New Version Of The ICT-Thermodynamic Code

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Abstract

The ICT-Thermodynamic Code together with the excerpt of the ICT-Database of Thermochemical Values has long been a powerful tool to calculate and predict the thermodynamical behavior of energetic materials. In 2014, updated versions of both will be released. Here the major changes and some application examples are shown.

Keywords: ICT-Thermodynamic Code, ICT-Database of Thermochemical Values, ICT-Code, Thermodynamics, Propellant, Combustion, Modeling, Interior Ballistics, Rocket Propellants, Energetic Materials

Introduction

The calculation of chemical equilibria is not only of interest for the evaluation of the performance of rocket and gun propellants; it is also useful for optimization purposes of different combustion processes with regard to temperature, pressure and formation of products. Such calculations can be performed with the ICT-Thermodynamic Code [1], [2].

The ICT-Thermodynamic Code is based on a method developed by the National Aeronautics and Space Administration (NASA). This method uses mass action and mass balance expressions to calculate chemical equilibria. The origin of the ICT-Thermodynamic Code, described in this Manual, lies in the year 1969. At that time, the Fraunhofer Institute for Chemical Technology developed a FORTRAN program for the calculation of chemical equilibria. The program was expanded in the following years making different calculation types, e.g. ETC or gas detonations possible. A major milestone in the development was the graphical user interface, which was released in the year 2000. This enabled a user friendly

handling of the thermodynamic calculations and consolidated its position as an international standard.

In the year 2014 a new version of the ICT-Thermodynamic Code will be released. The new version will run on current and future operating systems, e.g. Windows 7 or higher. The graphical user interface was completely new implemented while keeping the familiar looks to make the transition to the new version easy. In addition to the known features a new handling of user substances has been realized and a database manager has been included.

The reliability of thermodynamic calculations depends primarily on the availability and accuracy of thermochemical data. Therefore the Fraunhofer Institute for Chemical Technology (ICT) began very early to collect data on energetic materials. In 1971 tables with properties of substances related to the formulation of rocket and gun propellants were published [3]. This publication contains enthalpies of formation and other data like heat of combustion, molecular weight, oxygen balance, density and structural formulas of 500 substances. Data of 147 additional substances were published in 1981 [4].

Meanwhile properties of a lot of new energetic substances have been published. Therefore, instead of compiling an additional supplement, we decided to store the main properties of all these substances in a thermochemical database. This has the advantage – compared to printed tables – that data can be retrieved very fast and updates can be made easily and regularly.

The first database published in 1994 contained data of 1850 substances. The eighth update of the database now contains data of 14,100 substances [5]. Not all of them belong to the field of explosives. Enthalpies of formation of a lot of important substances were incorporated. Therefore it is possible to use the database for general purpose. From the database the excerpt for the ICT-Thermodynamic Code, that provides the input data for the calculations, is derived. A new excerpt will be released together with the new version of the ICT-Thermodynamic Code in 2014.

Use of the new ICT-Thermodynamic Code

Although the new graphical user interface of the ICT-Thermodynamic Code was completely redesigned, the looks and handling of the surface is almost exactly the same as in the previous version. This can be seen for example in Figure 1, which shows the first input form of the code.

But there are also differences and new features which were not implemented in the previous version. The main difference is the handling of user substances. In the previous version the user substances were stored in the same database as the data from the ICT-Database of

Thermochemical Values. This made the transfer of user created substances between different installations of the ICT-Thermodynamic Code cumbersome. Now user substances are stored in a separate database called the user database. The creation, editing, importing and deleting of user created substances is done using the new database manager. An example of the user interface of the database manager can be seen in Figure 2. With the database manager it is also possible to extract user created substances from an older database used in the previous version of the ICT-Thermodynamic Code and to import them in the new user database as well as to import data from other users.

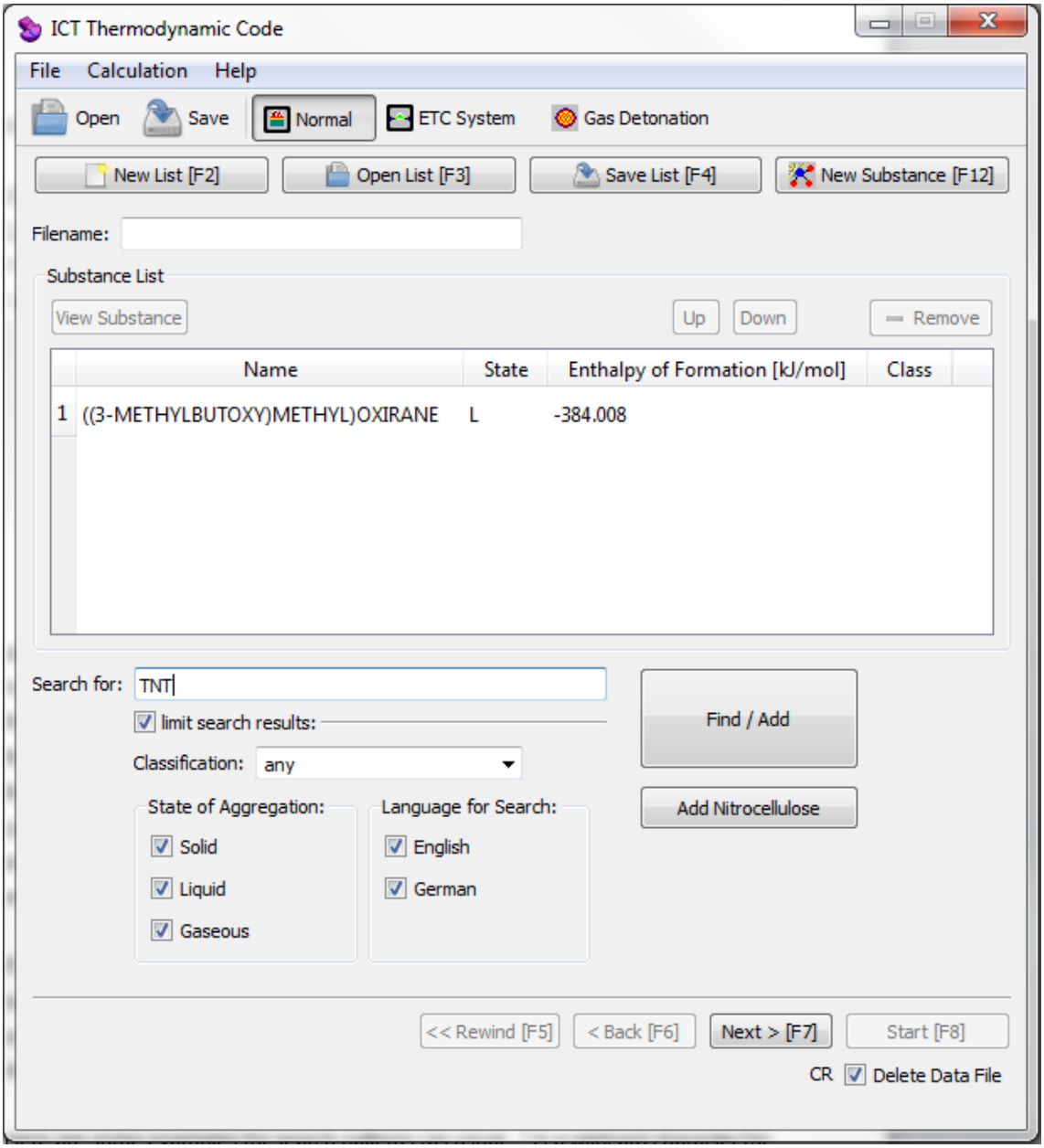

Figure 1: Reworked input form of the ICT-Thermodynamic-Code

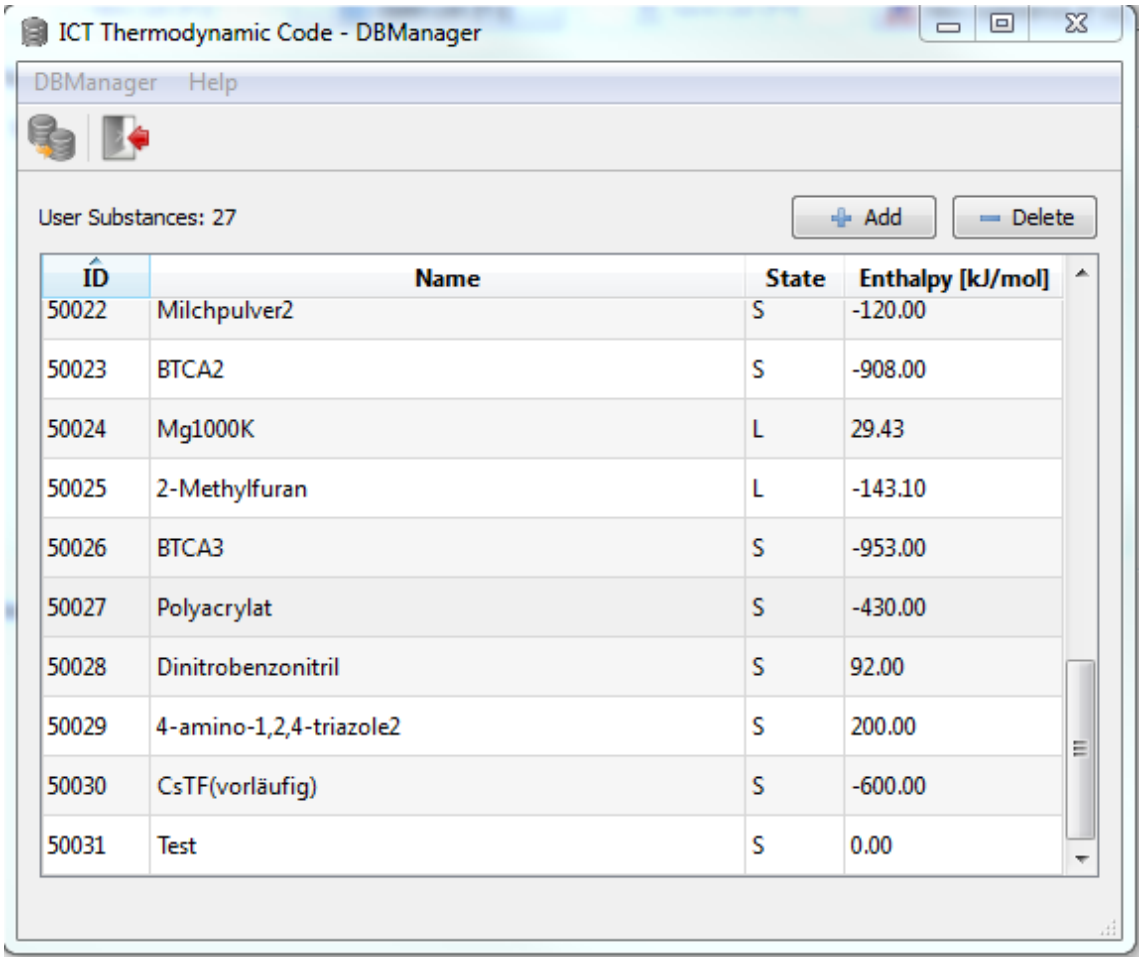

Figure 2: New database manager in the ICT-Thermodynamic Code

To show the possibilities and broad range of applications that the new version of the ICT-Thermodynamic Code gives to the user, some exemplary results for a model formulation of a solid rocket propellant mixture are given. The calculations aimed at the optimization of the composition with respect to the specific impulse, while keeping the adiabatic combustion temperature as low as possible. The results of the calculations can be seen in Figure 3 and Figure 4.

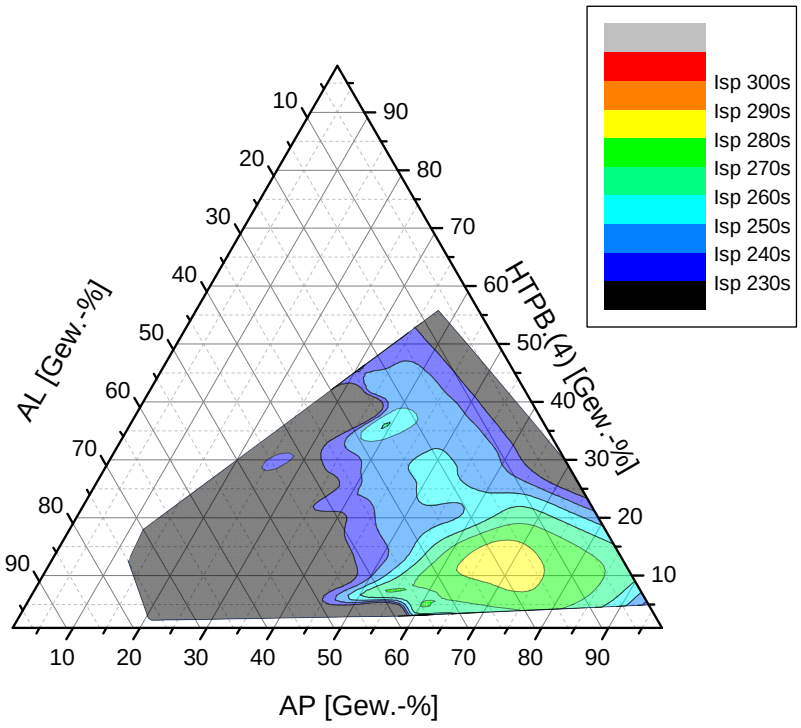

Figure 3: Specific impulse of an AP/HTPB/AL solid rocket propellant mixture

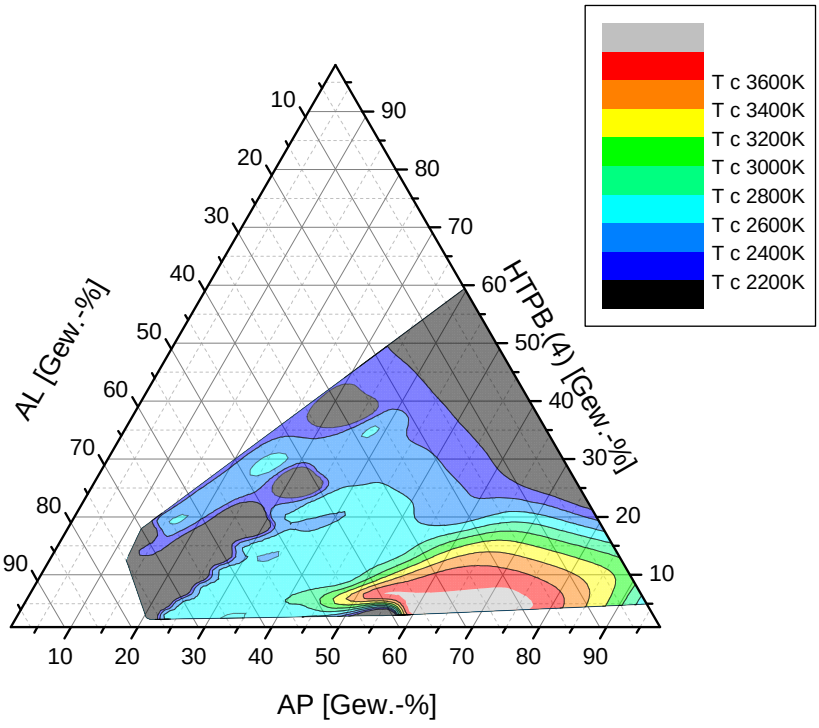

Figure 4: Adiabatic combustion temperature of an AP/HTPB/AL solid rocket propellant mixture

Content of the Database

The Database contains all the known names of the 14,100 substances stored in the eighth update. The CAS-Numbers are also included for other applications like search in commercial databases (STN). For each stored substance a sum formula and a structural formula are available. The structural formulas, shown on the screen, can be printed together with the other data. Further it can easy be transferred to the clipboard for the use in presentations etc.

3,817 references and 53,247 properties of the stored substances are recorded in the database, including molecular weight, density, melting and boiling point, state of aggregation, energy of combustion and other important values for thermodynamic calculations like oxygen balance, energy and enthalpy of formation.

Figure 5 shows the main window of the database showing the sum formula, the structural formula and properties of a chosen substance.

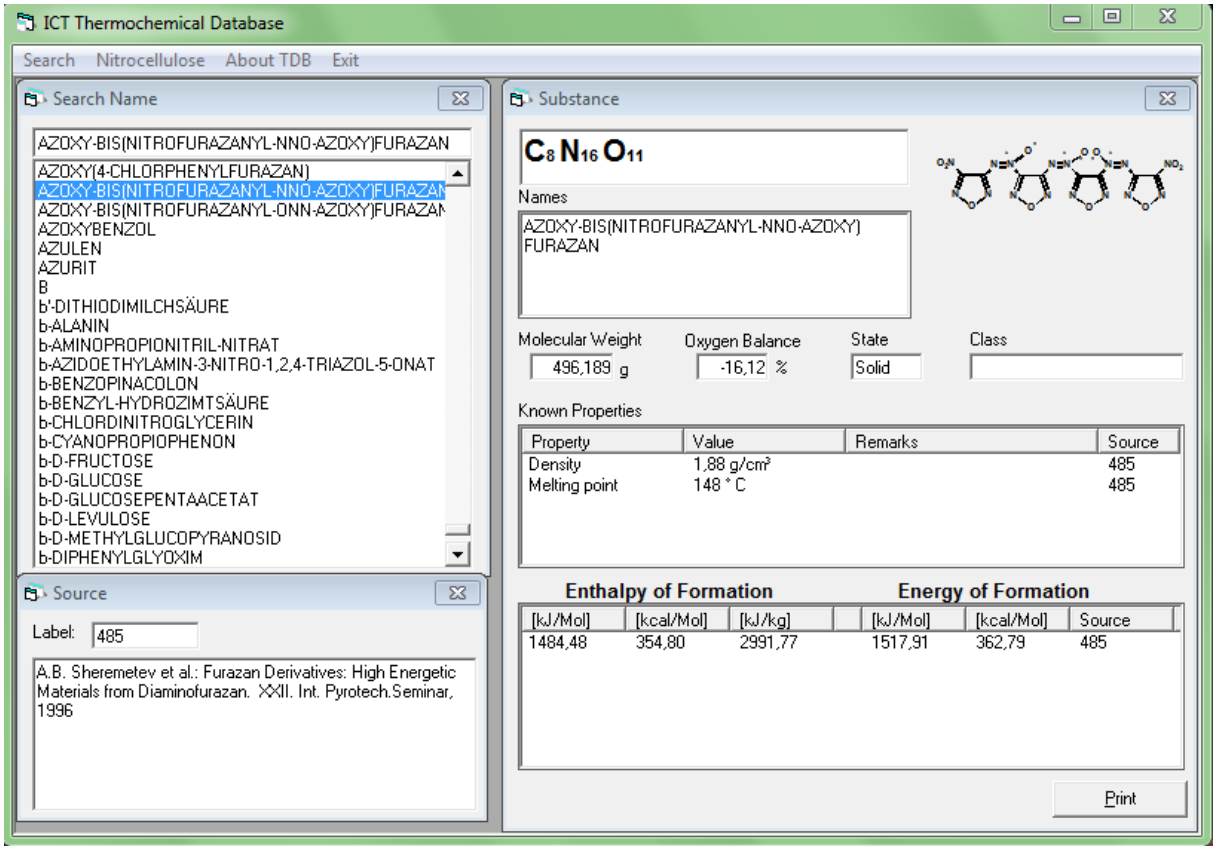

Figure 5: Result window of a substance search

From the ICT-Database of Thermochemical Values an excerpt is prepared that provides the necessary input data for the calculations of the ICT-Thermodynamic Code. The previous version of the excerpt contained data of 10491 substances. The new excerpt which will be shipped together with the new version of the ICT-Thermodynamic Code in 2014 contains the data for 11499 substances.

Handling of the Thermochemical Database

The use of the database is very easy. It enables you to search for substances in four different ways. Search by name, by part of a name, by sum formula or elements and by properties is possible. The search by properties, where different properties or ranges of properties can be used for the identification of certain substances, is of particular interest. If the expression „search by properties" is chosen, a window as shown in Figure 6 appears. You chose the desired properties and get a result window with a list of substances that fit the defined properties (Figure 7). By clicking one of the substances of the result list of the search, you get the window shown in Figure 5.

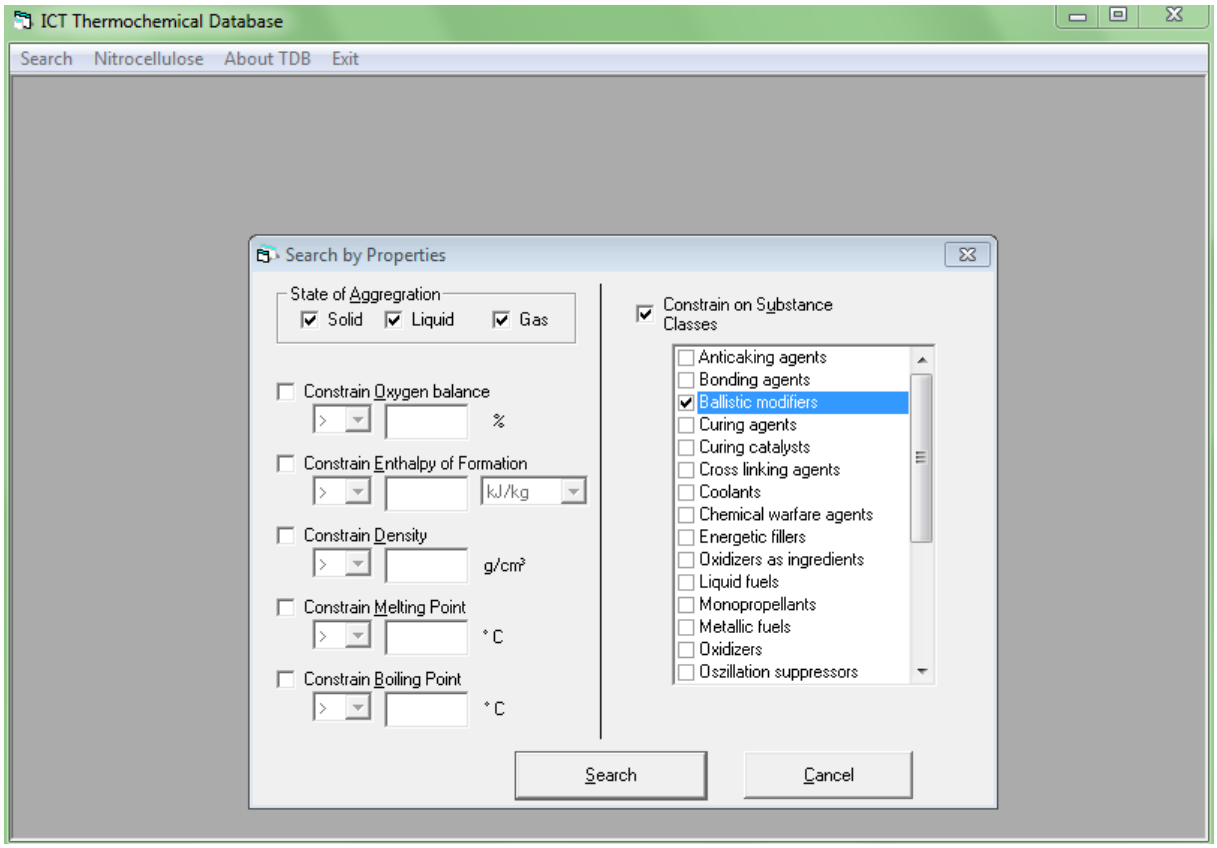

Figure 6: Window for search by properties

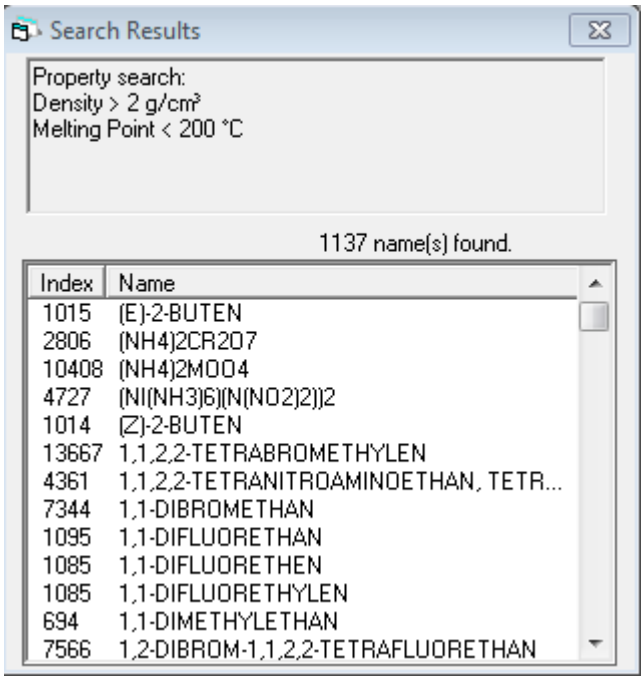

Figure 7: Result window of a properties search

Summary

A new version of the ICT-Thermodynamic Code will be released in 2014. The new version will run on current and future operating systems, e.g. Windows 7 or higher. The graphical user interface was redesigned while keeping the looks and functionality of the previous version. Some new features include a new and improved handling of user created data using the database manager.

Together with the ICT-Database of Thermochemical Values from which the input data for the ICT-Thermodynamic Code are derived, the new version is a powerful tool to understand and design the thermodynamical behavior of energetic systems.

References

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