | −0.255* | 8452.7263* | −0.090* |
| 8714.1402 | 0 0 0 4 | 8714.0897 | 0.051 | 8714.2578* | −0.117* | 8714.2449* | −0.105* |
| 8877.0415 | 1 2 0 3 | 8876.9422 | 0.099 | 8877.3664* | −0.325* | 8877.1327* | −0.091* |
| 8976.4890 | 2 0 0 3 | 8976.2535* | 0.235* | 8976.9883* | −0.499* | 8976.7048* | −0.216* |
| 9108.3216 | 2 4 0 2 | 9108.2860 | 0.036 | 9108.7161* | −0.394* | 9108.4572* | −0.136* |
| 9219.0555 | 3 2 0 2 | 9218.9379* | 0.118* | 9219.7128* | −0.657* | 9219.3962* | −0.341* |
| 9294.9938 | 4 0 0 2 | 9294.8469* | 0.147* | 9295.6477* | −0.654* | 9295.4103* | −0.416* |
| 9517.8741 | 4 4 0 1 | 9517.8689 | 0.005 | 9518.4044* | −0.530* | 9518.2872* | −0.413* |
| 9606.3360 | 5 2 0 1 | 9606.2331 | 0.103 | 9607.2162* | −0.880* | 9606.8245* | −0.488* |
| 9888.5800 | 1 0 0 4 | 9888.3582* | 0.222* | 9889.2836* | −0.704* | 9888.8626* | −0.283* |
| 10079.5560 | 2 2 0 3 | 10 079.5057 | 0.050 | 10080.8183* | −1.262* | 10080.0464* | −0.490* |
| 10163.5927 | 3 0 0 3 | 10 163.5338 | 0.059 | 10165.3785* | −1.786* | 10164.4924* | −0.900* |
| 10429.1510 | 4 2 0 2 | 10429.2853* | −0.134* | 10431.0674* | −1.916* | 10430.4631* | −1.312* |
| 10815.2510 | 0 0 0 5 | 10815.1098* | 0.141* | 10816.5578* | −1.307* | 10815.7119* | −0.461* |
| 10820.1280 | 0 4 0 4 | 10 820.1433 | −0.015 | 10821.5756* | −1.448* | 10820.4244* | −0.296* |
| 11844.9700 | 0 2 0 5 | 11 844.9216 | 0.048 | 11848.4292* | −3.459* | 11845.9308* | −0.961* |
| 11964.1220 | 1 0 0 5 | 11963.6569* | 0.465* | 11968.6000* | −4.478* | 11965.6175* | −1.495* |
| 12891.0787 | 0 0 0 6 | 12 890.9752 | 0.103 | 12899.5539* | −8.475* | 12892.5241* | −1.445* |
| 14009.6900 | 1 0 0 6 | 14007.8996* | 1.790* | 14007.8454* | 1.845* | 14013.4874* | −3.797* |
| 14934.2700 | 0 0 0 7 | 14933.4816* | 0.788* | 14928.9969* | 5.273* | 14937.9654* | −3.695* |

in comparison with the experiment. Meanwhile, our present results (column PES60f.Radau.ai) show discrepancies of less than 2% for six out of eight lines; the two less accurately predicted line intensities from this work may be actually due to some experimental issues. Our experience suggests that lines close together in $J$ for an isolated band should only give changes in the discrepancies as large as 3% if there are issues with the experimental values: a similar situation occurred with the $^{12}C^{16}O_2$ measurements from the same laboratory [19,30]. We calculated obs.-calc. values [19] for the previously-measured $^{12}C^{16}O_2$ line intensities [31]. Some of them were accurate to about 0.3%, in line with the stated experimental uncertainties. For other lines differences of 2 to 3% were found. We suggested that these larger discrepancies were

**Table 3**
Differences from dipole intensities ($I$ in cm/molecule at $T$ = 296 K scaled to 100% $^{14}N_2{}^{16}O$) given by HITRAN [1] for strong bands. Ames denotes the Ames-296K calculation [7] and TYM the ExoMol TYM line list [8]. Our calculations used PESs designated p60 – PES60, 60hj – PES60hJ, 60f – PES60f, Var – PES96G, and DMS ai – our *ab initio* DMS and Sch – Schröder et al.'s DMS [22], for nuclear motion calculations performed using the given coordinates, with p60.Quad.ai denoting a Jacobi calculation without use of the quadrature approximation.

| Line | $\tilde{\omega}$ | Band | $I$ | Ames | 60hj.aiRadau | 60f.aiRadau | Var.aiRadau | p60.aiJacobi | p60.SchJacobi | p60.Quad.ai | TYM |
|---|---|---|---|---|---|---|---|---|---|---|---|
| R 4 | 4.1900 | 0000 | 8.394E−24 | 8.4 | 36.93 | 36.05 | 36.49 | 36.6 | 2.0 | 38.0 | 14.8 |
| R 8 | 7.5416 | 0000 | 4.364E−23 | 8.1 | 36.38 | 35.53 | 36.38 | 36.2 | 2.1 | 37.8 | 14.5 |
| R 4 | 1172.3495 | 0200 | 2.798E−21 | 2.8 | 4.79 | 4.01 | 4.40 | −0.5 | −0.3 | 0.1 | −1.5 |
| R 8 | 1175.7552 | 0200 | 4.566E−21 | 3.0 | 4.72 | 4.01 | 4.72 | −0.5 | −0.3 | −0.4 | −1.4 |
| R 4 | 1289.0406 | 1000 | 8.313E−20 | −3.3 | 1.88 | 2.00 | 1.88 | 1.0 | −1.0 | 2.1 | −0.5 |
| R 8 | 1292.2870 | 1000 | 1.354E−19 | −2.9 | 2.58 | 2.58 | 2.58 | 1.3 | −0.8 | 1.8 | −0.3 |
| R 4 | 2326.8111 | 0400 | 2.313E−22 | 2.7 | −11.72 | −6.73 | −9.65 | −13.6 | −13.9 | −17.5 | −4.5 |
| R 8 | 2330.2577 | 0400 | 3.737E−22 | 2.3 | −11.86 | −7.04 | −9.95 | −14.1 | −14.6 | −18.0 | −5.2 |
| R 4 | 2466.1605 | 1200 | 2.677E−21 | 3.2 | 1.79 | 2.18 | 1.79 | 0.0 | 0.0 | 1.4 | 5.6 |
| R 8 | 2469.4599 | 1200 | 4.354E−21 | 3.2 | 1.97 | 2.21 | 1.97 | −0.2 | −0.3 | 0.6 | 5.3 |
| R 4 | 2567.4273 | 2000 | 1.202E−20 | −0.6 | 0.17 | −0.66 | 0.17 | −1.3 | −1.4 | −0.3 | 0.5 |
| R 8 | 2570.5747 | 2000 | 1.939E−20 | −1.1 | −0.05 | −1.07 | −0.56 | −1.8 | −2.1 | −0.9 | 0.0 |
| R 4 | 3625.1260 | 1400 | 3.919E−23 | 3.8 | −4.41 | −1.53 | −3.71 | −4.2 | −5.2 | −5.9 | 4.1 |
| R 8 | 3628.4623 | 1400 | 6.354E−23 | 3.3 | −4.88 | −2.10 | −4.16 | −4.8 | −4.9 | −6.2 | 3.4 |
| R 4 | 3752.3612 | 2200 | 3.283E−22 | 1.6 | −2.00 | −1.41 | −2.29 | −3.2 | −3.6 | −1.9 | 1.1 |
| R 8 | 3755.5516 | 2200 | 5.333E−22 | 1.4 | −2.33 | −1.79 | −2.50 | −3.5 | −4.0 | −2.1 | 0.7 |
| R 4 | 3840.4155 | 3000 | 7.212E−22 | 1.6 | −0.39 | −0.66 | −0.80 | −2.2 | −2.1 | −1.4 | 0.2 |
| R 8 | 3843.4763 | 3000 | 1.162E−21 | 0.9 | −0.68 | −1.53 | −1.53 | −2.9 | −2.9 | −2.5 | −0.5 |
| R 4 | 4771.3396 | 1600 | 3.566E−25 | −10.7 | −4.91 | −1.49 | −4.91 | −6.5 | −7.1 | 1.2 | 4.5 |
| R 8 | 4774.7042 | 1600 | 5.828E−25 | −10.5 | −4.93 | −1.39 | −4.78 | −6.3 | −7.1 | −0.1 | 4.6 |
| R 4 | 4915.1220 | 2400 | 4.273E−24 | −1.0 | −3.33 | −0.40 | −3.33 | −2.5 | −3.6 | −3.8 | 1.2 |
| R 8 | 4918.3457 | 2400 | 6.970E−24 | −1.1 | −3.33 | −0.57 | −3.33 | −2.6 | −3.8 | −3.6 | 1.4 |
| R 4 | 5030.3546 | 3200 | 2.424E−23 | −0.3 | −1.86 | 0.17 | −2.26 | −3.3 | −4.1 | −1.8 | −1.4 |
| R 8 | 5033.4295 | 3200 | 3.939E−23 | −0.6 | −2.01 | −0.28 | −2.50 | −3.5 | −4.5 | −3.1 | −1.6 |
| R 4 | 5109.6882 | 4000 | 2.505E−23 | −1.6 | −2.15 | −0.99 | −2.91 | −3.2 | −3.3 | −2.9 | −2.7 |
| R 8 | 5112.6830 | 4000 | 4.061E−23 | −1.5 | −2.14 | −0.95 | −2.61 | −3.1 | −3.3 | −2.7 | −2.5 |
| R 4 | 6196.3380 | 3400 | 4.232E−25 | −6.0 | −6.78 | −3.16 | −7.19 | −4.2 | −4.5 | −6.2 | −3.8 |
| R 8 | 6199.4436 | 3400 | 6.919E−25 | −6.0 | −6.75 | −3.23 | −7.13 | −4.1 | −4.5 | −6.1 | −2.7 |
| R 4 | 6299.4395 | 4200 | 1.495E−24 | −2.4 | −2.29 | 1.01 | −2.92 | −3.6 | −4.3 | −1.5 | −3.9 |
| R 8 | 6302.3948 | 4200 | 2.434E−24 | −2.4 | −2.25 | 0.58 | −3.03 | −3.5 | −4.3 | −1.3 | −3.8 |
| R 4 | 6377.2978 | 5000 | 7.000E−25 | −3.5 | −1.27 | 1.45 | −2.23 | 8.1 | 7.3 | 5.6 | −2.5 |
| R 8 | 6380.2504 | 5000 | 1.131E−24 | −3.6 | −1.65 | 0.98 | −2.50 | 8.0 | 7.2 | 4.9 | −2.6 |
| R 4 | 592.9627 | 0110 | 5.919E−21 | −6.7 | −7.66 | −7.52 | −7.66 | −8.6 | −1.8 | −7.7 | −3.6 |
| R 8 | 596.3244 | 0110 | 9.121E−21 | −6.6 | −7.49 | −7.40 | −7.49 | −4.7 | 2.3 | −4.1 | 0.5 |
| R 4 | 1753.2724 | 0310 | 1.051E−23 | 6.4 | 1.06 | 2.04 | 2.04 | 26.7 | 8.0 | 28.0 | 26.2 |
| R 8 | 1756.6582 | 0310 | 1.515E−23 | 6.9 | 1.68 | 1.68 | 1.68 | 14.5 | −2.0 | 13.3 | −1.4 |
| R 4 | 2227.8432 | 0001 | 4.929E−19 | −2.2 | 2.26 | 2.26 | 2.26 | 1.4 | 1.0 | 2.4 | 0.8 |
| R 8 | 2230.9878 | 0001 | 8.020E−19 | −1.8 | 2.82 | 2.82 | 2.82 | 1.7 | 0.9 | 3.1 | 1.1 |
| R 4 | 2802.3854 | 0111 | 4.889E−22 | 1.4 | 1.85 | 1.64 | 1.64 | −34.8 | −18.4 | −34.1 | −34.6 |
| R 8 | 2805.5426 | 0111 | 7.333E−22 | 1.2 | 1.42 | 1.28 | 1.28 | −34.7 | −18.3 | −33.8 | −34.6 |
| R 4 | 3368.0939 | 0201 | 7.980E−22 | −2.3 | −1.12 | 0.00 | −0.99 | 3.7 | 1.9 | 4.8 | 4.6 |
| R 8 | 3371.2972 | 0201 | 1.303E−21 | −2.0 | −0.53 | 0.23 | −0.53 | 3.8 | 1.9 | 4.3 | 4.7 |
| R 4 | 3484.8524 | 1001 | 1.626E−20 | −5.0 | −4.35 | −3.79 | −4.35 | −5.4 | −5.2 | −4.5 | −6.5 |
| R 8 | 3487.8906 | 1001 | 2.636E−20 | −5.0 | −4.15 | −3.44 | −4.15 | −5.4 | −5.4 | −4.4 | −6.5 |
| R 4 | 3935.3551 | 0311 | 2.880E−25 | −− | −1.37 | 0.35 | −1.37 | 2.1 | −25.4 | −26.2 | 5.8 |
| R 4 | 4066.0208 | 1111 | 6.232E−24 | 1.3 | −1.08 | −0.13 | −0.92 | 53.1 | 12.8 | 54.9 | 46.4 |
| R 8 | 4069.0748 | 1111 | 8.960E−24 | 0.9 | −1.54 | −0.67 | −1.43 | 39.5 | 3.4 | 41.8 | 33.5 |
| R 4 | 4421.3604 | 0002 | 5.828E−22 | 33.8 | 7.93 | 5.77 | 7.33 | 4.1 | 6.1 | 5.7 | 26.2 |
| R 8 | 4424.2974 | 0002 | 9.404E−22 | 33.7 | 7.72 | 5.78 | 7.23 | 2.8 | 4.7 | 4.4 | 24.5 |
| R 4 | 4495.6812 | 0401 | 9.535E−25 | −− | 3.64 | 2.42 | 1.87 | 8.3 | 27.7 | 41.0 | 25.0 |
| R 8 | 4498.9298 | 0401 | 1.566E−24 | −− | 3.03 | 1.69 | 1.69 | 9.0 | 28.6 | 41.5 | 25.0 |
| R 4 | 4634.2236 | 1201 | 5.091E−23 | −9.0 | −2.47 | 0.02 | −2.28 | −1.2 | −5.4 | 0.5 | −7.4 |
| R 8 | 4637.3198 | 1201 | 8.273E−23 | −9.4 | −2.90 | −0.33 | −2.78 | −1.3 | −5.6 | 0.3 | −7.5 |
| R 4 | 4734.8083 | 2001 | 3.606E−22 | −4.0 | −0.39 | 1.86 | −0.11 | −0.7 | −1.0 | 0.0 | −5.3 |
| R 8 | 4737.7465 | 2001 | 5.869E−22 | −3.7 | −0.19 | 2.25 | 0.15 | −0.3 | −0.7 | 0.4 | −4.9 |
| R 4 | 4981.6881 | 0112 | 2.232E−24 | 2.5 | −2.96 | −3.79 | −2.96 | −90.0 | −74.0 | −89.9 | −88.7 |
| R 8 | 4984.6404 | 0112 | 3.333E−24 | 2.4 | −3.11 | −3.95 | −3.11 | −90.1 | −74.2 | −90.2 | −88.7 |
| R 4 | 5533.7095 | 0202 | 4.273E−25 | 30.6 | 23.50 | 23.14 | 22.09 | 675.6 | 492.8 | 492.2 | 454.5 |
| R 8 | 5536.7099 | 0202 | 6.970E−25 | 31.0 | 23.80 | 23.58 | 22.50 | 652.6 | 477.7 | 476.5 | 437.8 |
| R 4 | 5650.6691 | 1002 | 8.556E−24 | 57.1 | 7.76 | 8.30 | 7.08 | −16.4 | 4.5 | −13.1 | 66.5 |
| R 8 | 5653.4986 | 1002 | 1.374E−23 | 56.3 | 7.34 | 7.34 | 6.51 | −18.0 | −2.1 | −14.9 | 62.6 |
| R 4 | 5892.1134 | 2201 | 3.242E−24 | −12.7 | −7.64 | −4.37 | −7.37 | −11.9 | −17.1 | −9.0 | −16.8 |
| R 8 | 5895.0997 | 2201 | 5.293E−24 | −12.7 | −7.63 | −4.29 | −7.30 | −11.6 | −16.8 | −8.5 | −16.4 |
| R 4 | 5978.7849 | 3001 | 8.798E−24 | −9.0 | −2.46 | 0.89 | −2.14 | 8.5 | 1.0 | 7.2 | −11.0 |
| R 8 | 5981.6365 | 3001 | 1.434E−23 | −8.5 | −1.78 | 0.99 | −1.78 | 9.2 | 1.7 | 8.3 | −10.4 |
| R 4 | 6584.7324 | 0003 | 1.182E−23 | 25.7 | 12.57 | 13.65 | 12.57 | 67.8 | 3.0 | 65.4 | −21.4 |
| R 8 | 6587.4616 | 0003 | 1.909E−23 | 25.7 | 12.29 | 13.63 | 12.29 | 65.1 | 1.8 | 64.5 | −22.3 |
| R 4 | 6872.4284 | 2002 | 3.091E−25 | −18.4 | 13.22 | 11.19 | 15.77 | 4561.5 | 104.7 | −95.7 | −52.6 |
| R 8 | 6875.1572 | 2002 | 5.010E−25 | −18.3 | 13.35 | 11.09 | 15.70 | 4545.3 | 106.1 | −94.3 | −52.6 |
| R 4 | 7141.0757 | 3201 | 3.545E−25 | −10.2 | −6.96 | −3.67 | −6.22 | −10.9 | −24.2 | −6.3 | −20.3 |
| R 8 | 7143.9444 | 3201 | 5.747E−25 | −10.7 | −7.46 | −4.06 | −6.70 | −11.2 | −24.5 | −6.4 | −20.6 |
| R 4 | 7218.5881 | 4001 | 3.384E−25 | −16.7 | −11.41 | −8.54 | −10.71 | 103.3 | 50.9 | 80.5 | −24.1 |
| R 8 | 7221.3766 | 4001 | 5.495E−25 | −16.5 | −11.08 | −8.26 | −10.36 | 103.8 | 51.5 | 81.4 | −23.9 |

**Table 4**
Comparison with the intensity measurements of Odintsova et al. [2] in cm/molecule at $T$ = 296 K. Ames gives the obs.-calc. values for the Ames-296K line list [7], p60.ai represents our calculations with the PES60 and our *ab initio* DMS [9] while p60.Sch calculations used PES60 and the DMS due to Schroder et al. [22]; in both cases Jacobi coordinates were used in the DVR3D calculations. The next three columns used Radau coordinates with our *ab initio* DMS [9] and three different PESs: PES60hJ, PES96G and PES60f. The final column, designated PES60f.Radau.ai, gives the final result of this work.

| line | $\tilde{\omega}$ cm$^{-1}$ | Band | Obs. | Ames | p60.ai | p60.Sch. | PES60hJ.Radau.ai | PES96G.Radau.ai | PES60f.Radau.ai |
|---|---|---|---|---|---|---|---|---|---|
| P41 | 4984.29 | (3200) | 6.23E−24 | −2.5 | | | −5.61 | −5.89 | −3.86 |
| R7 | 4983.92 | (0112) | 3.19E−24 | 7.6 | −89.6 | −73.2 | −0.31 | −0.31 | −1.24 |
| P43 | 4983.76 | (3310)–(0110) | 2.67E−25 | −0.3 | | | −2.91 | −3.26 | −1.11 |
| R6 | 4983.19 | (0112) | 2.83E−24 | 4.3 | −89.9 | −73.9 | −3.41 | −3.41 | −4.07 |
| P42 | 4983.06 | (3200) | 5.55E−24 | 0.3 | | | −2.80 | −3.31 | −1.07 |
| P43 | 4981.83 | (3200) | 4.84E−24 | 1.5 | | | −1.63 | −2.02 | 0.21 |
| R4 | 4981.69 | (0112) | 2.28E−24 | 6.8 | −89.6 | −73.2 | −0.87 | −0.87 | −1.72 |
| P44 | 4980.58 | (3200) | 4.21E−24 | 2.9 | | | −0.24 | −0.71 | 1.45 |

**Table 5**
Differences between measured intensities for the (4200) band ($I$ in cm/molecule at $T$ = 296 for 100% $^{14}N_2{}^{16}O$) due to Adkins et al. [3] and calculations: Ames – Ames-296K line list [7], PES60hJ.R.ai/PES60f.R.ai/PES96G.R.ai – PES60hJ/PES60f/PES96G obtained in Radau coordinates and our *ab initio* DMS, TYM – Exomol TYM list [8].

| Line | $\tilde{\omega}$/cm$^{-1}$ | $I$ | Ames | PES60hJ.R.ai | PES96G.R.ai | PES60f.R.ai | TYM |
|---|---|---|---|---|---|---|---|
| P17e | 6279.406202 | 2.80E−24 | −1.4 | | | 0.72 | |
| P16e | 6280.455528 | 2.84E−24 | −1.0 | | | 1.43 | |
| P15e | 6281.491611 | 2.86E−24 | −0.2 | | | 1.78 | |
| P14e | 6282.514458 | 2.80E−24 | −1.6 | | | 0.36 | |
| P13e | 6283.524079 | 2.76E−24 | −1.2 | | | 0.73 | |
| P12e | 6284.52048 | 2.80E−24 | 0.2 | | | 4.87 | |
| P11e | 6285.503667 | 2.56E−24 | −2.5 | | | −0.39 | |
| P10e | 6286.473645 | 2.46E−24 | −2.3 | −2.38 | −3.15 | 0.82 | −4.1 |
| P9e | 6287.430421 | 2.29E−24 | −3.1 | −2.97 | −3.78 | 0.00 | −4.8 |
| P8e | 6288.373997 | 2.18E−24 | 0.0 | 0.00 | −0.91 | 3.32 | −1.7 |
| P7e | 6289.304378 | 1.92E−24 | −2.6 | −2.54 | −3.52 | 0.52 | −4.3 |
| P6e | 6290.221565 | 1.69E−24 | −2.8 | −2.87 | −3.43 | 0.00 | −4.5 |
| P5e | 6291.125559 | 1.45E−24 | −2.4 | −2.68 | −3.33 | 0.69 | −4.1 |
| P4e | 6292.016361 | 1.19E−24 | −2.0 | −1.65 | −2.46 | 0.85 | −3.7 |
| P3e | 6292.893972 | 9.06E−25 | −2.2 | −2.27 | −2.89 | 0.89 | −3.8 |
| P2e | 6293.758388 | 6.03E−25 | −3.6 | −3.67 | −4.29 | −0.50 | −5.2 |
| P1e | 6294.609609 | 2.99E−25 | −5.3 | −5.38 | −5.97 | −2.29 | −6.7 |
| R0e | 6296.272448 | 3.07E−25 | −3.3 | −3.46 | −4.06 | −0.32 | −4.7 |
| R1e | 6297.084057 | 6.22E−25 | −1.8 | −1.74 | −2.51 | 1.30 | −3.3 |
| R2e | 6297.882451 | 9.23E−25 | −2.1 | −2.22 | −2.84 | 0.98 | −3.6 |
| R3e | 6298.667624 | 1.21E−24 | −2.7 | −2.42 | −3.2 | 0.00 | −4.2 |
| R4e | 6299.439566 | 1.50E−24 | −2.0 | −1.96 | −2.92 | 1.35 | −3.6 |
| R5e | 6300.198270 | 1.75E−24 | −2.9 | −2.78 | −3.85 | 0.00 | −4.4 |
| R6e | 6300.943725 | 2.03E−24 | −1.2 | −1.46 | −1.93 | 2.01 | −2.7 |
| R7e | 6301.675921 | 2.23E−24 | −2.4 | −2.62 | −3.04 | 0.45 | −3.9 |
| R8e | 6302.394846 | 2.24E−24 | −10.1 | −10.04 | −10.76 | −7.44 | −11.5 |
| R9e | 6303.100487 | 2.62E−24 | −2.0 | −2.24 | −2.60 | 1.16 | −3.5 |
| R10e | 6303.792831 | 2.76E−24 | −1.3 | | | 0.73 | |
| R11e | 6304.471864 | 2.89E−24 | −1.4 | | | 1.05 | |
| R12e | 6305.137572 | 2.98E−24 | −1.5 | | | 0.68 | |
| R13e | 6305.789939 | 3.07E−24 | −0.9 | | | 1.32 | |
| R14e | 6306.428948 | 3.10E−24 | −1.0 | | | 0.98 | |
| R15e | 6307.054582 | 3.11E−24 | −1.5 | | | 0.65 | |
| R16e | 6307.666825 | 3.11E−24 | −1.1 | | | 0.97 | |

caused by experimental problems, which was borne out by subsequent re-measurement of the intensities [30].

Tables 5 and 6 compare calculations of the (4200) and (5000) bands with sub-percent accuracy measurements [3]. For the (4220) band the calculations taken from the Ames-296K line list and our Jacobi coordinate calculations [9] give discrepancies of about 3%. Calculations in Radau coordinates show much higher accuracy, which is close to the experimental uncertainty. In particular, 29 out of 34 lines presented for $J \leq 17$ are predicted with either of sub-percent or one percent accuracy. Only 5 lines show discrepancies between 2 and 7.5%. For these 5 lines the arguments presented above are valid: we would encourage re-measurement of the intensities of these 5 lines. We are confident this would confirm the sub-percent accuracy of our calculations.

### 3.1.1. Comparisons with HITRAN

To estimate the accuracy of the intensity calculations using the various PESs plus our *ab initio* DMS [9] and that from the Schröder et al. [22], we calculated intensities for the R4 and R8 lines of the many bands presented in the HITRAN database [1]; the HITRAN database data is mostly based on somewhat less accurate intensity measurements than those considered above. The results of these comparisons are given in Table 3 where the differences are again represented as (Obs/Calc – 1) · 100, %. Table 3 also presents corresponding line intensities taken from Ames-296K line list [7] for comparison.

An important result is that swapping the coordinate system used to compute the wavefunctions from Jacobi coordinates, used in all calculations of our previous paper [9], to Radau coordinate system, completely solves the problem of large discrepancies found previously for some bands when using Jacobi coordinates calculations. All the bands presented in Table 3 calculated in Radau coordinates give very reasonable discrepancies, comparable or better than the error code given for them by HITRAN. All the ridiculous discrepancies have disappeared in these calculations. The worst discrepancies are 23% for the (0202) band and 36% for the (0000) band. Only two other bands are more than 10% off the values presented in HITRAN. 22 out of 37 bands

**Table 6**
Differences between measured intensities for the (5000) band ($I$ in cm/molecule at $T$ = 296 for 100% $^{14}N_2{}^{16}O$) due to Adkins et al. [3] and calculations. Ames – Ames-296K line list [7], PES60hJ.R.ai/PES60f.R.ai/PES96G.R.ai – PES60hJ/PES60f/PES96G obtained in Radau coordinates and our *ab initio* DMS, Ames.ai – Ames-296K PES and our *ab initio* DMS, Ames.Sch – Ames-296K and DMS by Schröder et al. , YYM – ExoMol TYM line list [8].

| Line | $\tilde{\omega}$/cm$^{-1}$ | $I$ | Ames | PES60hJ.R.ai | PES96G.R.ai | PES60f.R.ai | Ames.ai | Ames.Sch | TYM |
|---|---|---|---|---|---|---|---|---|---|
| P17e | 6357.260952 | 1.271E−24 | −3.1 | | | 0.87 | | | |
| P16e | 6358.309647 | 1.274E−24 | −4.0 | | | 0.31 | | | |
| P15e | 6359.345443 | 1.290E−24 | −3.2 | | | 0.78 | | | |
| P14e | 6360.368289 | 1.282E−24 | −3.4 | | | 0.94 | | | |
| P13e | 6361.378139 | 1.272E−24 | −2.8 | | | 0.95 | | | |
| P12e | 6362.374947 | 1.234E−24 | −3.3 | | | 0.33 | | | |
| P11e | 6363.358674 | 1.186E−24 | −3.8 | | | 0.51 | | | |
| P10e | 6364.329281 | 1.130E−24 | −4.7 | −2.59 | −3.42 | 0.00 | 10.4 | 8.1 | −3.6 |
| P9e | 6365.286733 | 1.080E−24 | −3.2 | −0.92 | −1.82 | 1.89 | 12.2 | 9.8 | −2.0 |
| P8e | 6366.231001 | 1.087E−24 | 5.5 | 7.62 | 6.57 | 10.92 | 22.2 | 19.6 | 6.7 |
| P7e | 6367.162054 | 8.929E−25 | −4.3 | −2.09 | −3.05 | 0.55 | 10.8 | 8.5 | −3.2 |
| P6e | 6368.079869 | 7.778E−25 | −5.7 | −3.50 | −4.45 | −0.79 | 9.2 | 6.9 | −4.6 |
| P5e | 6368.984422 | 6.707E−25 | −4.9 | −2.66 | −3.64 | −0.04 | 10.0 | 7.8 | −3.9 |
| P4e | 6369.875696 | 5.485E−25 | −4.9 | −2.75 | −3.60 | −0.09 | 10.0 | 7.8 | −3.9 |
| P3e | 6370.753673 | 4.111E−25 | −6.6 | −4.40 | −5.28 | −1.89 | 8.0 | 5.8 | −5.6 |
| P2e | 6371.618341 | 2.859E−25 | −3.9 | −1.75 | −2.76 | 1.02 | 11.1 | 8.9 | −2.9 |
| P1e | 6372.469689 | 1.434E−25 | −4.5 | −2.45 | −3.11 | 0.28 | 10.4 | 8.3 | −3.4 |
| R0e | 6374.132400 | 1.394E−25 | −7.7 | −5.81 | −6.44 | −3.19 | 10.3 | 4.6 | −6.7 |
| R1e | 6374.943758 | 2.939E−25 | −2.3 | −0.03 | −1.04 | 2.76 | 10.3 | 10.7 | −1.3 |
| R2e | 6375.741786 | 4.242E−25 | −5.3 | −3.15 | −4.03 | −0.42 | 9.4 | 7.4 | −4.3 |
| R3e | 6376.526487 | 5.586E−25 | −5.3 | −3.19 | −4.02 | −0.43 | 9.3 | 7.3 | −4.3 |
| R4e | 6377.297871 | 6.838E−25 | −5.8 | −3.55 | −2.23 | −0.90 | 7.3 | 6.8 | −4.8 |
| R5e | 6378.055947 | 8.121E−25 | −4.8 | −2.63 | −3.55 | 0.14 | 9.8 | 7.9 | −3.8 |
| R6e | 6378.800729 | 9.202E−25 | −5.2 | −3.03 | −3.95 | −0.41 | 9.3 | 7.4 | −4.3 |
| R7e | 6379.532233 | 1.077E−24 | −0.1 | 2.57 | 1.60 | 4.56 | 15.2 | 13.2 | 0.9 |
| R8e | 6380.250481 | 1.125E−24 | −4.1 | −2.17 | −3.02 | 0.45 | 10.6 | 8.7 | −3.1 |
| R9e | 6380.955494 | 1.202E−24 | −4.3 | −2.28 | −3.06 | 0.01 | 10.4 | 8.4 | −3.3 |
| R10e | 6381.647299 | 1.264E−24 | −3.7 | | | 0.32 | | | |
| R11e | 6382.325924 | 1.307E−24 | −4.4 | | | −0.23 | | | |
| R12e | 6382.991403 | 1.356E−24 | −3.7 | | | 0.44 | | | |
| R13e | 6383.643771 | 1.380E−24 | −3.9 | | | 0.00 | | | |
| R14e | 6384.283066 | 1.417E−24 | −2.3 | | | 1.94 | | | |
| R15e | 6384.909332 | 1.441E−24 | −0.8 | | | 2.93 | | | |
| R16e | 6385.522614 | 1.387E−24 | −3.9 | | | −0.22 | | | |

are only about 1 to 2% off their HITRAN values. Altogether this is an excellent result: for nearly half the bands our predictions are between 2 and 10 times more accurate than those of the Ames-296K line list [7].

There is one more interesting result which follows from the Tables 3–6. Previously [17] we found that improving the PES for the water molecule so that the standard deviation with which we predicted energy levels dropped from about 0.025 to 0.013 cm$^{-1}$ resulted in a change of the line intensities by up to 2 percent for about 20% of the bands; while the majority of the line intensities were unchanged within 0.1%. A very different situation can be seen in Tables 3 to 6. A small change in the standard deviation of the PES of $^{14}N_2{}^{16}O$ from $\sigma$ = 0.006 to 0.004 cm$^{-1}$ results in a change of more than 1% in the line intensities for very many band lines. In Table 4 the column PES96G.Radau.ai corresponds to the calculations with PES, fitted to experimental levels in Jacobi coordinates, which gives $\sigma$ = 0.006 cm$^{-1}$ in Radau coordinates, and the column PES60f.Radau.ai represents the results with the PES fitted in Radau coordinates with $\sigma$ < 0.004 cm$^{-1}$. The same behavior can also be seen in Tables 3, 5 and 6.

The conclusion from this finding is that even a seemingly insignificant change of the PES can result in a serious change of the intensity even for an isolated band. This finding needs to be borne in mind in the quest of generating sub-percent or even sub-per-mille calculated line intensities for the molecules important for atmospheric studies. Even more important is the role this might play in metrology where attempts to achieve line intensity accurate to $10^{-2}$ or even $10^{-3}$ % for measurement of temperature, pressure and isotopic substitution [32, 33].

## 4. Conclusion

In this paper we resolve the problem of inaccurately calculated $^{14}N_2{}^{16}O$ intensities for lines involving excitation of $\upsilon_3$ and/or $l$ identified by us previously [9] for calculations performed using Jacobi coordinates. Our solution is to change the coordinate system used to calculate the wavefunctions to Radau coordinates. Excellent reproduction of the experimental line intensities is achieved, superseding those presented in line lists such as Ames-296K [7], and ExoMol TYM [8], as well as our previous study [9]. In particular, four bands intensities, presented in Tables 4, 5, and 6 and measured with the sub-percent accuracy in [3] and [2] are reproduced within the experimental error. The previous variational calculations of these accurately measured bands gave the accuracy about 3 to 5 percent.

We also solve the problem of extremely large deviations of the line intensities of some bands which turned out to be due to the use of Jacobi coordinates. The reason why the Jacobi coordinates could not be used for the intensity calculations of $^{14}N_2{}^{16}O$ still remains unclear. Practically all the bands presented in HITRAN are reproduced in our calculations more accurately than in the variational calculations given in the literature [7–9].

The solution of the intensity problem combined with the near experimental accuracy achieved for calculated line centers [9] facilitates the computation of a highly accurate line list for $^{14}N_2{}^{16}O$.

## CRediT authorship contribution statement

**Irina I. Mizus:** Writing – review & editing, Investigation, Formal analysis, Data curation. **Mikhail A. Rogov:** Investigation. **Nikolai F. Zobov:** Writing – review & editing, Investigation. **Roman I. Ovsyannikov:** Methodology, Investigation, Formal analysis. **Evgenii I. Lebedev:** Investigation. **Jonathan Tennyson:** Writing – review & editing, Formal analysis. **Oleg L. Polyansky:** Writing – original draft, Methodology, Formal analysis, Conceptualization.

## Declaration of competing interest

The authors declare no conflict of interest.

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## Appendix A. Supplementary data

The supplementary material contains (A) the potential energy surfaces created in this work; (B) full results of the fits in terms of observed minus calculated comparisons.

Supplementary material related to this article can be found online at https://doi.org/10.1016/j.jms.2025.112034.

## Data availability

The data is all supplied as supplementary material.

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