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STATTHERMO® – НОВАЯ ПРОГРАММА ДЛЯ РАСЧЕТА ТЕРМОДИНАМИЧЕСКИХ ФУНКЦИЙ

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StatThermo – это новое программное обеспечение для расчета термодинамических функций молекул и ионов в состоянии идеального газа по молекулярным постоянным в приближении «жесткий ротатор-гармонический осциллятор». Программа содержит различные встроенные алгоритмы для расчета координат атомов большинства простых молекул (с числом атомов N ≤ 8). Разработанное программное обеспечение может проводить расчеты для двух референтных температур (0 или 298,15 K) и различных давлений. Одной из отличительных черт StatThermo является возможность учета энергии и степени вырождения низколежащих электронных уровней. Программа была протестирована на различных органических и неорганических молекулах, в результате чего были получены следующие средние погрешности расчетов: 0,05 кДж·моль$^{-1}$ (H°(T)-H°(0)), 0,01 Дж·моль$^{-1}$·K^{-1} (Ф°(T)) и 0,002 Дж·моль$^{-1}$·K^{-1} (S°(T)). Программа также обладает способностью проводить аппроксимацию готовых наборов термодинамических функций, введенных пользователем. Аппроксимация производится при помощи полиномиальной функции методом LU-разложения. Большой набор функциональных возможностей, гибкие параметры расчета и способность экспорта в виде макросов Visual Basic делают StatThermo мощным инструментом для термодинамических расчетов. StatThermo может взаимодействовать с серверами наиболее широко распространенных табличных процессоров, таких как MS Office и OpenOffice для экспорта полученных данных. Программное обеспечение может обрабатывать выходные файлы наиболее популярных программ для квантово-химических расчетов, среди которых Gaussian, Gamess, FireFly, Jaguar, MolPro, CFour, NWChem, ORCA, Priroda, PSI4, Q-Chem и VASP. Мультиязычная и кросс-платформенная поддержка делают StatThermo доступной для широкого круга пользователей.

Ключевые слова: термодинамические функции, программное обеспечение, жесткий ротатор-гармонический осциллятор, MS Excel, Open Office

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STATTHERMO® – NEW SOFTWARE FOR CALCULATION OF THERMODYNAMIC FUNCTIONS

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A new software StatThermo for calculation of thermodynamic functions using the molecular constants in Rigid Rotator – Harmonic Oscillator approximation has been developed. Program includes various prebuilt algorithms to calculate atom coordinates for the majority of simple compounds (with a number of atoms N ≤ 8). The developed software can make the calculation for two reference temperatures (0 or 298.15 K) and different pressures. One of the prominent features of StatThermo is taking into account the low-lying electronic levels. The software was tested on different organic and inorganic molecules and average errors was found as follows: 0.05 kJ·mol^{-1} ($H°(T)-H°(0)$), 0.01 J·mol^{-1}·K^{-1} ($Φ°(T)$), and 0.002 J·mol^{-1}·K^{-1} ($S°(T)$). The program can also approximate by the polynomial the thermodynamic functions defined by user. A wide range of functional possibilities, flexible parameters of calculation, and feature of export results in the Visual Basic macro do the StatThermo powerful software for thermodynamic computations. StatThermo can connect to the MS Office and OpenOffice servers for the export of calculated data. The software can treat the Gaussian, Gamess, FireFly, Jaguar, MolPro, CFour, NWChem, ORCA, Priroda, PSI4, Q-Chem, and VASP output files. A multilingual and cross-platform support makes the StatThermo accessible for a lot of users.

Key words: thermodynamic functions, software, rigid rotator – harmonic oscillator, Gaussian, MS Excel, Open Office

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INTRODUCTION

Nowadays owing to a great progress in quantum chemistry many structural and energetic data on different organic and inorganic molecules were appeared. Unfortunately, existing databases [1-3] on thermodynamic properties of individual substances include restricted number of objects only and do not cover the requests of specialists. Statistical thermodynamics enables to carry out the calculations of thermodynamic functions on the basis of theoretical data of quantum chemistry. However, to date a cross-platform multilingual software for calculation of thermodynamic functions on molecular constants and energy levels of molecules is absent. In this regard, the development of such program forming thermodynamic databases and convenient for a wide range of users is a topical problem.

This paper presents a description of a new program StatThermo [4] for calculating thermodynamic functions of the molecules in the state of ideal gas on the base of molecular parameters.

METODOLOGICAL ASPECTS

The developed software uses the Rigid Rotator – Harmonic Oscillator (RRHO) approximation. The fundamental constants and atomic masses were taken from [5]. The main formulas were taken from [6, 7]. The software was written on the Object Pascal language using Lazarus IDE [8]. The program structure was based on the principles of an object-oriented programming. The hierarchy of classes is shown on Fig. 1.

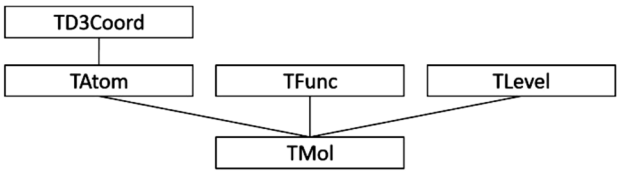

Fig. 1. The hierarchy of classes used in the StatThermo
Рис. 1. Иерархия классов в StatThermo

The TAtom class included the atom designation, the mass, and the Cartesian coordinates gives the description of atom properties. The array of atoms forms the class TMol corresponding to selected molecule. The fields of the TMol class include: type of molecule (nonlinear or linear), point group of symmetry, arrays of internuclear distances, angles and vibrational frequencies, symmetry number, molecular weight, and number of atoms. The low-lying electronic energy levels and their degeneracy factors are also given. Resulting thermodynamic functions of internal energy $U(T)$, enthalpy increment $H(T)$, free energy $Φ(T)$, Helmholtz energy $F(T)$, isobaric and isochoric specific heat capacity $C_p(T)$ and $C_v(T)$, and entropy $S(T)$) form the two-dimensional array (temperature – function values).

RESULTS AND DISCUSSION

The user interface is very convenient (Fig. 2). A distinctive feature of the program is availability of various prebuilt algorithms to calculate atom coordinates for the majority of simple compounds (with a number of atoms $N \leq 8$) included. User could simply choose a number of atoms, the structure of molecule, and insert the molecular constants. It is very convenient because literature data contain molecular constants in this format. Nevertheless, user can input the geometry of the molecule manually. To do this user must click on "Manual input of geometry" checkbox. The table containing fields with the masses of atoms and their coordinates will appear. Also user must set the type of molecule (nonlinear or linear) as well as the symmetry number.

The StatThermo has its own format of files of input data (*.stf). User can save the initial parameters of calculation by clicking on "Save initial data" button. The software also supports the Gaussian [9], Gamess [10], FireFly [11], Jaguar [12], MolPro [13], CFour [14], NWChem [15], ORCA [16], Priroda [17], PSI4 [18], Q-Chem [19], and VASP [20] output files as input data along with its own format.

The developed software produces calculation for two reference temperatures (0 or 298.15 K) and different pressures (101325 Pa by default). Also user can select the thermodynamic functions for calculation into the corresponding checkboxes, set the temperature interval and increment.

As was recently shown [21] the electronic states are very important for evaluating of thermodynamic functions. The possibility to take into account the low-lying electronic states is one of the remarkable features of the program. It should be noted that software treats all low-lying electronic levels instead of simple splitting of ground state.

After the calculation the window automatically switches on next tab "Results". Here in the table the calculated thermodynamic functions are shown.

However to work with tabulated data is not so convenient as with polynomials. For this purpose the feature of approximation of the thermodynamic functions was added to the program. The software approximates the thermodynamic functions by the polynomial recommended in [7]:

$$Func(T) = a\ln x + bx^{-2} + cx^{-1} + dx + ex^2 + fx^3, \quad (x = T/1000), \qquad (1)$$

here $Func(T)$ is a thermodynamic function.

The StatThermo can also approximate the functions in any specified temperature range. The reference pressure can also be adjusted. To find the coefficients of polynomial (1) the LU-decomposition is used.

The obtained polynomial together with tabulated data can be exported into the MS Excel or OpenOffice (LibreOffice) Calc. To export these results as macro of Visual Basic user must enter the macro name and push the "Export" button. After the export the chosen application will be open and new macro file will be linked to it. All exported files are saved in the "Export" folder inside the main directory of StatThermo.

User can also approximate by the polynomial its own functions. To do this the user must clear the results table and paste into it the prepared functions. First column always must contain the temperature values, other columns should correspond to the order of functions in results table ($H°(T)$ – first, $\Phi°(T)$ – second, etc.).

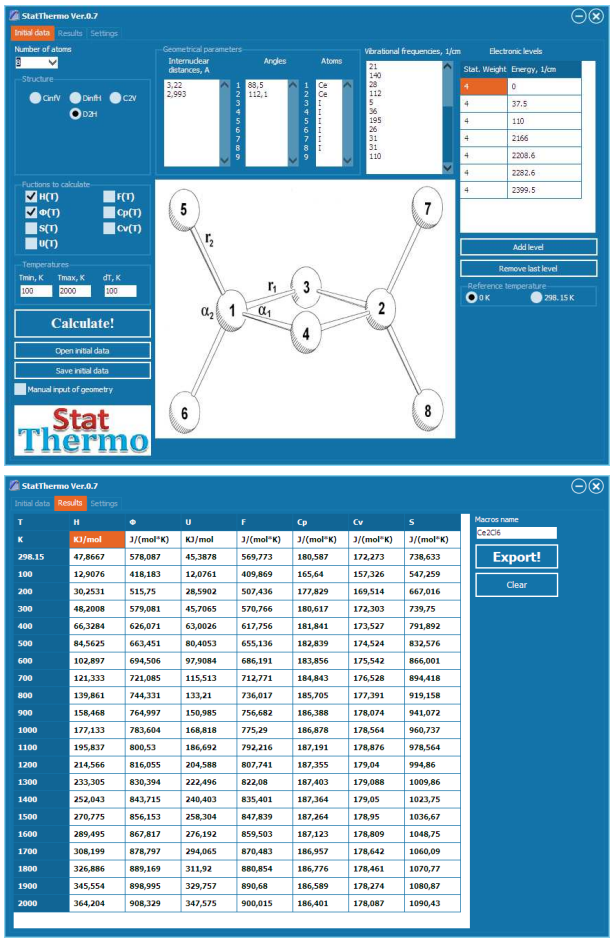

Fig. 2. User interface of StatThermo
Рис. 2. Интерфейс StatThermo

The software StatThermo has been tested by comparison the calculation results of the thermodynamic functions for reference molecules with those from the databases [1, 2]. They were chosen to cover more wide set of input parameters (linear or nonlinear structure, different point group of symmetry, number of atoms, and electronic levels). Table 1 contains the molecular constants for selected molecules from [7].

The relative differences of tabulated [2] and calculated thermodynamic functions are collected in Table 2. Analysis of Table 2 shows a good agreement between the tabulated values and calculated by StatThermo. None of the errors exceeds the 1%. The average errors of StatThermo are as follows: 0.05 kJ·mol^{-1} ($H°(T)$-$H°(0)$), 0.01 J·mol^{-1}·K^{-1} ($\Phi°(T)$), and 0.002 J·mol^{-1}·K^{-1} ($S°(T)$). Mainly they explained by the divergence of the fundamental constants.

Table 1

Molecular constants of reference molecules

Таблица 1. **Молекулярные постоянные молекул стандартов**

Molecule	Point group of symmetry	Internuclear distances, Å	Angles	Vibrational frequencies, cm^{-1}	Electronic levels, cm^{-1}
GeO_2	$D_{\infty h}$	1.65	180.0	860; 280(2) [1]; 1062	0(1) [1]
$GeCl_2$	C_{2v}	2.186	100.4	395; 160; 370	0(1)
Be_2O	$D_{\infty h}$	1.4	180.0	620; 320(2); 1200	0(3)
Na_2F_2	D_{2h}	2.08	95.0	406; 229; 271; 176; 350; 371	0(1)
Al_2I_6	D_{2h}	2.449 (r_t)[2]; 2.634 (r_r)	115.0 (α_t); 99.6 (α_r)	340; 145; 93; 42; 20; 310; 82; 82; 415; 90; 13; 405; 54; 291	0(1)
CeI_3	D_{3h}	2.92	120.0	142; 27; 191(2); 35(2)	0(2); 40(2); 110(2); 2200(8)
COOH	C_1	r(O-H) = 0.97; r(C-O) = 1.32; r(C=0) = 1.23	107 (C-O-H); 123 (O-C-O)	3316; 1797; 1261; 1088; 620; 615	0(2)
CBr_4	T_d	1.942	109.28	268; 122(2); 680(3); 182(3)	0(1)

Notes: 1) – the degeneracy of level or vibrational frequency is given in parentheses, 2) – the values corresponding to the torsion and ring attributes are designated by "t" and "r", respectively

Примечания: 1) – в скобках дана степень вырождения частот колебаний, 2) – величины, соответствующие торсионному и кольцевому участку, обозначены как "t" и "r" соответственно

Table 2

Comparison of tabulated and calculated by StatThermo (ST) thermodynamic functions of some molecules

Таблица 2. **Сравнение табличных и рассчитанных StatThermo (ST) термодинамических функций некоторых молекул**

Molecule	T, K	Thermodynamic function		Error, %
		[2]	ST	
$H(T)$-$H(0)$, kJ·mol^{-1}				
GeO_2	298.15	11.268	11.258	0.091
	1000	50.344	50.330	0.028
$GeCl_2$	298.15	13.277	13.277	0.002
	1000	53.125	53.123	0.003
Be_2O	298.15	11.190	11.190	-0.003
	1000	50.460	50.451	0.018
Na_2F_2	298.15	16.682	16.682	0.001
	1000	73.194	73.191	-0.004
Al_2I_6	298.15	40.920	40.598	-0.786
	1000	166.836	166.38	-0.272
CeI_3	298.15	22.018	22.018	0.001
	1000	81.581	81.596	0.019
COOH	298.15	10.813	10.813	-0.003
	1000	52.059	52.046	0.024
CBr_4	298.15	20.365	20.365	0.001
	1000	91.818	91.804	0.015
$\Phi(T)$, J·mol^{-1}·K^{-1}				
GeO_2	298.15	203.374	203.365	0.004
	1000	256.677	256.655	0.009
$GeCl_2$	298.15	251.185	251.191	-0.002
	1000	310.872	310.877	-0.002
Be_2O	298.15	190.312	190.265	0.025
	1000	243.681	243.628	0.022
Na_2F_2	298.15	241.840	241.838	-0.001
	1000	321.247	321.242	-0.002
Al_2I_6	298.15	452.271	453.215	0.209
	1000	638.732	638.767	0.005
CeI_3	298.15	357.992	357.990	-0.001
	1000	452.275	452.280	0.002
COOH	298.15	215.355	215.398	-0.020
	1000	267.640	267.675	-0.013
CBr_4	298.15	289.643	289.641	0.001
	1000	387.647	387.631	0.004
$S(T)$, J·mol^{-1}·K^{-1}				
GeO_2	298.15	241.134	241.124	0.004
	1000	307.020	306.985	0.011
$GeCl_2$	298.15	295.716	295.722	-0.002
	1000	363.998	364.000	-0.001
Be_2O	298.15	227.843	227.798	0.020
	1000	294.141	294.078	0.021
Na_2F_2	298.15	297.792	297.790	-0.001
	1000	394.441	394.434	-0.002
Al_2I_6	298.15	589.517	589.382	-0.023
	1000	805.567	805.149	-0.052
CeI_3	298.15	431.841	431.840	0.000
	1000	533.856	533.883	0.005
COOH	298.15	251.622	251.666	-0.017
	1000	319.700	319.721	-0.005
CBr_4	298.15	357.948	357.945	0.001
	1000	479.465	479.435	0.006

The software can work under the MS Windows operating system (XP, Vista, 7, 8, 10) as well as Linux (Debian based distributives). Both x86 and x64 architecture is supported. The minimal system requirements depend on chosen exporting server (MS Excel XP, MS Excel 2007, OpenOffice Calc etc.). If user won't use the export function it is enough 512 Mb RAM, 1 GHz processor frequency, and 3 Mb free disk space.

The StatThermo has multilingual support: English and Russian language available. Nevertheless, user interface is easily translatable. In "languages" folder user can duplicate the STATThermo.en.po file, change the language code suffix, and edit the file in any appropriate editor (PoEdit [22], for example).

CONCLUSION

The new software StatThermo for calculation of the thermodynamic functions of molecules in the state of ideal gas using the molecular constants has been developed. Program has a lot of prebuilt algorithms for calculation of the geometry of small molecules, takes into account low-lying electronic states, and can perform calculation for different reference temperatures and pressures. A wide range of functionality, flexible parameters of calculation and possibility to approximate and export results as a macro do the StatThermo powerful software for thermodynamic chemical calculations. Low hardware requirements, multilingual and cross-platform support makes the StatThermo accessible for a lot of users. To download the StatThermo please visit official website www.isuct.ru/htms/en/statthermo.

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