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Computation of vibrational partition function: a comparative analysis between Poisson summation and classical limit

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Abstract

The computation of partition function (Z) is the bedrock of the study of statistical mechanics as it plays a significant role in the thermodynamic properties (TP) where microscopic properties are connected to macroscopic properties. Several studies have reported TP via the Z using one of the classical limit approach or Poisson summation formula. No study however justifies the agreement or discrepancy between the methods. This study therefore, investigates the two methods for theoretical determination of the vibrational partition function by considering the energy levels of Tietz molecular potential. The first approach employs Poisson summation method with a defined energy levels of the Tietz molecular potential while the second approach adopts the utilization of the classical limit approach with the same energy levels of the Tietz molecular potential. By comparing the results of the two approaches, our result reveals discrepancy between the analytic equations for Z. However, the numerical results obtained for the thermal properties of NaBr and CuCl molecules showed a perfect agreement between the two approaches and the experimental data with the results from classical limit approach closer to the experimental data. This study therefore, provides guidelines for choosing the appropriate approach based on the characteristics of the system under study for theoretical research.

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1. Introduction

The study of bound states is a crucial concept in quantum mechanics that has motivated and drawn the attention of various researchers in theoretical physics and theoretical chemistry for years. Extensive studies have been conducted on this concept, considering various physical potential systems of interest. Some of the potentials reported include the Manning-Rosen potential, the Rosen-Morse potential, Eckart potential, Morse potential, Hellmann potential, Yukawa potential, shifted Deng-Fan potential, Varshni potential, Coulomb potential, a class of Yukawa potential, modified shifted Morse potential, generalized Morse potential, Tietz potential, and others. Some of these potential systems have been studied for specific models with appreciable results due to their parameterization. For instance, the generalized Morse potential was studied for hydrogen fluoride (HF) by Zhang *et al.* [1] and Onate *et al.* [2]. Deng-Fan potential was studied for TP by Oyewumi *et al.* [3]. Oluwadare and Oyewumi [4] studied the shifted Deng-Fan potential for some molecules. Onate *et al.* [5] examined the Morse potential for scandium and nitrogen monoiodides. Varshni potential

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was studied for scattering states by Oluwadare and Oyewumi [6]. Other potentials have been studied for molecular spectra and TP [7, 8].

The study of TP via energy levels obtained from bound states links quantum mechanics and statistical mechanics, which have applications in science and engineering. TP are crucial for analyzing and designing heat engines and determining the efficiency of engine work output, combustion analysis, adsorption, phase transition, fluorescence microscopy [9–17] and others. Thus, the study of TP cannot be overemphasized. The microscopic properties and macroscopic properties in TP from energy levels are obtained via the Z existing as a crucial link between the energy levels and the TP such as mean energy, free energy, entropy, heat capacity, enthalpy, and Gibbs free energy.

Several reports on the TP analytically determined the vibrational Z using either the classical approach [18–23] or the Poisson summation formula [24–32]. The results of the two approaches have been extensively reported for different potential models. However, to the best of our understanding, it has not been clearly reported whether the two methods reproduce the same result or not. If these methods reproduced different results, then, which of the method will be more accurate? This has become a subject of discussion in the minds of the authors that necessitates the present study.

This study therefore, analyzes the analytical expressions and numerical computations of the vibrational Z of the energy levels of Tietz molecular potential with the two approaches. The approaches are similar but differ in the evaluation of the integral. In the classical approach, the summation turns to integral at classical limit while in the Poisson summation, the lower-order gives an approximate value of a summation to an accurate value. The physical structure of the Tietz molecular potential is [33]:

$$V(r) = D_e\left(1 - \frac{e^{ar_e} + q}{e^{ar} + 1}\right)^2, \tag{1}$$

where D_e is a dissociation energy, and r_e is equilibrium bond length. The parameter α and q are given as [25]:

$$\alpha = 2\pi c\omega_e\sqrt{\frac{2\mu}{D_e} - \frac{8\pi^2 c^2\mu^2 r_e^3\alpha_e\omega_e}{3\hbar^2} - \frac{1}{r_e}}, \tag{2}$$

$$q = \left[\frac{1}{\pi c\omega_e}\sqrt{\frac{D_e}{2\mu}} - 1\right]e^{ar_e}, \tag{3}$$

The energy levels of the Tietz molecular potential [25] is given as:

$$E_n = D_e - \frac{\alpha^2\hbar^2}{2\mu}\left[\frac{\frac{\mu D_e}{\alpha^2\hbar^2}\left(\frac{e^{2\alpha r_e}}{q^2} - 1\right)}{n + \frac{1}{2} + \frac{1}{2}\sqrt{1 + \frac{8\mu D_e}{\alpha^2\hbar^2}\left(\frac{e^{\alpha r_e}}{q}\right)^2}}\right. \\ \left. - \frac{n + \frac{1}{2} + \frac{1}{2}\sqrt{1 + \frac{8\mu D_e}{\alpha^2\hbar^2}\left(\frac{e^{\alpha r_e}}{q} + 1\right)^2}}{2}\right]^2, \tag{4}$$

2. Partition function from energy levels

The Partition function is the key concept for the computations of TP from energy levels that connects microscopic properties to macroscopic properties. It is a serving tool for proper understanding of the TP of a system. Generally, the vibrational partition function Z_v is obtained from energy levels using the formula [34–48]:

$$Z_y = \sum_{n=0}^{n_{max}} e^{-\beta E_n}, \tag{5}$$

where β is the inverse of the product of Boltzmann constant k_β and absolute temperature T written as $\beta = \frac{1}{k_\beta T}$. The E_n is the energy of the system and n_{max} is the maximum quantum state that is obtained from the first derivative of equation (4). The maximum quantum state is given is obtained as

$$n_{max} = \sqrt{\frac{2\mu D_e}{\alpha^2\hbar^2}\left(\frac{e^{2\alpha r_e}}{q^2} - 1\right)} - \\ \left(\frac{1}{2} + \frac{1}{2}\sqrt{1 + \frac{8\mu D_e}{\alpha^2\hbar^2}\left(\frac{e^{\alpha r_e}}{q} + 1\right)^2}\right). \tag{6}$$

2.1. The Poisson summation formula

Plugging equation (4) into equation (5), the partition function becomes:

$$Z_p = e^{-\beta D_e}\sum_{n=0}^{n_{max}} e^{\frac{\beta\hbar^2}{2\mu}\left[\frac{\Lambda}{n+\delta} - \frac{n+\delta}{2}\right]^2}, \tag{7}$$

where

$$\Lambda = \frac{\mu D_e e^{2\alpha r_e}}{\alpha^2\hbar^2 q^2} - \frac{\mu D_e}{\alpha^2\hbar^2}, \tag{8}$$

$$\delta = \frac{1}{2} + \frac{1}{2}\sqrt{1 + \frac{8\mu D_e}{\alpha^2\hbar^2}\left(\frac{e^{\alpha r_e}}{q} + 1\right)^2}. \tag{9}$$

In the Poisson summation formula [49], the summation in equation (6) can be approximated using the formula:

$$\sum_{n=0}^{n_{max}} f(n) = \frac{1}{2}\left[f(0) - f(n_{max} + 1)\right] + \int_0^{n_{max}+1} f(x)\,dx. \tag{10}$$

Plugging equation (6) into equation (10), the vibrational partition function for the Poisson summation formula becomes:

$$Z_p = \frac{e^{-\beta D_e}}{2}\left(e^{\Lambda_1^2} - e^{\Lambda_2^2} + \frac{\sqrt{\pi}}{\Lambda_0}\left[erfi(\Lambda_1)\right.\right. \\ \left.\left. -erfi(\Lambda_2)\right]\right), \tag{11}$$

where

$$\Lambda_1 = \Lambda_0\left(\frac{\Lambda}{n_{max} + 1 + \delta} - \frac{n_{max} + 1 + \delta}{2}\right), \tag{12}$$

$$\Lambda_2 = \Lambda_0\left(\frac{\Lambda}{\delta} - \frac{\delta}{2}\right), \quad \Lambda_0 = \alpha\hbar\sqrt{\frac{\beta}{2\mu}}. \tag{13}$$

2.2. Classical limit approach

To use this approach, we transform the summation in equation (7) to an integral of the form:

$$Z_c = e^{-\beta D_e} \int_0^{n_{max}} e^{\frac{\beta\alpha^2\hbar^2}{2\mu}} \left(\frac{\Lambda}{n+\delta} - \frac{n+\delta}{2} \right)^2 dn. \tag{14}$$

Defining

$$n+\delta = \frac{\Lambda_3 + \sqrt{\Lambda_3^2 + 2\Lambda\Lambda_0^2}}{\Lambda_0}, \tag{15}$$

then,

$$dn = \Lambda_0 \left(\frac{\Lambda}{n+\delta} - \frac{n+\delta}{2} \right) d\Lambda_3. \tag{16}$$

The integral in equation (15) turns to:

$$Z_c = \frac{e^{-\beta D_e}}{\Lambda_0} \int_{\Lambda_1}^{\Lambda_4} e^{\Lambda_3^2} \left(1 + \frac{\Lambda_3}{\sqrt{2\Lambda\Lambda_0^2 + \Lambda_3^2}} \right) d\Lambda_3, \tag{17}$$

$$\Lambda_4 = \Lambda_0 \left(\frac{\Lambda}{n_{max}+\delta} - \frac{n_{max}+\delta}{2} \right). \tag{18}$$

This gives a partition function for classical limit as

$$\begin{aligned} Z_c = {} & \frac{e^{-\beta D_e}\sqrt{\pi}}{2\Lambda_0} \left[erfi(\Lambda_4) - erfi(\Lambda_1) \right] + \\ & e^{-\beta D_e - 2\Lambda\Lambda_0^2} \left[erfi(\Lambda_5) - erfi(\Lambda_6) \right], \end{aligned} \tag{19}$$

$$\Lambda_5 = \Lambda_0 \left(\frac{\Lambda}{n_{max}+\delta} + \frac{n_{max}+\delta}{2} \right), \ \Lambda_6 = \Lambda_0 \left(\frac{\Lambda}{\delta} + \frac{\delta}{2} \right). \tag{20}$$

Here, we compute vibrational Gibbs free energy using equations (11) and (19), respectively, as the TP.

To compare the analytic result with experimental data, the contribution of the vibrational partition functions Z_v, the rotational partition function Z_r and the translational partition function Z_t are considered. Thus, molar partition function can be written as:

$$Z = Z_v Z_r Z_t, \tag{21}$$

where

$$Z_r = \frac{T}{\tau\Theta} \left(1 + \frac{1}{3}\frac{\Theta}{T} + \frac{1}{15}\left(\frac{\Theta}{T}\right)^2 + \frac{4}{315}\left(\frac{\Theta}{T}\right)^3 \right), \tag{22}$$

$$Z_t = \left(\frac{2\pi k_B T m}{h^2} \right)^{3/2} V. \tag{23}$$

$$\Theta = \frac{\hbar^2}{8\mu k_B \pi^2 r_e^2}, \tag{24}$$

$Z_v = Z_p$ or Z_c as the case may be. m is the mass and V is the volume of the gas. Having obtained the molar partition function, we can now calculate the various analytical expression for the thermal properties as follows:

2.2.1. Molar entropy

The molar entropy (S) is related to the molar partition function by the formula:

$$S = RlnZ + RT \left(\frac{\partial \ln Z}{\partial T} \right)_v, \tag{25}$$

where R is the gas constant.

2.2.2. Molar heat capacity

The molar heat capacity at constant pressure is given as

$$C_p = \frac{\partial H}{\partial T}, \tag{26}$$

where

$$H = RT^2 \left(\frac{\partial \ln Q}{\partial T} \right)_v + VRT \left(\frac{\partial \ln Q}{\partial V} \right), \tag{27}$$

2.2.3. Molar Gibbs free energy

This is calculated using:

$$G = VRT \left(\frac{\partial \ln Z}{\partial V} \right)_T - k_\beta T \ln Z. \tag{28}$$

3. Discussion

Equation (11) and equation (19) are the analytic equations of the Z for the two approaches. These equations are not physically the same. Since the computation of thermal properties depend on the partition function, and we do not have access to the experimental data for partition function, we obtained analytic expression for molar entropy, Gibbs free energy and molar heat capacity at constant pressure using the partition functions from the two approaches. for NaBr and CuCl molecules. Using equations (25), (26) and (28), respectively, for molar entropy, molar heat capacity at constant pressure and molar Gibbs free energy, we generate numerical values for these thermal properties of NaBr and CuCl from both methods and compare with experimental data as shown in Tables 1 and 2.

The comparison covers a temperature range of 0 K to 6000 K in 500 K increment. Both molecules showed a steady increase in the molar entropy with rise in temperature which reflects the degree of disorderliness as the temperature rises due to thermal agitation. At different temperatures, the entropy of NaBr is slightly higher than the entropy of CuCl suggesting *NaBr′s* vibrational and rotational states may be more thermally accessible due to mass and bonding discrepancies. However, the result from Poisson summation are higher at lower temperatures but as the temperature rises, the result from the classical limit approach outburst the result from Poisson summation formula. The Poisson summation formula includes the quantum corrections while the classical limit approach assumes a continuum. Thus, at low temperatures, the corrections raise the entropy above the classical prediction while at higher temperatures, the corrections vanished and the classical limit begins to

Table 1: Molar entropy S (in $Jmol^{-1}K^{-1}$), Gibbs free energy G in ($Jmol^{-1}K^{-1}$), and heat capacity C_p in ($Jmol^{-1}K^{-1}$) at constant pressure as a function of temperature for NaBr. Spectroscopic constants for NaBr: $D_e = 27,200\ cm^{-1}$, $r_e = 2.342$ Å, $\omega_e = 262\ cm^{-1}$ and $\alpha_e = 0.0009\ cm^{-1}$.

$T(K)$	NIST	S_p	Sc	NIST	$-G_p$	$-G_c$	NIST	$-Cp_p$	Cp_c
500	260.278	263.147	262.902	245.379	248.265	247.762	37.301	37.087	37.527
1000	286.410	289.012	288.952	260.089	262.901	262.587	38.065	37.510	37.652
1500	301.934	304.263	304.244	271.619	274.315	274.094	38.526	37.722	37.792
2000	313.075	315.141	315.138	280.655	283.226	283.058	38.941	37.911	37.954
2500	321.808	323.622	323.627	288.034	290.488	290.353	39.342	38.117	38.148
3000	329.016	330.593	330.603	294.288	296.608	296.497	39.739	38.364	38.389
3500	335.171	336.528	336.542	299.700	301.897	301.804	40.132	38.664	38.686
4000	340.555	341.713	341.729	304.477	306.557	306.477	40.524	39.006	39.027
4500	345.351	346.328	346.346	308.757	310.724	310.655	40.916	39.359	39.376
5000	349.682	350.492	350.512	312.636	314.496	314.436	41.307	39.677	39.691
5500	353.638	354.286	354.307	316.187	317.944	317.891	41.697	39.921	39.930
6000	357.282	357.766	357.788	319.461	321.119	321.073	42.088	40.066	40.067

Table 2: Molar entropy S (in $Jmol^{-1}K^{-1}$), Gibbs free energy G in ($Jmol^{-1}K^{-1}$), and heat capacity C_p in ($Jmol^{-1}K^{-1}$) at constant pressure as a function of temperature for CuCl. Spectroscopic constants for CuCl: $D_e = 28,300cm^{-1}$, $r_e = 2.091A$, $\omega_e = 377cm^{-1}$ and $\alpha_e = 0.00173cm^{-1}$.

$T(K)$	NIST	S_p	Sc	NIST	$-G_p$	$-G_c$	NIST	$-Cp_p$	Cp_c
500	255.861	256.999	256.414	241.270	242.379	241.297	36.730	36.574	37.510
1000	281.675	282.617	282.445	255.733	256.808	256.097	37.641	37.275	37.614
1500	297.012	297.788	297.717	267.105	268.107	267.596	38.008	37.554	37.728
2000	307.986	308.619	308.588	276.017	276.945	276.549	38.290	37.749	37.856
2500	316.558	317.062	317.051	283.299	284.155	283.834	38.546	37.928	38.002
3000	323.607	323.994	323.994	289.447	290.234	289.966	38.792	38.117	38.174
3500	329.605	329.885	329.894	294.766	295.488	295.259	39.033	38.335	38.381
4000	334.833	335.020	335.034	299.455	300.115	299.916	39.272	38.589	38.630
4500	339.472	339.582	339.600	303.648	304.252	304.077	39.509	38.877	38.914
5000	343.647	343.694	343.716	307.443	307.994	307.838	39.745	39.181	39.214
5500	347.446	347.442	347.467	310.090	311.412	311.273	39.981	39.475	39.504
6000	350.935	350.888	350.935	314.101	314.003	314.435	40.216	39.733	39.755

overestimate entropy due to its assumptions of unlimited continuous energy levels and degree of freedom. Though the results from the two methods agreed with the experimental data, but the results from the classical limit agreed more than the results from the Poisson summation formula. The Gibbs free energy decreases as the temperature rises for both molecules but not linearly. This is consistent with the temperature contribution to the Gibbs free energy $G = H - TS$. At different temperatures, the Gibbs free energy of CuCl is higher than the Gibbs free energy of NaBr. Similarly, the Gibbs free energy obtained from the Poisson summation formula is lower than the Gibbs free energy obtained from the classical limit approach for the two molecules. Though the results from the two methods agreed with the experimental data, but the results from the classical limit agreed more than the results from the Poisson summation formula. The heat capacity increases as the temperature rises for both molecules. This is consistent with the relationship between heat and temperature. Again, the heat capacity obtained from the Poisson summation formula are lower than the heat capacity obtained from the classical limit approach at different temperatures. Though the results from the two methods agreed with the experimental data, but the results from the classical limit agreed more than the results from the Poisson summation formula. Having observed the three thermal properties from the two method for both NaBr and CuCl, it can be clearly seen that though the results from the two method perfectly agreed with the experimental data, but the results from the classical limit approach consistently aligned more with the experimental data than the results from the Poisson summation formula.

4. Conclusion

The partition function from the energy levels of Tietz molecular potential model was calculated from two distinct approaches. The analytic equations for the partition function from the two approaches are not exactly the same. However, the results of the two approaches demonstrated consistent behaviours following the variation of temperature with the various thermal properties affirming the reliability and coherence of the two approaches in capturing thermodynamic trends. However, the numerical values calculated from the classical limit approach is always higher and more in agreement with the experimental data than that of Poisson summation formula. The results from classical limit approach align more closely with the experimental data probably because. the experimental data often reflect macroscopic average where classical assumptions hold. It may also be due to convergence limitations in the Poisson summation formula. Thus, the classical limit approach is recommended for a more accurate result.

Data availability

All relevant data are within the manuscript.

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APPENDIX 1

MATLAB Script For the Computation of Thermodynamic Properties of Diatomic Molecules Based on The Improved Tietz Oscillator

```
clear all
close all
clc

h = 6.62607e-34;            % Planck constant
hbar = h/(2*pi);            % Reduced Planck constant
e = 1.60217662e-19;         % electronic charge
amu = 1.6605402e-27;        % atomic mass unit
c = 299792458;              % Speed of light
cm_1 = 100*h*c;             % Wave number energy unit (cm^-1) to Joule
kcalpermol = 349.757*cm_1;  % kcal mol^-1 to Joule
R = 8.31446;                % Gas constant in J mol^-1 K^-1
kB = 1.3806485e-23;         % Boltzmann constant
NA = 6.0221409e23;          % Avogadro number
kJpermol = (1000/NA);       % conversion from kJmol^-1 to Joule
sap = 1e5;                  % Standard atmospheric pressure

% Molecular and NIST-JANAF Data for NaBr (X ^1Sigma^+)
% https://doi.org/10.1016/j.chemphys.2018.09.037
muNaBr = (22.98976928^-1+78.918338^-1)^-1*amu;
mNaBr = (22.98976928+78.918338)*amu;
reNaBr = 2.539e-10;
DeNaBr = 27270.21*cm_1;
weNaBr = 293.2e2;
aeNaBr = 0.000879e2;
TNaBr = [300 350 400 450 500 600 700 800 900 1000 1100 1200 1300 1400 ...
1500 1600 1700 1800 1900 2000 2100 2200 2300 2400 2500 2600 ...
2700 2800 2900 3000 3100 3200 3300 3400 3500 3600 3700 3800 ...
3900 4000 4100 4200 4300 4400 4500 4600 4700 4800 4900 5000 ...
5100 5200 5300 5400 5500 5600 5700 5800 5900 6000];
CpNaBr = [36.339 36.699 36.957 37.150 37.301 37.529 37.699 37.837 37.957 ...
38.065 38.165 38.260 38.351 38.440 38.526 38.611 38.695 38.778 ...
38.860 38.941 39.022 39.103 39.183 39.263 39.342 39.422 39.501 ...
39.580 39.660 39.739 39.817 39.896 39.975 40.054 40.132 40.211 ...
40.289 40.368 40.446 40.524 40.603 40.681 40.759 40.837 40.916 ...
40.994 41.072 41.150 41.228 41.307 41.385 41.463 41.541 41.619 ...
41.697 41.775 41.853 41.931 42.010 42.088];
SNaBr = [241.443 247.073 251.991 256.356 260.278 267.100 272.899 277.942 ...
282.405 286.410 290.043 293.368 296.434 299.279 301.934 304.423 ...
306.767 308.981 311.080 313.075 314.977 316.794 318.534 320.203 ...
321.808 323.352 324.841 326.279 327.670 329.016 330.320 331.585 ...
332.814 334.009 335.171 336.303 337.405 338.481 339.530 340.555 ...
341.557 342.536 343.495 344.433 345.351 346.251 347.134 347.999 ...
348.849 349.682 350.501 351.305 352.096 352.873 353.638 354.390 ...
355.130 355.858 356.576 357.282];
GNaBr = -[241.219 241.663 242.653 243.937 245.379 248.447 251.536 254.529 ...
257.383 260.089 262.649 265.073 267.369 269.547 271.619 273.592 ...
275.476 277.276 279.000 280.655 282.244 283.774 285.247 286.669 ...
288.043 289.371 290.658 291.904 293.114 294.288 295.430 296.540 ...
297.621 298.673 299.700 300.701 301.678 302.632 303.565 304.477 ...
305.369 306.243 307.098 307.936 308.757 309.562 310.352 311.128 ...
```

```
311.889 312.636 313.371 314.093 314.802 315.500 316.187 316.862 ...
317.527 318.182 318.826 319.461];
HNaBr = [0.067 1.894 3.735 5.588 7.450 11.192 14.954 18.731 22.520 26.322 ...
30.133 33.954 37.785 41.625 45.473 49.330 53.195 57.069 60.950 ...
64.840 68.739 72.645 76.559 80.481 84.412 88.350 92.296 96.250 ...
100.212 104.182 108.160 112.146 116.139 120.141 124.150 128.167 ...
132.192 136.225 140.265 144.314 148.370 152.434 156.506 160.586 ...
164.674 168.769 172.873 176.984 181.103 185.230 189.364 193.506 ...
197.657 201.815 205.981 210.154 214.336 218.525 222.722 226.927];
HTrNaBr = 12088.0708; % H(29815)

% Molecular and NIST-JANAF Data for CuCl (X ^1Sigma^+)
muCuCl = ((62.929597^-1+34.9688527^-1)^-1)*amu;
mCuCl = (62.929597+34.9688527)*amu;
reCuCl = 2.05e-10;
DeCuCl = 91.5*kcalpermol;
weCuCl = 415.3e2;
aeCuCl = 0.001e2;
TCuCl = [300 350 400 450 500 600 700 800 900 1000 1100 1200 1300 1400 ...
1500 1600 1700 1800 1900 2000 2100 2200 2300 2400 2500 2600 ...
2700 2800 2900 3000 3100 3200 3300 3400 3500 3600 3700 3800 ...
3900 4000 4100 4200 4300 4400 4500 4600 4700 4800 4900 5000 ...
5100 5200 5300 5400 5500 5600 5700 5800 5900 6000];
CpCuCl = [35.285 35.83 36.22 36.509 36.73 37.044 37.257 37.415 37.538 ...
37.641 37.729 37.807 37.879 37.945 38.008 38.068 38.126 38.182 ...
38.236 38.29 38.342 38.394 38.445 38.496 38.546 38.595 38.645 ...
38.694 38.743 38.792 38.84 38.889 38.937 38.985 39.033 39.081 ...
39.129 39.176 39.224 39.272 39.319 39.367 39.414 39.462 39.509 ...
39.556 39.604 39.651 39.698 39.745 39.793 39.84 39.887 39.934 ...
39.981 40.028 40.075 40.122 40.169 40.216];
SCuCl = [237.425 242.908 247.719 252.003 255.861 262.587 268.315 273.3 ...
277.715 281.675 285.267 288.553 291.582 294.392 297.012 299.467 ...
301.777 303.957 306.023 307.986 309.855 311.64 313.348 314.985 ...
316.558 318.07 319.528 320.934 322.293 323.607 324.88 326.114 ...
327.311 328.474 329.605 330.705 331.777 332.821 333.839 334.833 ...
335.803 336.751 337.678 338.585 339.472 340.341 341.192 342.027 ...
342.845 343.647 344.435 345.208 345.967 346.713 347.446 348.167 ...
348.876 349.573 350.26 350.935];
GCuCl = -[237.208 237.639 238.605 239.86 241.27 244.279 247.314 250.257 ...
253.067 255.733 258.258 260.647 262.912 265.061 267.105 269.052 ...
270.909 272.685 274.386 276.017 277.585 279.092 280.545 281.946 ...
283.299 284.608 285.874 287.101 288.292 289.447 290.57 291.661 ...
292.723 293.758 294.766 295.749 296.708 297.645 298.56 299.455 ...
300.329 301.185 302.023 302.844 303.648 304.436 305.209 305.968 ...
306.712 307.443 308.16 308.865 309.558 310.239 310.909 311.568 ...
312.216 312.855 313.483 314.101];
HCuCl = [0.065 1.844 3.646 5.464 7.295 10.985 14.701 18.435 22.183 25.942 ...
29.71 33.487 37.272 41.063 44.86 48.664 52.474 56.289 60.11 ...
63.937 67.768 71.605 75.447 79.294 83.146 87.003 90.865 94.732 ...
98.604 102.481 106.362 110.249 114.14 118.036 121.937 125.843 ...
129.753 133.668 137.588 141.513 145.443 149.377 153.316 157.26 ...
161.209 165.162 169.12 173.083 177.05 181.022 184.999 188.981 ...
192.967 196.958 200.954 204.954 208.959 212.969 216.984 221.003];
HTrCuCl = 12505.8087; % H(298.15)

% MATLAB Input
tau = 1; % for heteronuclear
```

```
% tau = 2; % for homouclear
mu = muNaBr;
m = mNaBr;
re = reNaBr;
De = DeNaBr;
we = weNaBr;
ae = aeNaBr;
T = TNaBr;
SNIST = SNaBr;
GNIST = GNaBr;
HNIST = HNaBr;
CpNIST = CpNaBr;
HTr = HTrNaBr;
bet = 1./(kB*T);
lam = 2*mu/hbar^2;

% Vibrational partition function
alp = pi*c*we*sqrt(8*mu/De)-32*pi^4*c^2*mu^2*re^3*ae*we/(3*h^2)-1./re;
q = ((alp./(pi*c*we)).*sqrt(De./(2*mu))-1)*exp(alp*re);
sig = 0.5+sqrt(0.25+(2*mu*De./(alp^2*hbar^2*q^2)).*(exp(alp*re)+q).^2);
eta = (mu*De./(alp^2*hbar^2)).*(exp(2*alp*re)/q^2-1);
omg = bet*De;
numax = sqrt(2*eta)-sig;
eps = alp*hbar.*sqrt(bet./(2*mu));
energy = De-(alp.^2.*hbar^2./(2*mu)).*(eta./(numax+sig)-(numax+sig)./2).^2;
EE = energy./cm_1;

Alp1 = eps.*(eta./sig-sig./2);
Alp2 = eps.*(eta./(numax+1+sig)-(numax+1+sig)./2);
Alp3 = eps.*(eta./sig+sig./2);
Alp4 = eps.*(eta./(numax+1+sig)+(numax+1+sig)./2);

Z1 = 0.5*exp(Alp1.^2-omg);
Z2 = 0.5*exp(Alp2.^2-omg);
Z3 = (sqrt(pi)./(2*eps)).*exp(-omg).*erfi(Alp1);
Z4 = (sqrt(pi)./(2*eps)).*exp(-omg).*erfi(Alp2);
Z5 = (sqrt(pi)./(2*eps)).*exp(-omg-2*eta.*eps.^2).*erfi(Alp3);
Z6 = (sqrt(pi)./(2*eps)).*exp(-omg-2*eta.*eps.^2).*erfi(Alp4);
Z7 = -Z5+Z6;

Z1prime = (Alp1.^2-omg).*(Z1./bet);
Z2prime = (Alp2.^2-omg).*(Z2./bet);
Z3prime = Alp1.*Z1./(bet.*eps)-(omg+0.5).*(Z3./bet);
Z4prime = Alp2.*Z2./(bet.*eps)-(omg+0.5).*(Z4./bet);
Z5prime = Alp3.*exp(Alp3.^2-omg-2*eta.*eps.^2)./(2*bet.*eps)-(omg+2*eta.*eps.^2+0.5).*(Z5./bet);
Z6prime = Alp4.*exp(Alp4.^2-omg-2*eta.*eps.^2)./(2*bet.*eps)-(omg+2*eta.*eps.^2+0.5).*(Z6./bet);
Z7prime = -Z5prime+Z6prime;

Z1primeprime = (Alp1.^2-omg).^2.*(Z1./bet.^2);
Z2primeprime = (Alp2.^2-omg).^2.*(Z2./bet.^2);
Z3primeprime = Alp1.*Z1./(bet.^2.*eps).*(Alp1.^2-2*omg-1.5)+(omg.^2+omg+0.75).*(Z3./bet.^2);
Z4primeprime = Alp2.*Z2./(bet.^2.*eps).*(Alp2.^2-2*omg-1.5)+(omg.^2+omg+0.75).*(Z4./bet.^2);
rho = 4*eta.*eps.^2+2*omg+1.5;
kap = 4*eta.^2.*eps.^4+4*eta.*eps.^2.*omg+2*eta.*eps.^2+omg.^2+omg+0.75;
Z5primeprime = (Alp3./(2*bet.^2.*eps)).*exp(Alp3.^2-2*eta.*eps.^2-omg).*(Alp3.^2-rho)+kap.*Z5./bet.^2;
Z6primeprime = (Alp4./(2*bet.^2.*eps)).*exp(Alp4.^2-2*eta.*eps.^2-omg).*(Alp4.^2-rho)+kap.*Z6./bet.^2;
Z7primeprime = -Z5primeprime+Z6primeprime;
```

```
Zvib = Z1-Z2+Z3-Z4;
Zvibprime = Z1prime-Z2prime+Z3prime-Z4prime;
Zvibprimeprime = Z1primeprime-Z2primeprime+Z3primeprime-Z4primeprime;
Svib = R*log(Zvib)-R.*bet.*(Zvibprime./Zvib);
Hvib = -NA.*Zvibprime./Zvib;
Gvib = -R.*T.*log(Zvib);
Cvib = R*bet.^2.*(Zvibprimeprime./Zvib-Hvib.^2./NA^2);

% Rotational functions
the = h^2./(8*pi^2*mu*re^2*kB);
Zrot = (T./(tau*the)).*(1+(1/3)*(the./T)+(1/15)*(the./T).^2+(4/315)*(the./T).^3);
Zrotprime = (1./(tau*the)).*(1-(1/15)*(the./T).^2-(8/315)*(the./T).^3);
Zrotprimeprime = (2*the./(15*tau*T.^3)).*(1+(4/7).*(the./T));
Srot = R.*(1+log(T./(tau.*the)));
Hrot = R*T.^2.*Zrotprime./Zrot;
Grot = -R*T.*log(Zrot);
Crot = -Hrot.^2./(R.*T.^2)+2.*Hrot./T+R.*T.^2.*Zrotprimeprime./Zrot;

% Translational functions
Ztra = ((2*pi*m./(bet*h.^2))).^1.5.*(1./(sap*bet));
Stra = R.*(2.5+log(Ztra));
Htra = 2.5*R.*T;
Gtra = -R*T.*log(Ztra);
Ctra = 2.5*R;

Sana = Srot+Stra+Svib;
Hana = Hrot+Htra+Hvib;
Gana = Grot+Gtra+Gvib;
Cana = Crot+Ctra+Cvib;

Sred = Sana;
Hred = (Hana-HTr)*1e-3;
Gred = (Gana-HTr)./T;
Cred = Cana;

S = Sred;
H = Hred;
G = Gred;
Cp = Cred;

% OUTPUT IN WORKSPACE
AA_S = [S;SNIST]';
AA_H = [H;HNIST]';
AA_G = [G;GNIST]';
AA_Cp = [Cp;CpNIST]';
```