A theoretical room-temperature line list for $^{15}$NH$_3$

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Abstract

A new room temperature line list for $^{15}$NH$_3$ is presented. This line list comprised of transition frequencies and Einstein coefficients has been generated using the ‘spectroscopic’ potential energy surface NH3-Y2010 and an ab initio dipole moment surface. The $^{15}$NH$_3$ line list is based on the same computational procedure used for the line list for $^{14}$NH$_3$ BYTe reported recently and should be as accurate. Comparisons with experimental frequencies and intensities are presented. The synthetic spectra show excellent agreement with experimental spectra.

1. Introduction

Although the abundance of $^{15}$N is 450 times lower than that of $^{14}$N [1], $^{15}$NH$_3$ is an important astrophysical molecule. It is a maser source detected in interstellar molecular clouds [2] and is also a tracer of the N$^{15}$/N$^{14}$ isotopic ratio in interstellar medium [3–5], planetary [6, 7] and Earth [8] atmospheres, meteorites [9], comets [10], important as a probe of chemical processes in the astrophysical environment, of planetary atmospheric and formation processes etc. Very recently Fletcher et al. [11] used the $^{14}$NH$_3$ and $^{15}$NH$_3$ spectral features to study the N$^{15}$/N$^{14}$ ratio for Jupiter and Saturn.

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Experimentally the ro-vibrational spectra of $^{15}$NH$_3$ have been studied in a large number of works, including rotation-inversion spectrum [12–17], fundamental bands [18–27], overtone bands [28–33], hot bands [34–37], and intensity measurements [38–41]. Some of these data are now collected in the HITRAN database [42]. The electric dipole moment was experimentally studied by Orr and Oka [43] and Dilonardo et al. [44] using the Stark spectroscopy. The ground state energies were reported by Urban et al. [22]. Very recently a VECSEL laser source study of the 2.3 $\mu$m region of $^{15}$NH$_3$ was presented by Čermák et al. [45] and a tentative assignment of new $^{15}$NH$_3$ lines in the 1.51 $\mu$m region was suggested by Földes et al. [46].

Huang et al. [47] presented theoretical ro-vibrational energies of $^{15}$NH$_3$ computed variationally using an empirical PES HSL-2 for $J = 0\ldots6$. These energies helped them to reassign and correct a number of transitions in HITRAN. An extensive hot line list BYTe for $^{14}$NH$_3$ was recently generated [48] using the TROVE approach [49]. Containing 1.1 billion transitions BYTe was designed to be applicable for temperatures up to 1500 K. It has proven to be useful for astrophysical and spectroscopic applications (see, for example, Refs. [45, 50, 51]). In this work we build a room temperature line list for the N$^{15}$ isotopologue of ammonia using the same computational approach based on the ‘spectroscopic’ potential energy surface (PES) NH3-Y2010 [52] and the \textit{ab initio} dipole moment surface (DMS) from Ref. [53]. The highest $J$ considered in this work is 18 defining the temperature limit of the current line list to be 300 K. It should be noted that TROVE was also used in the study of the thermal averaging properties of the spin-spin coupling constants of $^{15}$NH$_3$ by Yachmenev et al. [54] and a high-temperature partition function for $^{14}$NH$_3$ [55].

The paper is structured as follows. In Section 2 we outline the theoretical approach used for the line list production. In Section 3 the structure of the line list and the description of the quantum numbers are presented, where some
comparisons with experimental data are also given and the accuracy of the line list is discussed. In Section 4 some conclusions are offered.

2. Theoretical approach

We use the same computational procedure and the associated program TROVE [49] as was employed to generate the hot ammonia line list BYTe [48], therefore the reader should refer to this paper for a detailed description. Here we present only a short outline of this approach.

In order to obtain energies and associated wavefunctions required for building the line list of $^{15}$NH$_3$ we solve the Schrödinger equation for the nuclear motion variationally. Both the kinetic and potential energy terms of the Hamiltonian were expanded to 6th and 8th orders, respectively, in terms of five linearized coordinates around the reference geometry, defined as a non-rigid reference configuration associated with the inversion motion characterized by a relatively low barrier to the planarity. The linearized coordinates are chosen to be close to the three stretching modes associated with the N-H vibrations and two asymmetric bending modes combined from the three bending vibrations of the interbond angles H–N–H. Our vibrational basis set is a product of six one-dimensional (1D) basis functions. The stretching, bending, and inversion 1D basis sets are obtained by solving the corresponding reduced 1D Schrödinger equations using the Numerov-Cooley approach [56, 57] for each degree of freedom independently. This so-called primitive basis set is then improved through a number of pre-diagonalizations and consecutive contractions. The latter is controlled by the polyad number

$$P = 2(v_1 + v_2 + v_3) + v_4 + v_5 + v_6/2,$$

where $v_1, v_2, v_3$ are the quantum numbers associated with the three stretching modes, $v_4, v_5$ are associated with the asymmetric bending modes, and $v_6$ counts
the inversion mode functions. As in Ref. [48], we define the size of the basis
set using the condition $P \leq 14$. We use the so-called $J = 0$ representation,
where the final contracted ro-vibrational basis functions are represented by direct
symmetrized products of the vibrational $J = 0$ eigenfunctions and the rigid rotor
wavefunctions $|J, K, \tau_{\text{rot}}\rangle$, where $J$ is the rotational angular momentum, $K$ is
the projection of the rotational angular momentum to the molecular axis $z$, and $\tau_{\text{rot}}$
is the rotational parity (see [58] for further details). The $J = 0$ eigenfunctions
are the eigensolutions of the pure vibrational problem. The highest rotational
excitation presently considered is $J = 18$. We only compute and store the energy
term values and wavefunctions below $14\,000\,\text{cm}^{-1}$ above the zero point energy
(ZPE) obtained as $7414.08\,\text{cm}^{-1}$. These thresholds are chosen to get a reasonable
population at room temperature according with the Boltzmann distribution.

As in [53] here we employ the EBSC (empirical basis set correction) scheme,
where some of the $J = 0$ band centers are substituted with the corresponding
experimental values, where available. For $^{15}\text{NH}_3$ however there are only very
few band centers known experimentally with high enough accuracy, namely for $\nu_1$, $\nu_2$, $\nu_3$, $\nu_4$, $\nu_1 + \nu_2$, $\nu_1 + \nu_3$, $2\nu_2$, $\nu_2 + \nu_3$, $2\nu_4$, $2\nu_4$, $2\nu_4$, $2\nu_3$, $\nu_3 + 2\nu_4$, as well as the ground state inversion splitting [18–23, 25, 27–
30, 32, 33, 35–37, 45, 53, 60]. Therefore the effect of this otherwise very efficient
procedure is rather limited. With this approach the $J = 0$ energies are reproduced
exactly, while the ro-vibrational coupling leads to a gradual ‘de-focus’ of the
$J > 0$ energies. In Table 1 we compare the original theoretical term values
with the experimental band centres used in our EBSC approach. The Obs.-Calc.
residuals in this table illustrate the deficiency of our model based on the $^{14}\text{NH}_3$
PES applied for the 15th isotopologue. Although the accuracy of these particular
bands is recovered through the EBSC approach, the error of other band centers
can be expected to be as large as up to about $0.2\,\text{cm}^{-1}$ at least, as illustrated in
Table 1.

4
Figure 1: Absorption of $^{15}\text{NH}_3$ at $T = 296$ K (log-scale): The theoretical (BYTe-15 in the upper display) vs. experimental line intensities (bottom) from HITRAN 2012, by Devi et al. [39], and Lins et al. [41]. The experimental data points are repeated in the upper display as crosses for a better illustration of the agreement between theoretical and experimental intensities, where a number of outliers in the HITRAN data set is also clearly visible.

The same PES and DMS as in [48] were used. The potential energy surface NH3-Y2010 was obtained by Yurchenko et al. [52] by fitting to the experimentally derived term values of the main isotopologues only, with $J \leq 8$ covering term values up to $E = 10300$ cm$^{-1}$. Because of the approximations used in the fitting, this ‘spectroscopic’ PES is an effective object. Therefore it does not guarantee, at least in principle, the same accuracy for $^{15}\text{NH}_3$ as was reached for $^{14}\text{NH}_3$. We make a comparison with the experiment in the next section. The ab initio dipole moment surface ATZfc DMS used here was developed by Yurchenko et al. [61] which should be capable of accurate modelling of $^{15}\text{NH}_3$ spectra. For the description of the intensity calculations see Refs. [48, 62].

In Tables 2-5 we compare our theoretical term values of $^{15}\text{NH}_3$ with their ‘experimental’ counterparts for the vibrational ($J = 0$) and pure rotational
Figure 2: Absorption of $^{15}$NH$_3$ at $T = 296$ K: The theoretical (BYTE-15) vs. experimental line intensities (bottom) from HITRAN 2012, by Devi et al. [39], and Lins [41]. The intensities of the strong 3 $\mu$m band, which is also shown, are not known experimentally.

$(J = 0 \ldots 4)$ states available in the literature (see Introduction). As far as the accuracy of these term values is concerned it is comparable to the accuracy of the vibrational term values for the main isotopologue using the same PES. The pure rotational and rotation-inversional term values also show a very good agreement with experiment. This is reassuring especially if the underlying PES was generated using the main isotopologue only, although the effect from the isotopic substitution $^{14}$ → $^{15}$ is not expected to be large.
In Table 6 some vibrational term values \((J = 0)\) of \(^{15}\text{NH}_3\) from this work are compared to the theoretical values computed by Huang et al. \[47\] using their empirical PES HSL-II. The agreement at lower energies is very good but deteriorates at about 5000 cm\(^{-1}\). It is difficult to claim the better accuracy for any of these two approaches based on this comparison only. We believe that at least some of our band centers above 6000 cm\(^{-1}\) should be more accurate, see e.g. Table 5. However according to Čermák et al. \[45\] the line positions of \(^{15}\text{NH}_3\) reported by Huang et al. \[47\] are more precise at least for the 2.3 \(\mu\)m region.

We have compared our intensities to the HITRAN data \[42\] as well as to those reported by Devi et al. \[39\] (\(\nu_4\)) and Lins et al. \[41\] (near infrared). In Figs. 1 and 2 we show a generated absorption spectrum of \(^{15}\text{NH}_3\) at \(T = 296\) K compared to the HITRAN intensities. The agreement is similar to that achieved by BYTe for \(^{14}\text{NH}_3\) \[48\]. The \(^{15}\text{NH}_3\) experimental data is rather sparse compared to the data available for the main isotopologue. A number of obvious outliers (5014.4776, 5084.8734, 5104.2963, and possibly 5103.8909 cm\(^{-1}\)) in the experimental spectra indicate problems with the assignment of the \(^{15}\text{NH}_3\) transitions in HITRAN. Similar problems have recently been studied and resolved for the \(^{14}\text{NH}_3\) data \[63\]. Another outlier is at 6586.747 cm\(^{-1}\) from the recent work by Lins et al. \[41\] which also appears to be too strong, see Figs. 1 and 2.

3. The line list

Our room temperature \(^{15}\text{NH}_3\) line list contains \(80\,515\,767\) transitions representing all non-zero \((T = 300\) K\) intensities covering the wavenumber range up to 8000 cm\(^{-1}\) constructed from \(270\,646\) upper state term values below 14 000 cm\(^{-1}\) and \(9772\) lower state term values below 6 000 cm\(^{-1}\) with rotational excitations up to \(J = 18\). Following Refs. \[48, 64\] we use the two-files ExoMol format \[65\] to organize the line list for \(^{15}\text{NH}_3\). The Energy file (see an extract in Table 7) contains the energy term values \(\tilde{E}_i\) (cm\(^{-1}\)), quantum numbers both in the local
and normal mode representations. Each energy record is indexed with a running number \(i\). These indexes are then used in the Transition file (see extract in Table 8) to refer to a pair of states \(i'\) and \(i''\) participating in the transition \(i'' \rightarrow i'\). Apart from these indexes, only the Einstein coefficient \(A(i', i'')\) is needed to complete the transition record. With this format the size of the line list is significantly reduced. The line list can be also found via [www.exomol.com](http://www.exomol.com) as a part of the ExoMol project [66]. We also supply a sample Fortran code to be used together with our line list to simulate intensities or cross sections [67]. In fact the unified ExoMol-format of the present \(^{15}\)NH\(_3\) line list makes this code useful with any line lists stored in this format.

The largest expansion coefficients of the ro-vibrational eigenfunctions were used to assign the corresponding final eigenvalues with the vibrational quantum numbers \(v_1, v_2, v_3, v_4, v_5, v_6\), the rotational quantum numbers \(J\) and \(K\), the total symmetry \(\Gamma_{\text{tot}}\) as well as the symmetry of the \(J = 0\) vibrational basis function \(\Gamma_{\text{vib}}\). Here \(\Gamma_{\text{tot}}\) and \(\Gamma_{\text{vib}}\) are represented by six irreducible representations \(A'_1, A'_2, E', A''_1, A''_2, E''\) in the molecular symmetry group \(D_{3h}(M)\) [68]. In this case our ‘local’ mode basis functions are used as reference and provide approximate labels for the eigenstates. The problem with this approach (as well as many other assigning approaches) is the strong mixing of basis set functions at high excitations which gives rise to the ambiguity in assignment. As a manifestation of the quality of the assignment we also provide values of the corresponding largest expansion coefficients, see the \(|C_i|^2\)-column in Table 7: small numbers (less than 0.5) indicate strong mixing of reference states and show that that the suggested quantum numbers can be ambiguous.

Recognizing the importance of the conventional ‘normal’ mode quantum numbers, we map our ‘local’ modes to the ‘normal’ mode quantum numbers using the same procedure as in Ref. [48]. It should be noted however that there is no direct transformation between these two labelling schemes. Furthermore due to
the approximate nature of the assignment in some cases we obtain ambiguous normal mode quantum numbers, which do not always correspond to the experimental normal mode labels. Again, the value $|C_i|^2$ can be used as measure of this ambiguity.

We follow Ref. [63] and define the normal mode quantum numbers as given by

$$n_1, n_2, n_3, n_4, L_3, L_4, L, \Gamma_{\text{vib}}, J, K, i, \Gamma_{\text{rot}}, \Gamma_{\text{tot}},$$

(2)

where $L_3 = |l_3|, L_4 = |l_4|, L = |l|, K = |k|$. Here $n_i, (i = 1, 2, 3, 4)$ are the vibrational normal mode quantum numbers, $l_3$, $l_4$, and $l$ are the vibrational angular momentum labels; $J$ is the total angular momentum quantum number, $k = -J, \ldots, J$ is the projection of the total angular momentum on the molecule fixed axis $z$; $i = s/a$ is the inversion symmetry of the vibrational motion; and $\Gamma_{\text{vib}}$, $\Gamma_{\text{rot}}$ and $\Gamma_{\text{tot}}$ are the symmetry species of the rotational, vibrational, and total internal wave-functions in the molecular symmetry group $D_{3h}(M)$, respectively, spanning $A'*1, A''*1, A'*2, A''*2, E', E''$. As was argued by Down et al. [63], the definition of the signs of the vibrational angular momentum quantum numbers $l_3, l_4$ and $l$ is ambiguous (as ambiguous the sign of $k$). Therefore we follow the suggestion of Down et al. [63] and use the absolute values $L_i = |l_i| = n_i, n_i - i, \ldots, 0$ (1) instead.

The symmetries of the initial and final states are important for the line intensities, which is manifested by the selection rules and the nuclear statistical weights $g_{ns}$. Similar to the main isotopologue of ammonia, the ro-vibrational states with the symmetries of $A_1'$ and $A_2''$ do not exist (i.e. the corresponding $g_{ns} = 0$). The non-zero nuclear statistical weights factors are 8, 4, 8, 4 for $A_2', E', A_2'', E''$, respectively, which are different from those of $^{14}$NH$_3$ owning to the different nuclear spin of $^{15}$N, 1 against 1/2 of $^{14}$N. The TROVE approach uses the symmetrically adapted basis set, which gives the symmetry labels of the
eigenstates automatically. The selection rules are the following

\[ A'_2 \leftrightarrow A''_2, E' \leftrightarrow E'' \]  

and

\[ \Delta J = J' - J'' = 0, \pm 1, \quad J' + J'' \geq 1. \]  

The non-existing pure vibrational \((J = 0)\) \(A'_1\) and \(A''_1\) term values are also included into the line list with the total statistical weight \(g_{\text{tot}} = 0\), which can be useful as band centers.

With our computed energies of \(^{15}\text{NH}_3\) we obtain the partition function of 1165.4 which can be compared to the room-temperature partition function supplied by HITRAN of 1152.7 by Fischer et al. \[69\].

4. Conclusion

In this paper a new synthetic line list for \(^{15}\text{NH}_3\) is presented. This line list should be applicable for describing absorption of this molecule for temperatures up to 300 K. The \(^{15}\text{NH}_3\) line list has already proven useful for analysis of the experimental spectra by Čermák et al. \[45\] where it was applied for assignment of the 2.3 \(\mu\text{m}\) VECSEL spectra of \(^{15}\text{NH}_3\).

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References

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Table 1: Comparison of the theoretical term values (cm\(^{-1}\)) of \(^{15}\text{NH}_3\) before EBSC replacement and experimental ones used in the EBSC approach. See Table 7 for the description of the notations.

| \(v_{ij}\) | \(v_1\) | \(v_2\) | \(v_3\) | \(L_3\) | \(L_4\) | \(L_4\) | Obs. | Calc. | Obs.-Calc. | Ref. |
|---------|-------|-------|-------|--------|--------|--------|------|------|----------|-----|
| \(A''\) | 0 0 0 0 0 0 0 0.761 0.758 0.003 | [35] |
| \(A'\) | 1 0 0 0 0 0 0 928.509 928.457 0.052 | [35] |
| \(A''\) | 0 1 0 0 0 0 0 962.912 962.894 0.018 | [35] |
| \(A'\) | 2 0 0 0 0 0 0 1591.236 1591.185 0.051 | [28] |
| \(E'\) | 0 0 0 0 1 1 1 1623.130 1623.149 -0.020 | [28] |
| \(E''\) | 0 0 0 0 1 1 1 1624.190 1624.202 -0.012 | [28] |
| \(A''\) | 2 0 0 0 0 0 0 1870.823 1870.853 -0.030 | [30] |
| \(A'\) | 3 0 0 0 0 0 0 2369.274 2369.314 -0.041 | [28] |
| \(E'\) | 0 1 0 0 1 1 1 2533.382 2533.380 0.002 | [28] |
| \(E''\) | 0 1 0 0 1 1 1 2577.571 2577.590 -0.020 | [28] |
| \(A''\) | 0 3 0 0 0 0 0 3210.614 3210.430 0.184 | [27] |
| \(A'\) | 0 0 0 0 2 0 0 3212.355 3212.120 0.215 | [27] |
| \(E'\) | 0 0 0 0 2 2 2 3234.107 3233.925 0.182 | [27] |
| \(E''\) | 0 0 0 0 2 2 2 3235.504 3235.338 0.165 | [27] |
| \(A''\) | 1 0 0 0 0 0 0 3333.306 3333.220 0.086 | [27] |
| \(A'\) | 1 0 0 0 0 0 0 3334.252 3334.160 0.092 | [27] |
| \(E'\) | 0 0 1 1 0 0 1 3435.167 3435.143 0.024 | [27] |
| \(E''\) | 0 0 1 1 0 0 1 3435.540 3435.475 0.065 | [27] |
| \(A''\) | 1 1 0 0 0 0 0 4288.186 4288.024 0.162 | [22] |
| \(A'\) | 1 1 0 0 0 0 0 4312.345 4312.304 0.041 | [22] |
| \(E'\) | 1 0 0 0 2 2 2 6546.951 6546.987 -0.036 | [60] |
| \(E''\) | 1 0 0 0 2 2 2 6548.560 6548.449 0.111 | [60] |
| \(E'\) | 1 0 1 1 0 0 1 6597.607 6597.498 0.109 | [60] |
| \(E''\) | 1 0 1 1 0 0 1 6664.486 6664.627 -0.141 | [60] |
| \(E'\) | 1 0 1 1 0 0 1 6665.480 6665.303 0.177 | [60] |

\(^a\) Estimated from the a \(\rightarrow\) s band centers.

\(^b\) Estimated from the corresponding \(^3P(J = 1, k = 1)\) transition frequencies.
Table 2: Calculated term values (cm\(^{-1}\)) of \(^{15}\)NH\(_3\) compared to the experimental values \(^{22}\):
ground vibrational state. Here \(J\) is the rotational angular momentum, \(K\) is its projection, \(\Gamma_{\text{tot}}\) is the symmetry of the rotational states \(D_{3h}(M)\), and \(s/a\) is the inversion parity.

| \(J\) | \(K\) | \(\Gamma_{\text{tot}}\) | \(s/a\) | Obs. | Calc. | Obs.-Calc. |
|-------|-------|-----------------|-------|------|------|------------|
| 0     | 0     | \(A''\) a       | 0.7577| 0.7577| 0.0000|            |
| 1     | 1     | \(E''\) s       | 16.1491| 16.1495| -0.0004|            |
| 1     | 0     | \(A'_1\) s       | 19.8413| 19.8416| -0.0003|            |
| 1     | 0     | \(A''_1\) a      | 20.5892| 20.5895| -0.0003|            |
| 2     | 2     | \(E''\) s       | 44.7490| 44.7502| -0.0011|            |
| 2     | 2     | \(E''''\) a     | 45.5046| 45.5058| -0.0012|            |
| 2     | 1     | \(E''\) s       | 55.8176| 55.8186| -0.0010|            |
| 2     | 0     | \(A'_2\) s       | 59.5035| 59.5044| -0.0009|            |
| 2     | 0     | \(A''_2\) a      | 60.2322| 60.2332| -0.0010|            |
| 3     | 3     | \(A''_1\) s      | 85.7924| 85.7948| -0.0024|            |
| 3     | 2     | \(A''_2\) s      | 85.7924| 85.7948| -0.0024|            |
| 3     | 2     | \(A'_2\) s       | 86.5526| 86.5550| -0.0025|            |
| 3     | 1     | \(E''''\) s     | 104.2293| 104.2314| -0.0021|            |
| 3     | 1     | \(E''\) s       | 115.2695| 115.2715| -0.0019|            |
| 3     | 1     | \(E''''\) s     | 115.9768| 115.9789| -0.0021|            |
| 3     | 0     | \(A'_2\) s       | 118.9460| 118.9479| -0.0019|            |
| 3     | 0     | \(A''_2\) s      | 119.6469| 119.6490| -0.0021|            |
| 4     | 4     | \(E''\) s       | 139.2674| 139.2715| -0.0041|            |
| 4     | 4     | \(E''''\) s     | 140.0361| 140.0403| -0.0042|            |
| 4     | 3     | \(A''_2\) s      | 165.0675| 165.0711| -0.0037|            |
| 4     | 3     | \(A'_2\) s       | 165.7832| 165.7931| -0.0099|            |
| 4     | 2     | \(E''\) s       | 183.4416| 183.4450| -0.0035|            |
| 4     | 2     | \(E''''\) s     | 184.1315| 184.1352| -0.0038|            |
| 4     | 1     | \(E''\) s       | 194.4443| 194.4477| -0.0034|            |
| 4     | 1     | \(E''''\) s     | 195.1158| 195.1196| -0.0037|            |
| 4     | 0     | \(A'_2\) s       | 198.1083| 198.1117| -0.0034|            |
| 4     | 0     | \(A''_2\) s      | 198.7738| 198.7775| -0.0037|            |
Table 3: Calculated term values (cm\(^{-1}\)) of \(^{15}\)NH\(_3\) compared to the experimental values\(^{22}\). \(\nu_2\) state. Here \(J\) is the rotational angular momentum, \(K\) is its projection, \(\Gamma_{tot}\) is the total symmetry of the ro-vibrational states \(D_{3h}(M)\), and \(s/a\) is the inversion parity.

| \(J\) | \(K\) | \(\Gamma_{tot}\) | State | \(s/a\) | Obs. | Calc. | Obs.-Calc. |
|------|------|----------------|-------|--------|------|-------|------------|
| 0    | 0    | \(A_1^2\)     | \(\nu_2\) s | 928.457 | 928.457 | 0.000 |
| 1    | 1    | \(E^\prime\)  | \(\nu_2\) s | 944.594 | 944.590 | 0.004 |
| 1    | 0    | \(A_2^0\)     | \(\nu_2\) s | 948.550 | 948.544 | 0.006 |
| 0    | 0    | \(A_2^0\)     | \(\nu_2\) a | 962.894 | 962.894 | 0.000 |
| 2    | 2    | \(E^\prime\)  | \(\nu_2\) s | 972.908 | 972.898 | 0.010 |
| 1    | 1    | \(E^\prime\)  | \(\nu_2\) a | 978.924 | 978.922 | 0.003 |
| 2    | 1    | \(E^\prime\)  | \(\nu_2\) s | 984.763 | 984.749 | 0.015 |
| 2    | 2    | \(E^\prime\)  | \(\nu_2\) a | 1007.269 | 1007.262 | 0.007 |
| 3    | 3    | \(A_2^0\)     | \(\nu_2\) s | 1013.390 | 1013.371 | 0.019 |
| 2    | 1    | \(E^\prime\)  | \(\nu_2\) a | 1018.391 | 1018.382 | 0.009 |
| 2    | 0    | \(A_2^0\)     | \(\nu_2\) s | 1022.096 | 1022.086 | 0.010 |
| 3    | 2    | \(E^\prime\)  | \(\nu_2\) s | 1033.137 | 1033.111 | 0.027 |
| 3    | 1    | \(E^\prime\)  | \(\nu_2\) s | 1044.949 | 1044.918 | 0.031 |
| 3    | 3    | \(A_2^0\)     | \(\nu_2\) a | 1047.921 | 1047.908 | 0.013 |
| 3    | 0    | \(A_2^0\)     | \(\nu_2\) s | 1048.881 | 1048.848 | 0.032 |
| 4    | 4    | \(E^\prime\)  | \(\nu_2\) s | 1066.029 | 1065.998 | 0.030 |
| 3    | 2    | \(E^\prime\)  | \(\nu_2\) a | 1066.450 | 1066.433 | 0.017 |
| 3    | 1    | \(E^\prime\)  | \(\nu_2\) a | 1077.544 | 1077.531 | 0.013 |
| 4    | 3    | \(A_2^0\)     | \(\nu_2\) s | 1093.666 | 1093.626 | 0.040 |
| 4    | 4    | \(E^\prime\)  | \(\nu_2\) a | 1100.870 | 1100.848 | 0.022 |
| 4    | 2    | \(E^\prime\)  | \(\nu_2\) s | 1113.317 | 1113.270 | 0.047 |
| 4    | 1    | \(E^\prime\)  | \(\nu_2\) s | 1125.071 | 1125.020 | 0.051 |
| 4    | 3    | \(A_2^0\)     | \(\nu_2\) s | 1126.801 | 1126.774 | 0.026 |
| 4    | 2    | \(E^\prime\)  | \(\nu_2\) s | 1145.279 | 1145.249 | 0.030 |
| 4    | 1    | \(E^\prime\)  | \(\nu_2\) s | 1156.349 | 1156.317 | 0.032 |
| 4    | 0    | \(A_2^0\)     | \(\nu_2\) s | 1160.036 | 1160.003 | 0.032 |
Table 4: Calculated term values (cm$^{-1}$) of $^{15}$NH$_3$ compared to the experimental values\textsuperscript{[22]}.

The $\nu_1 + \nu_2$ band. Here $J$ is the rotational angular momentum, $K$ is its projection, $\Gamma_{tot}$ is the total symmetry of the ro-vibrational states $D_{3h}$ (M), and $s/a$ is the inversion parity.

| $J$ | $K$ | $\Gamma_{tot}$ | $s/a$ | Obs. | Calc. | Obs.-Calc. |
|-----|-----|----------------|-------|------|-------|------------|
| 0   | 1   | $A_2^0$        | a     | 4312.303 | 4312.304 | −0.001     |
| 1   | 1   | $E^0$          | a     | 4328.148 | 4328.151 | −0.003     |
| 2   | 1   | $A_2^1$        | a     | 4370.642 | 4370.654 | −0.012     |
| 2   | 1   | $E^1$          | a     | 4367.042 | 4367.050 | −0.008     |
| 2   | 1   | $E''$          | a     | 4356.231 | 4356.232 | −0.001     |
| 3   | 1   | $E'$           | a     | 4425.344 | 4425.364 | −0.020     |
| 3   | 1   | $E''$          | a     | 4414.552 | 4414.563 | −0.011     |
| 3   | 1   | $A_2^2$        | a     | 4396.541 | 4396.539 | 0.001      |
| 1   | 1   | $E^3$          | s     | 4307.725 | 4307.720 | 0.006      |
| 1   | 1   | $E''$          | s     | 4303.949 | 4303.944 | 0.005      |
| 2   | 1   | $E''$          | s     | 4332.010 | 4332.002 | 0.008      |
| 3   | 1   | $A_2^3$        | s     | 4406.116 | 4406.086 | 0.029      |
| 3   | 1   | $E^3$          | s     | 4402.357 | 4402.330 | 0.028      |
| 3   | 1   | $E'$           | s     | 4391.069 | 4391.046 | 0.024      |
| 1   | 1   | $A_2^4$        | s     | 4372.198 | 4372.192 | 0.006      |
| 1   | 1   | $E'$           | a     | 4328.149 | 4328.151 | −0.002     |
| 2   | 1   | $E''$          | a     | 4367.042 | 4367.050 | −0.009     |
| 2   | 1   | $E''$          | a     | 4356.230 | 4356.232 | −0.002     |
| 3   | 1   | $E'$           | a     | 4425.347 | 4425.364 | −0.016     |
| 3   | 1   | $E''$          | a     | 4414.552 | 4414.563 | −0.011     |
| 3   | 1   | $A_2^5$        | a     | 4396.543 | 4396.539 | 0.003      |
| 1   | 1   | $E^6$          | a     | 4503.017 | 4503.050 | −0.033     |
| 1   | 1   | $E''$          | a     | 4492.247 | 4492.272 | −0.025     |
| 1   | 1   | $A_2^6$        | a     | 4474.275 | 4474.288 | −0.013     |
| 1   | 1   | $E''$          | a     | 4449.066 | 4449.061 | 0.005      |
| 1   | 1   | $E'$           | s     | 4303.949 | 4303.944 | 0.005      |
| 2   | 1   | $E''$          | s     | 4334.336 | 4334.320 | 0.015      |
| 2   | 1   | $E'$           | s     | 4332.010 | 4332.002 | 0.007      |
| 3   | 1   | $E''$          | a     | 4402.358 | 4402.330 | 0.029      |
| 3   | 1   | $E'$           | s     | 4391.074 | 4391.046 | 0.028      |
| 3   | 1   | $A_2^7$        | s     | 4372.207 | 4372.192 | 0.015      |
| 4   | 1   | $E^8$          | s     | 4480.955 | 4480.908 | 0.047      |
| 4   | 1   | $E'$           | s     | 4469.708 | 4469.668 | 0.040      |
| 4   | 1   | $A_2^9$        | s     | 4450.918 | 4450.890 | 0.028      |
| 3   | 1   | $E'$           | a     | 4424.519 | 4425.364 | −0.845     |
| 2   | 1   | $A_2^7$        | a     | 4370.642 | 4370.654 | −0.012     |
| 2   | 1   | $E^7$          | a     | 4367.042 | 4367.050 | −0.008     |
| 3   | 1   | $E''$          | a     | 4425.346 | 4425.364 | −0.018     |
| 3   | 1   | $E'$           | a     | 4414.552 | 4414.563 | −0.011     |
| 0   | 0   | $A_2^0$        | a     | 4506.607 | 4506.966 | −0.359     |
| 1   | 1   | $E^0$          | a     | 4503.020 | 4503.050 | −0.030     |
| 1   | 1   | $E''$          | a     | 4492.248 | 4492.272 | −0.024     |
| 1   | 1   | $A_2^1$        | a     | 4474.268 | 4474.288 | −0.020     |
| 1   | 1   | $A_2^2$        | a     | 4307.724 | 4307.720 | 0.005      |
| 1   | 1   | $E^1$          | a     | 4367.042 | 4367.050 | −0.008     |
| 1   | 1   | $E''$          | s     | 4406.115 | 4406.086 | 0.029      |
| 1   | 1   | $E'$           | s     | 4391.069 | 4391.046 | 0.023      |
| 4   | 1   | $E''$          | s     | 4480.955 | 4480.908 | 0.048      |
| 4   | 1   | $E'$           | s     | 4469.711 | 4469.668 | 0.043      |
| 4   | 1   | $A_2^5$        | s     | 4450.924 | 4450.890 | 0.033      |
Table 5: Calculated term values (cm\(^{-1}\)) of \(^{15}\)NH\(_3\) compared to the experimental values\(^{32,33}\) in the 1.5 \(\mu\)m band. Here \(J\) is the rotational angular momentum, \(K\) is its projection, \(\Gamma_{tot}\) is the total symmetry of the ro-vibrational states \(D_{10}(\text{M})\), and \(s/a\) is the inversion parity.

| \(J\) | \(K\) | \(\Gamma_{tot}\) | State | \(s/a\) | Obs. | Calc. | Obs.-Calc. |
|------|------|-----------------|-------|-------|------|-----|----------|
| 0    | 0    | \(E'\) \(v_1 + v_3\) | s     | 6596.605 | 6596.569 | 0.036 |
| 0    | 0    | \(E''\) \(v_1 + v_3\) | a     | 6597.498 | 6597.607 | -0.109 |
| 0    | 0    | \(E''\) \(v_1 + v_3\) | s     | 6644.627 | 6664.627 | 0.000 |
| 1    | 1    | \(E'\) \(v_1 + v_3\) | s     | 6612.935 | 6612.745 | 0.190 |
| 1    | 1    | \(E''\) \(v_1 + v_3\) | s     | 6613.111 | 6613.311 | -0.200 |
| 1    | 1    | \(E''\) \(v_1 + v_3\) | a     | 6613.987 | 6614.222 | -0.235 |
| 1    | 0    | \(E'\) \(v_1 + v_3\) | s     | 6616.563 | 6616.585 | -0.022 |
| 1    | 0    | \(E''\) \(v_1 + v_3\) | a     | 6617.389 | 6617.375 | 0.014 |
| 1    | 1    | \(E''\) \(v_1 + v_3\) | s     | 6680.448 | 6680.395 | 0.053 |
| 1    | 1    | \(E''\) \(v_1 + v_3\) | a     | 6681.159 | 6680.969 | 0.190 |
| 1    | 0    | \(E'\) \(v_1 + v_3\) | s     | 6684.445 | 6684.459 | -0.014 |
| 1    | 0    | \(E''\) \(v_1 + v_3\) | a     | 6655.051 | 6655.062 | -0.011 |
| 2    | 2    | \(E''\) \(v_1 + v_3\) | a     | 6641.024 | 6640.637 | 0.387 |
| 2    | 2    | \(A''\) \(v_1 + v_3\) | s     | 6642.655 | 6642.223 | 0.432 |
| 2    | 1    | \(E''\) \(v_1 + v_3\) | s     | 6651.538 | 6651.540 | -0.002 |
| 2    | 1    | \(E''\) \(v_1 + v_3\) | s     | 6653.082 | 6653.098 | -0.016 |
| 2    | 1    | \(E''\) \(v_1 + v_3\) | s     | 6653.864 | 6653.364 | 0.500 |
| 2    | 0    | \(E'\) \(v_1 + v_3\) | s     | 6656.415 | 6656.516 | -0.101 |
| 2    | 0    | \(E''\) \(v_1 + v_3\) | a     | 6657.122 | 6657.101 | 0.021 |
| 2    | 2    | \(A''\) \(v_1 + v_3\) | s     | 6709.141 | 6708.980 | 0.161 |
| 2    | 2    | \(A''\) \(v_1 + v_3\) | s     | 6709.962 | 6709.633 | 0.329 |
| 2    | 1    | \(A''\) \(v_1 + v_3\) | a     | 6720.105 | 6720.056 | 0.049 |
| 2    | 1    | \(E''\) \(v_1 + v_3\) | a     | 6720.618 | 6720.493 | 0.125 |
| 0    | 0    | \(E''\) \(v_1 + v_3\) | s     | 6724.162 | 6724.185 | -0.023 |
| 0    | 0    | \(E''\) \(v_1 + v_3\) | a     | 6724.623 | 6724.659 | -0.036 |
| 0    | 0    | \(E''\) \(v_1 + 2v_4\) | s     | 6546.987 | 6546.987 | 0.000 |
| 1    | 1    | \(A''\) \(v_1 + 2v_4\) | a     | 6548.449 | 6548.449 | 0.000 |
| 1    | 1    | \(A''\) \(v_1 + 2v_4\) | a     | 6559.895 | 6559.922 | -0.027 |
| 1    | 0    | \(E''\) \(v_1 + 2v_4\) | s     | 6567.492 | 6567.504 | -0.012 |
| 1    | 0    | \(E''\) \(v_1 + 2v_4\) | s     | 6567.904 | 6567.960 | -0.056 |
| 1    | 0    | \(E''\) \(v_1 + 2v_4\) | s     | 6568.657 | 6568.730 | -0.073 |
| 1    | 1    | \(E''\) \(v_1 + 2v_4\) | a     | 6569.257 | 6569.269 | -0.012 |
| 2    | 2    | \(E''\) \(v_1 + 2v_4\) | s     | 6582.047 | 6582.056 | -0.009 |
| 2    | 2    | \(E''\) \(v_1 + 2v_4\) | a     | 6583.439 | 6583.476 | -0.037 |
| 2    | 1    | \(A''\) \(v_1 + 2v_4\) | s     | 6599.495 | 6599.514 | -0.019 |
| 2    | 1    | \(A''\) \(v_1 + 2v_4\) | s     | 6601.051 | 6600.952 | 0.099 |
| 2    | 2    | \(A''\) \(v_1 + 2v_4\) | a     | 6602.177 | 6602.120 | 0.057 |
| 2    | 0    | \(E''\) \(v_1 + 2v_4\) | s     | 6608.463 | 6608.506 | -0.043 |
| 2    | 0    | \(E''\) \(v_1 + 2v_4\) | a     | 6609.322 | 6609.348 | -0.026 |
| 2    | 0    | \(E''\) \(v_1 + 2v_4\) | a     | 6609.323 | 6609.348 | -0.025 |
| 2    | 1    | \(E''\) \(v_1 + 2v_4\) | a     | 6609.784 | 6609.876 | -0.092 |
| 2    | 2    | \(E''\) \(v_1 + 2v_4\) | a     | 6640.194 | 6640.470 | -0.276 |
| 2    | 1    | \(E''\) \(v_3 + 2v_4\) | a     | 6700.714 | 6699.362 | 1.352 |
| 2    | 2    | \(E''\) \(v_3 + 2v_4\) | s     | 6702.047 | 6703.073 | -1.026 |
| 2    | 1    | \(A''\) \(v_3 + 2v_4\) | a     | 6713.529 | 6712.830 | 0.699 |
Table 6: Comparison of the theoretical term values (cm$^{-1}$) of $^{15}$NH$_3$, from this work (BYTe-15) and computed by Huang et al. [47]. See Table 7 for the description of the notations.

| $v_{10}$ | $v_1$ | $v_2$ | $v_3$ | $v_4$ | $v_5$ | $\tau_{0\omega}$ | BYTe-15 | HSL-2 | BYTe-HSL |
|---------|-------|-------|-------|-------|-------|------------------|---------|-------|----------|
| $A'_{20}$ | 0 | 0 | 0 | 0 | 0 | 0 | 0.00 | 0.00 | 0.00 |
| $A'_{22}$ | 0 | 0 | 0 | 0 | 0 | 1 | 0.76 | 0.76 | 0.00 |
| $A'_{40}$ | 0 | 1 | 0 | 0 | 0 | 0 | 928.46 | 928.47 | −0.01 |
| $A'_{42}$ | 0 | 1 | 0 | 0 | 0 | 1 | 962.89 | 962.93 | −0.04 |
| $A'_{44}$ | 0 | 2 | 0 | 0 | 0 | 0 | 1591.18 | 1591.18 | 0.00 |
| $A'_{50}$ | 0 | 2 | 0 | 0 | 0 | 1 | 1870.85 | 1870.82 | 0.03 |
| $A'_{60}$ | 0 | 3 | 0 | 0 | 0 | 0 | 2369.31 | 2369.33 | −0.02 |
| $A''_{20}$ | 0 | 0 | 0 | 2 | 0 | 0 | 2876.12 | 2876.12 | 0.01 |
| $A''_{22}$ | 0 | 0 | 0 | 2 | 0 | 1 | 3212.12 | 3212.08 | −0.08 |
| $A''_{40}$ | 0 | 0 | 0 | 2 | 0 | 0 | 3212.12 | 3212.08 | 0.04 |
| $A''_{42}$ | 1 | 0 | 0 | 0 | 0 | 0 | 3333.22 | 3333.27 | −0.05 |
| $A''_{44}$ | 1 | 0 | 0 | 0 | 0 | 1 | 3334.16 | 3334.25 | −0.09 |
| $A''_{46}$ | 0 | 4 | 0 | 0 | 0 | 0 | 4383.72 | 4383.70 | 0.02 |
| $A''_{50}$ | 0 | 4 | 0 | 0 | 0 | 1 | 4034.03 | 4033.67 | 0.36 |
| $A''_{52}$ | 0 | 1 | 0 | 2 | 0 | 0 | 4105.77 | 4105.95 | −0.18 |
| $A''_{54}$ | 0 | 1 | 0 | 2 | 0 | 1 | 4161.85 | 4161.73 | 0.12 |
| $A''_{56}$ | 0 | 1 | 0 | 2 | 0 | 0 | 4383.24 | 4383.26 | −0.01 |
| $A''_{60}$ | 1 | 1 | 0 | 0 | 0 | 0 | 4995.22 | 4992.68 | 2.54 |
| $A''_{62}$ | 1 | 1 | 0 | 0 | 0 | 1 | 4312.30 | 4312.29 | 0.01 |
| $A''_{64}$ | 0 | 5 | 0 | 0 | 0 | 0 | 4622.71 | 4622.23 | 0.48 |
| $A''_{66}$ | 0 | 5 | 0 | 0 | 0 | 1 | 4740.39 | 4743.57 | −3.18 |
| $A''_{70}$ | 0 | 0 | 0 | 3 | 0 | 3 | 4832.84 | 4832.55 | 0.29 |
| $A''_{72}$ | 0 | 0 | 0 | 3 | 0 | 3 | 4834.25 | 4834.26 | −0.01 |
| $A''_{74}$ | 0 | 1 | 2 | 0 | 0 | 0 | 4973.92 | 4970.92 | 3.02 |
| $A''_{76}$ | 0 | 1 | 2 | 0 | 0 | 1 | 4995.22 | 4992.68 | 2.54 |
| $A''_{80}$ | 0 | 0 | 1 | 1 | 1 | 1 | 5058.33 | 5055.98 | 2.35 |
| $A''_{82}$ | 0 | 0 | 1 | 1 | 1 | 1 | 5058.75 | 5056.20 | 2.55 |
| $A''_{84}$ | 0 | 2 | 0 | 2 | 0 | 0 | 5074.97 | 5076.68 | −1.71 |
| $A''_{86}$ | 1 | 2 | 0 | 2 | 0 | 0 | 5221.82 | 5220.15 | 1.67 |
| $A''_{90}$ | 0 | 5 | 0 | 0 | 0 | 0 | 5322.90 | 5322.97 | −0.07 |
| $A''_{92}$ | 0 | 3 | 0 | 2 | 0 | 0 | 5579.27 | 5582.89 | −3.62 |
| $A''_{94}$ | 0 | 1 | 0 | 3 | 0 | 3 | 5704.65 | 5705.12 | −0.47 |
| $A''_{96}$ | 1 | 3 | 0 | 0 | 0 | 0 | 5723.13 | 5721.57 | 1.56 |
| $A''_{100}$ | 0 | 1 | 0 | 3 | 0 | 3 | 5773.60 | 5774.00 | −0.40 |
| $A''_{102}$ | 0 | 6 | 0 | 0 | 0 | 0 | 6002.36 | 6001.83 | 0.53 |
| $A''_{104}$ | 0 | 1 | 1 | 1 | 1 | 1 | 6004.37 | 6007.44 | −3.07 |
| $A''_{106}$ | 0 | 1 | 1 | 1 | 1 | 1 | 6030.73 | 6031.88 | −1.15 |
| $A''_{110}$ | 0 | 3 | 0 | 2 | 0 | 0 | 6106.56 | 6109.59 | −3.03 |
| $A''_{112}$ | 1 | 3 | 0 | 0 | 0 | 0 | 6208.93 | 6208.84 | 0.09 |
| $A''_{114}$ | 0 | 2 | 0 | 2 | 0 | 0 | 6330.11 | 6333.51 | −3.40 |
| $A''_{116}$ | 0 | 0 | 0 | 4 | 0 | 0 | 6346.25 | 6343.14 | 3.11 |
| $A''_{120}$ | 0 | 0 | 0 | 4 | 0 | 1 | 6350.08 | 6344.21 | 5.87 |
| $A''_{122}$ | 2 | 0 | 0 | 0 | 0 | 0 | 6506.86 | 6512.69 | −5.83 |
| $A''_{124}$ | 2 | 0 | 0 | 0 | 0 | 1 | 6508.66 | 6514.29 | −5.63 |
| $A''_{126}$ | 1 | 0 | 0 | 2 | 0 | 0 | 6595.10 | 6597.04 | −1.94 |
| $A''_{130}$ | 1 | 0 | 0 | 2 | 0 | 1 | 6595.98 | 6597.93 | −1.95 |
| $A''_{132}$ | 1 | 0 | 0 | 2 | 0 | 0 | 6634.75 | 6637.61 | −2.86 |
| $A''_{134}$ | 1 | 0 | 0 | 2 | 0 | 1 | 6636.48 | 6638.79 | −2.31 |
| $A''_{136}$ | 0 | 4 | 0 | 2 | 0 | 0 | 6680.14 | 6682.30 | −2.16 |
| $A''_{140}$ | 0 | 2 | 0 | 3 | 0 | 3 | 6692.05 | 6694.31 | −2.26 |
Table 7: Extract from the Energy file.

| Column Notation | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 | 19 | 20 | 21 | 22 | 23 | 24 |
|-----------------|---|---|---|---|---|---|---|---|---|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|
| N               |   |   |   |   |   |   |   |   |   |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |
| E               |   |   |   |   |   |   |   |   |   |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |
| $g_{rot}$       |   |   |   |   |   |   |   |   |   |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |
| $J_{rot}$       |   |   |   |   |   |   |   |   |   |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |
| $n_1$ - $n_4$   |   |   |   |   |   |   |   |   |   |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |
| $L_3, L_4$      |   |   |   |   |   |   |   |   |   |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |
| $\Gamma_{vib}$^a |   |   |   |   |   |   |   |   |   |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |
| $s/a$           |   |   |   |   |   |   |   |   |   |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |
| $K$             |   |   |   |   |   |   |   |   |   |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |
| $\Gamma_{rot}$^a |   |   |   |   |   |   |   |   |   |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |
| $|C_i^2|^2$      |   |   |   |   |   |   |   |   |   |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |
| $v_1$ - $v_6$   |   |   |   |   |   |   |   |   |   |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |

\* The symmetry labels (1,2,3,4,5,6) are used for $(A_1', A_2', E', A_1'', A_2'', E'')$, respectively.

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1. The symmetry labels (1,2,3,4,5,6) are used for $(A_1', A_2', E', A_1'', A_2'', E'')$, respectively.
Table 8: Extract from the Transition file.

| $i'$ | $i''$ | $\lambda_{i'\gamma_{i''}} / \text{s}^{-1}$ |
|------|-------|------------------------------------------|
| 623528 | 445704 | 1.5466e-08 |
| 1737233 | 1846711 | 1.1752e-07 |
| 1334663 | 1430969 | 2.4884e-06 |
| 446023 | 393427 | 1.1053e-01 |
| 623718 | 688990 | 9.7052e-08 |
| 906264 | 688810 | 7.0643e-10 |
| 1334663 | 1430969 | 2.4884e-06 |
| 446023 | 393427 | 1.1053e-01 |
| 623718 | 688990 | 9.7052e-08 |
| 906264 | 688810 | 7.0643e-10 |
| 1334663 | 1430969 | 2.4884e-06 |
| 446023 | 393427 | 1.1053e-01 |
| 623718 | 688990 | 9.7052e-08 |
| 906264 | 688810 | 7.0643e-10 |
| 1334663 | 1430969 | 2.4884e-06 |
| 446023 | 393427 | 1.1053e-01 |
| 623718 | 688990 | 9.7052e-08 |
| 906264 | 688810 | 7.0643e-10 |
| 1334663 | 1430969 | 2.4884e-06 |
| 446023 | 393427 | 1.1053e-01 |
| 623718 | 688990 | 9.7052e-08 |
| 906264 | 688810 | 7.0643e-10 |
| 1334663 | 1430969 | 2.4884e-06 |
| 446023 | 393427 | 1.1053e-01 |
| 623718 | 688990 | 9.7052e-08 |
| 906264 | 688810 | 7.0643e-10 |
| 1334663 | 1430969 | 2.4884e-06 |
| 446023 | 393427 | 1.1053e-01 |
| 623718 | 688990 | 9.7052e-08 |
| 906264 | 688810 | 7.0643e-10 |
| 1334663 | 1430969 | 2.4884e-06 |
| 446023 | 393427 | 1.1053e-01 |
| 623718 | 688990 | 9.7052e-08 |
| 906264 | 688810 | 7.0643e-10 |
| 1334663 | 1430969 | 2.4884e-06 |

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