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Total internal partition sums for molecules of astrophysical interest

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Abstract

Total internal partition sums (TIPS) are calculated for several molecules, which are abundant in non-terrestrial planetary atmospheres. For all molecules, calculations are performed for the most abundant isotopic species. Partition sums for lesser abundant isotopomers of several molecules are determined as well. The calculations are made for temperatures between 70 and 300 K. The resulting TIPS are fit to a polynomial expression, which is fourth order in temperature. The methods of calculation of the TIPS, the convergence, and the quality of the polynomial fits for each isotopomer are discussed. © 2002 Published by Elsevier Science Ltd.

Keywords: Partition sums; Temperature dependence of partition sums; Planetary atmospheres

1. Introduction

Knowledge of the total internal partition sum (TIPS) is useful for a number of different applications. Many thermodynamic quantities can be derived from the partition sum. Relationships between the intensity of a spectral line and the transition moment squared, or Einstein A coefficient, or the oscillator strength require an accurate value for the partition sum [1–3]. The intensity of a spectral line at a given temperature can be calculated from the line intensity at a reference temperature and the TIPS at both temperatures. Such relationships are necessary when studying systems that are not isothermal, e.g. planetary atmospheres. Thus given a spectroscopic database of molecules for the particular atmosphere [4–6] and knowing the partition sum at the temperatures of the atmosphere, spectra can be inverted to obtain the desired profiles. It should be noted that in the literature, the terms partition function and partition sum are synonymous.

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In this paper, the calculations of the total internal partition sums for several molecular isotopomers, which are abundant in non-terrestrial planetary atmospheres and important to various astrophysical concerns, are presented. The list of species under consideration in this study and the temperature range of the study were chosen with regard to the temperatures and constituents of the Jovan atmosphere. In particular, the list of molecules and isotopomers comprises those studied by the NIMS project [7], a part of the Galileo mission, [8] for which TIPS were not readily available in the literature (e.g. the HITRAN database [4], JPL catalogue [6]). In order to be useful the TIPS must be recalled quickly and accurately. To facilitate the recall, the TIPS are fit to a fourth order in temperature polynomial expression, which minimizes storage of data and allows for rapid recall with the introduction of minimal error.

2. Total internal partition sums

The total internal partition sum of a molecule is defined as a direct sum over all states, s, of the factor $e^{-hcE_s/kT}$. In this expression, h is the Planck constant, c is the speed of light, k is the Boltzmann constant, T is the temperature in Kelvin and E_s is the total energy of state s in wavenumber units, including electronic, vibrational, rotational and any other quantized motion. This expression can be simplified by accounting for degenerate states with the following formula:

$$Q(T) = d_i \sum_s d_s e^{-hcE_s/kT}, \tag{1}$$

where d_s accounts for state-dependent degeneracy factors and d_i accounts for state-independent degeneracy factors. Examples of state-dependent degeneracy factors are the $2J+1$ degenerate states of total angular momentum J in the absence of an electric field or the coupling of rotational and nuclear wavefunctions due to the symmetry of a molecule such as dicyanogen ($^{14}N^{12}C^{12}C^{14}N$) which gives 6- and 3-fold degeneracy for even and odd rotational states, respectively. An example of a state-independent degeneracy factor is the product, $\Pi(2I_i+1)$, where I_i is the nuclear spin of each atom, present in a molecule where identical atoms are not exchanged by rotations which leave the symmetry of the molecule intact, such as HC_3N.

The calculation of the partition sum for a molecule requires the energy levels and degeneracy factors be known for the isotopomer in question. As the energy of state s increases, the exponential, $e^{-hcE_s/kT}$, approaches zero, and the partition sum can be truncated with no loss of accuracy. The state at which truncation can occur without loss of accuracy is dependent on temperature, as kT divides the energy of the state. An accurate calculation of the partition sum by direct summation can only be made by summing over energy levels until the exponential factor no longer contributes significantly to $Q(T)$. This can be determined by considering $Q(T)$ versus energy and noting the point beyond which $Q(T)$ remains constant as additional energies are summed over. At this point, the calculation of the partition sum is said to have converged.

For various reasons, it is often difficult to obtain the energy levels of a particular isotopomer to high enough states to accurately calculate the partition sum. For such cases, a number of approximations can be made. For molecules with large separations between the ground and excited electronic states, the total energy is taken as a sum of the vibrational and rotational energy, $E_{\mathrm{tot}} = E_{\mathrm{vib}} + E_{\mathrm{rot}}$. Ignoring vibrational–rotational interactions, the TIPS is given by

$$Q(T) = \sum_{\substack{\text{vibrational} \\ \text{states},v}} d_v \mathrm{e}^{-hcE_v/kT} \times d_i \sum_{\substack{\text{rotational} \\ \text{states},s}} d_s \mathrm{e}^{-hcE_s/kT} = Q_{\mathrm{vib}} Q_{\mathrm{rot}}. \tag{2}$$

This expression is called the product approximation of the partition function. This approximation is very useful when many rotational energy levels are available for the ground vibrational state but few rotational energy levels are available for excited vibrational states. The problem is then reduced to computing the rotational and vibrational partition sums. Partition functions calculated by the product approximation agree very well with those calculated by direct sum [1].

Often the rotational energy levels of an isotopomer are not known for high-energy states, hence Q_{rot} cannot be computed with high accuracy. For such cases, there are a number of analytical formulae [9–19] with varying degrees of complexity and accuracy, which can be used. Such formulae range from the approximate classical formulae, which rely only on the principle moment of inertia, to complicated analytical expressions utilizing dozens of terms.

Several of the species under consideration in this work are prone to reaction or are otherwise difficult to study in the laboratory. Therefore, only relatively low-energy levels are known. As a result of this, the following approach was used to calculate the TIPS. The TIPS were calculated by direct summation to the highest temperature at which $Q(T)$ converged. The TIPS were also calculated by analytical expression and compared to the direct summation $Q(T)$ to ensure agreement. The analytical expression was then used to calculate the partition sum over the entire temperature range under consideration. This is a reasonable approach since the analytical formulae are more valid in the limit of the temperature in this study [9].

To apply the product approximation, it is necessary to calculate Q_{vib}. The method used was the harmonic oscillator approximation (HOA) of Herzberg [9], which gives Q_{vib} as a product over the fundamental vibrational energies, ω_i, of the molecule,

$$Q_{\mathrm{vib}}(T) = \prod \left(\frac{1}{1 - \mathrm{e}^{-hc\omega_i/kT}} \right). \tag{3}$$

Once the partition functions are calculated, it is useful to reduce them to a form for rapid, accurate recall. While interpolation provides for a convenient accurate method of recall, the temperature range under consideration in this work is small (70–300 K) allowing a single polynomial to be used. The expression adopted is fourth order in temperature, requiring the storage of five coefficients for a given isotopomer

$$Q(T) = a + bT + cT^2 + dT^3 + eT^4. \tag{4}$$

A fourth-order polynomial in temperature expression was used, rather than the previous third order polynomial [1,2], because several of the species under consideration have many low-lying vibrational states. The low-lying states cause $Q_{\mathrm{vib}}(T)$ to increase quickly with temperature resulting in larger fit uncertainty for a given number of fitting coefficients. Tests showed that a fourth order expression is able to reproduce the calculated partition sum to better than 0.5% for most species at most temperatures and to better than 1% for all species at all temperatures within the specified temperature range. The temperature range for which the TIPS are calculated, 70–300 K, was selected based on the use of the TIPS to reduce data taken by the near infrared mapping spectrometer [7], of the Galileo project [8], as well as other astrophysical applications.

The total partition sums were calculated at 5 K steps from 70 to 300 K and these data are then fit to the polynomial expression, Eq. (4), where the coefficients are determined by fitting to the data using a simplex nonlinear minimization algorithm [20]. The fitting is based on minimizing the sum of the eighth powers of the percentage differences between the polynomial of Eq. (4) and the calculated partition functions. The use of the percentage differences reflects the way partition functions are used in calculations, as well as the accuracy of the calculations, better than absolute differences would. The use of least-eighth powers as a fitting criterion yields almost a minimax fit. A true minimax fit would produce insignificantly smaller maximum differences, but larger average differences in many cases. The resulting coefficients can then be used to recalculate the total internal partition sum within the range of the fit.

The analytical expressions used to calculate the TIPS for each species are described below, as well as the agreement between the analytical expression and the direct sum and the quality of the polynomial fit. In all cases, the state-dependent and state-independent factors are accounted for as accurately as possible.

3. Calculation of total internal partition sums

3.1. Cyanoacetylene (HC_3N)

Five isotopomers of cyanoacetylene were considered in this study; $H^{12}C^{12}C^{12}C^{14}N$, $H^{12}C^{12}C^{12}C^{15}N$, $H^{12}C^{12}C^{13}C^{14}N$, $H^{12}C^{13}C^{12}C^{14}N$, $H^{13}C^{12}C^{12}C^{14}N$, and $D^{12}C^{12}C^{12}C^{14}N$. For each species, the product approximation was used. Energy levels were calculated from the Hamiltonian constants of Lafferty and Lovas [21]. The Q_{rot} calculated by direct sum over rotational levels converges to about 60 K. Using the analytical expression of McDowell [10] and the constants from Ref. [21], the analytical rotational partition function was calculated from 1 to 300 K. A comparison between Q_{rot} calculated by direct sum and analytical expression is shown in Fig. 1. The two methods of calculating Q_{rot} agree to within 0.5% between 0 and 60 K. The point of greatest difference occurred at ~5 K for all species except for $H^{12}C^{12}C^{12}C^{15}N$. This difference is $< 3\%$ at 5 K and is due to the neglect of quantum mechanical structure at low temperature in the analytical expression. For $H^{12}C^{12}C^{12}C^{15}N$, the point of greatest difference occurred at ~60 K. The vibrational partition functions were calculated using the HOA method of Herzberg [9] with the vibrational frequencies of the principle species from Refs. [22–27,5].

For all species under consideration in this study except $H^{12}C^{12}C^{12}C^{15}N$, hyperfine splitting occurs. In calculating the direct sum, these hyperfine levels were individually accounted for. However, in the analytical expression, these levels factor in as a state-independent factor of 3. For $H^{12}C^{12}C^{12}C^{15}N$, the state-independent factor is 4. For all species of cyanoacetylene, the state-dependent factor is equal to $(2J+1)$.

The polynomial fit was made to the analytical partition sums. The absolute error of the polynomial fits never exceeds 0.3% for the non-deuterated species and never exceeds 0.65% for the deuterated isomer. Fig. 2 shows the percent error of the fit for the $H^{12}C^{12}C^{12}C^{14}N$ isotopomer. This figure is typical for all species of this study.

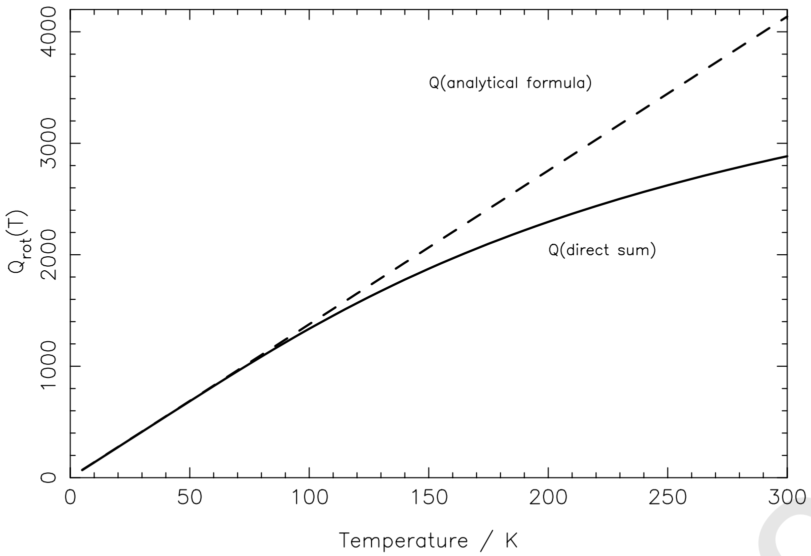

Fig. 1. Comparison of $Q(T)$ calculated by direct sum and by analytical expression for $H^{12}C^{12}C^{12}C^{14}N$ (cyanoacetylene).

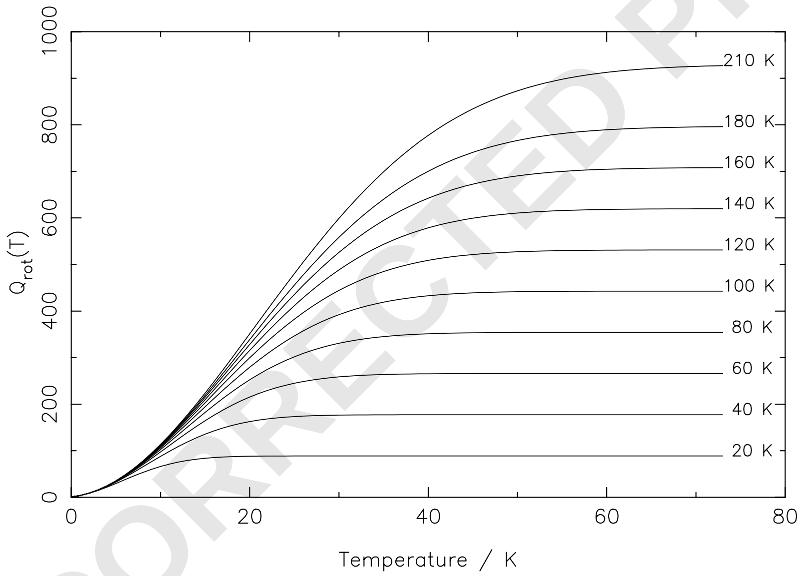

Fig. 2. Percent error between calculated $Q(T)$ and that calculated by polynomial fit coefficients versus temperature for $H^{12}C^{12}C^{12}C^{14}N$ (cyanoacetylene).

3.2. Dicyanogen (C_2N_2)

For both isotopomers of dicyanogen considered in this study, $^{14}N^{12}C^{12}C^{14}N$ and $^{15}N^{12}C^{12}C^{15}N$, the product approximation of $Q(T)$ was used. Energy levels were calculated from the Hamiltonian constants of Maki [28]. The Q_{rot} determined by direct sum converged to ~160 K, as shown in

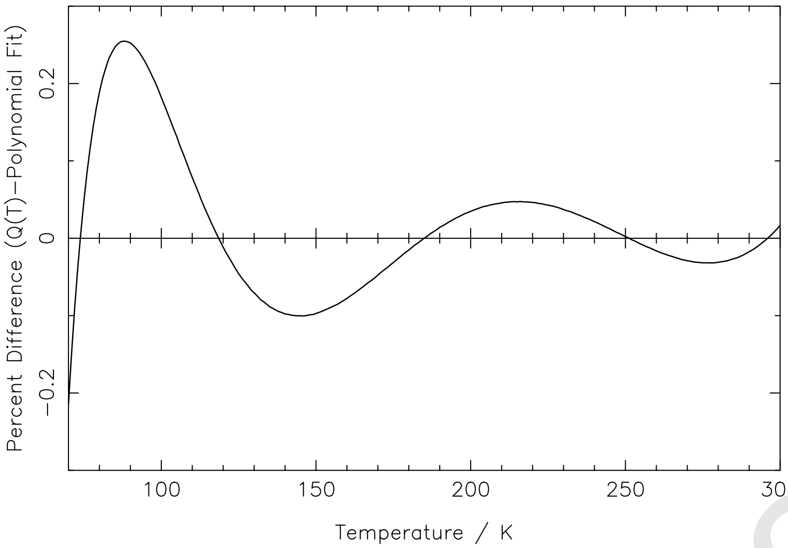

Fig. 3. Convergence of $Q_{\mathrm{rot}}(T)$ versus J'' for different temperatures for $^{14}\mathrm{N}^{12}\mathrm{C}^{12}\mathrm{C}^{14}\mathrm{N}$ (dicyanogen).

Fig. 3. This figure depicts graphs of $Q_{\mathrm{rot}}(T)$, determined by direct summation versus the quantum number J'' of the energy levels used to calculate to direct sum, at a number of temperatures. For a given temperature, as J increases, Q_{rot} increases, to a point, after which the graph exhibits a horizontal asymptoic structure as the increasingly high energy levels cease to contribute substantially to the exponential term. The highest temperature at which this asymptotic behavior is exhibited indicates the greatest temperature at which $Q_{\mathrm{rot}}(T)$ converges.

The analytical rotational partition functions were calculated between 1 and 300 K using linear molecule expression of McDowell [10] with the constants of Ref. [28]. A comparison between Q_{rot} calculated by direct sum and analytical expression shows that the two methods agree to within 0.36% between 1 and 160 K. The vibrational partition functions were calculated using the HOA method of Herzberg [9] with the vibrational frequencies of the principle species from Refs. [29–33,5].

For dicyanogen, the coupling of rotational motion with nuclear wavefunctions gives rise to state-dependent degeneracies. For the $^{14}\mathrm{N}^{12}\mathrm{C}^{12}\mathrm{C}^{14}\mathrm{N}$ isotopomer, these degeneracies are three-fold for the odd J levels and six-fold for the even J levels. For the $^{15}\mathrm{N}^{12}\mathrm{C}^{12}\mathrm{C}^{15}\mathrm{N}$ isomer, these degeneracies are three-fold for the odd J levels and one-fold for the even J levels. For both of these species, the state-independent degeneracy factor is equal to 1.

The polynomial fit was made to the analytical partition sums. The absolute error of the polynomial fits never exceeds 0.15% for either species under consideration.

3.3. Diacetylene ((Butadiyne), $^{12}C_4H_2$)

For diacetylene, the TIPS are calculated using the product approximation. Energy levels were calculated using the Hamiltonian constants of Arie and Johns [34]. The direct sum method converges to 60 K. The analytical expression used to determine Q_{rot} was McDowell's formulation for linear molecules [10]. The calculations were made with the constants of Ref. [34]. A comparison of Q_{rot} determined by direct sum and analytical expression demonstrates that the two methods agree to within 0.07% between 1 and 60 K. The vibrational partition function was calculated using the HOA method of Herzberg [9] with the vibrational frequencies of Refs. [35–41,5].

The interactions between rotational motion and the nuclear wavefunctions of this molecule give rise to state-dependent degeneracy factors. These degeneracies are three-fold for odd J levels and one-fold for even J levels. The state-independent degeneracy factor for this species is equal to 1.

The polynomial fit was made to the analytical partition sums. The absolute error of the polynomial fits never exceeds 0.2% between 70 and 300 K.

3.4. Germane ($^{74}GeH_4$)

For germane, $Q(T)$ was calculated using the product approximation. The rotational partition sum was calculated using the spherical top molecule analytical expression of McDowell [11] with the molecular Hamiltonian constants from Ref. [42]. However, the direct sum method converged to over 300 K, so the analytical expression was used only for comparison. The greatest difference between the two methods was $\approx$ 0.001%. The vibrational partition function was calculated using the HOA method of Herzberg [9] with the vibrational frequencies of Refs. [33,40,43,5].

The state-independent degeneracy factor of germane is equal to 1. This value is equal to twice the nuclear spin of the central germanium atom plus 1. The state-dependent degeneracy factors, which occur due to the interaction between the nuclear spin of the hydrogen atoms and the rotational wavefunction of the molecule, are five-fold for the A states, three-fold for the F states and two-fold for the E states. Since there are two A states, two F states and one E state, an average degeneracy factor may be obtained by taking a weighted average of the above degeneracies. This average factor is equal to 18/5.

A polynomial fit was made to the direct sum partition sums. The absolute error of the polynomial fits never exceeds 0.03%.

3.5. Propane (C_3H_8)

Six different species of propane were considered in this study: $^{12}C_3H_8$, $^{13}CH_3{}^{12}CH_2{}^{12}CH_3$, $^{12}CH_3{}^{13}CH_2{}^{12}CH_3$, $^{12}CH_3{}^{12}CHD^{12}CH_3$, $^{12}CH_2D^{12}CH_2{}^{12}CH_3$ (symmetric), and $^{12}CH_2D^{12}CH_2{}^{12}CH_3$ (asymmetric). The symmetric/asymmetric notation is that of Lide [44], where the symmetric configuration is defined as the deuterium atom on the methyl top being in the plane of the three carbon atoms and the asymmetric configuration is defined as the deuterium atom on the methyl top being out of this plane. For all species, $Q(T)$ was calculated using the product approximation. The rotational partition function was calculated using the asymmetric rotor expression of Watson [19], with the Hamiltonian constants of Lide [44]. The vibrational partition function was calculated using the HOA method of Herzberg [9] with the vibrational frequencies of Ref. [40].

The free rotation of the methyl tops on the propane molecule causes a four-fold torsional splitting [45]. The total state-independent factors for the various species of propane under consideration are the product of this torsional splitting and the state-independent factor caused by nuclear spin. This

Table 1
Coefficients of TIPS polynomial fit

Isotopomer	a	b	c	d	e
$H^{12}C^{12}C^{12}C^{14}N$	302.43	4.2331	9.3363×10^{-2}	-2.9987×10^{-4}	1.3540×10^{-6}
$H^{12}C^{12}C^{12}C^{15}N$	417.16	5.7515	1.2895×10^{-1}	-4.1549×10^{-4}	1.8678×10^{-6}
$H^{12}C^{12}C^{13}C^{14}N$	306.69	4.1519	9.4929×10^{-2}	-3.0701×10^{-4}	1.3730×10^{-6}
$H^{12}C^{13}C^{12}C^{14}N$	301.83	4.3132	9.3022×10^{-2}	-2.9745×10^{-4}	1.3514×10^{-6}
$H^{13}C^{12}C^{12}C^{14}N$	322.90	4.0106	1.0060×10^{-1}	-3.3075×10^{-4}	1.4456×10^{-6}
$D^{12}C^{12}C^{12}C^{14}N$	18.987	13.309	1.7221×10^{-2}	-9.0082×10^{-8}	1.0215×10^{-6}
$^{14}N^{12}C^{12}C^{14}N$	222.69	13.677	4.0879×10^{-2}	6.1373×10^{-5}	8.0557×10^{-7}
$^{15}N^{12}C^{12}C^{15}N$	105.21	6.4649	1.9320×10^{-2}	2.9014×10^{-5}	3.8075×10^{-7}
$H^{12}C^{12}C^{12}C^{12}CH$	208.45	2.1273	8.6027×10^{-2}	-3.9418×10^{-4}	1.5230×10^{-6}
$^{74}GeH_4$	−15.879	1.6483	1.9543×10^{-2}	-3.6955×10^{-5}	5.3202×10^{-8}
$^{12}C_3H_8$	2.1053×10^{6}	-6.2551×10^{4}	1319.6	−6.6120	2.0094×10^{-2}
$^{13}CH_3{}^{12}CH_2{}^{12}CH_3$	4.3258×10^{6}	-1.2853×10^{5}	2711.5	−13.586	4.1289×10^{-2}
$^{12}CH_3{}^{13}CH_2{}^{12}CH_3$	4.2605×10^{6}	-1.2658×10^{5}	2670.5	−13.381	4.0665×10^{-2}
$^{12}CH_3{}^{12}CHD^{12}CH_3$	3.4159×10^{6}	-1.0149×10^{5}	2141.2	−10.729	3.2605×10^{-2}
$^{12}CH_2D^{12}CH_2{}^{12}CH_3$ (sym)	3.4013×10^{6}	-1.0107×10^{5}	2132.1	−10.683	3.2467×10^{-2}
$^{12}CH_2D^{12}CH_2{}^{12}CH_3$ (asym)	3.4230×10^{6}	-1.0171×10^{5}	2145.7	−10.751	3.2673×10^{-2}

yields a total state-independent factor of 1024 for $^{12}C_3H_8$, 2048 for $^{13}CH_3{}^{12}CH_2{}^{12}CH_3$, 2048 for $^{12}CH_3{}^{13}CH_2{}^{12}CH_3$, 1536 for all of the deuterated species in this study.

The polynomial fit was made to the analytical partition sums. The absolute error of the polynomial fits never exceeds 0.66% for any species under consideration.

4. Summary

Total internal partition sums were calculated as a function of temperature in the range 70–300 K for many isotopomers of molecules of astrophysical interest: cyanoacetylene, dicyanogen, diacetylene, germane, and propane. The TIPS calculated by analytical formulae were compared to those calculated by direct summation to insure that quantum effects were negligible for the temperatures of interest. The TIPS were fit to a fourth order in temperature polynomial for rapid and accurate recall. The coefficients for the species studied are listed in Table 1. FORTRAN code to calculate the TIPS is available from one of the authors (Robert_Gamache@uml.edu).

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