ReSpecTh: a joint reaction kinetics, spectroscopy, and thermochemistry information system

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Abstract

Reaction kinetics, high-resolution molecular spectroscopy, and thermochemistry data are frequently used together to help the interpretation of complex experiments and to carry out simulations of complex gas-phase chemical systems. The relevant systems may involve combustion reactions, and atmospheric, stellar and interstellar environments. The principal aim of the newly set-up active information system `ReSpecTh` is to provide useful, accurate searchable data and utility programs that can be used in several engineering and scientific fields either separately or simultaneously. The present status of `ReSpecTh`, set up at http://respecth.hu/, is described. `ReSpecTh` is under constant development and significant extensions are expected to come regularly.

Introduction

Accurate experimental data have an eminent role in chemical research. In the fourth age of quantum chemistry we live in [1] it is also viable, through high-level, complex algorithms and related computer codes, to validate the experimental data, to generate new data augmenting the measured data, and to utilize the experimental and computed data within diverse scientific and engineering applications. The experimental and computed data and the related codes help (a) to understand our wider natural environment (*e.g.*, star forming regions, and the atmospheres of planets and exoplanets), (b) to answer important questions related to the origin of life on Earth and our special role in its maintenance, and (c) to protect the quality of life on our own planet (*e.g.*, via an improved scientific understanding of the greenhouse effect on Earth and of combustion systems, and research and development related to climate change). An improved science-based understanding of the environments and processes mentioned requires the creation of modern, preferably active chemical information systems containing carefully validated data of traceable origin. Several such information systems exist in the fields of reaction kinetics [2-6], high-resolution molecular spectroscopy [7-10], and thermochemistry [11-13].

`ReSpecTh`, an information system containing reaction kinetics, high-resolution molecular spectroscopy, and thermochemistry data, is not just another information system set up by our laboratories but it has several unique and noteworthy features. `ReSpecTh` is a dynamic website written in PHP with client-side jQuery services. Most data are stored in MySQL databases. One of the unique features of `ReSpecTh` is the joint and extended utilization of all available experimental and computational information. The information system is active, meaning that all the experimental and computed data that `ReSpecTh` contains in its three branches and all new data influence the values and the uncertainties of all the derived data, and thus improvement of the quality of the data through appropriate refinement procedures is a constantly ongoing effort. Furthermore, some of the datasets contained in `ReSpecTh` are built upon data mining using novel methods of discrete mathematics, including graph theory. `ReSpecTh` includes a searchable bibliographical chemical kinetics data collection, a database of high-temperature gas kinetics elementary reactions with information on the available experimental data, and capacity for a detailed assessment of derived quantities, like the uncertainty of rate parameters and vibrational energy levels and thermochemical quantities. Another `ReSpecTh` dataset includes raw experimental data in the field of combustion chemistry. Some of these specialized datasets are cross referenced with each other and with the spectroscopic and thermochemical datasets.

The `ReSpecTh` website was set up at the dedicated address http://respecth.hu/. The methods, codes, and the final datasets are either available to the general public for the benefit of interested scientists and engineers, or can be accessed freely by approved parties via a login system.

Reaction kinetics

The reaction kinetics part of `ReSpecTh` includes experimental data, detailed reaction mechanisms of exemplary combustion systems, and utility programs.

The experimental kinetic data are currently all related to the combustion of hydrogen but will be extended to include other systems, like the combustion of syngas, hydrocarbons, and alcohols. The data consist of indirect combustion experiments related to ignition delays, measured in shock tubes and rapid compression machines (RCMs), as well as laminar flame velocities and concentration profiles, measured in various facilities. Direct measurements of rate coefficients of elementary reactions are also included in the database. Our strategy is to provide a comprehensive coverage of hydrogen combustion experiments first and of other systems later. The hydrogen data have already been used for testing published reaction mechanisms [14] and for the production of a new reaction mechanism via mechanism optimization [15].

The database of indirect experiments is searchable according to the type of the experiment, the

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experimental conditions (initial pressure and temperature), and the type of fuel and bath gas. This way ReSpecTh can easily be used to locate all experimental data at a given set of experimental conditions, which can be of great assistance for mechanism development. Currently the ReSpecTh site contains 223 XML files related to indirect hydrogen combustion experiments (including 54, 72, 73, and 24 data sets related to ignition delays measured in shock tubes, ignition delays measured in RCMs, laminar flame velocity measurements, and concentration profiles measured in reactors, respectively). The direct experiments can be searched according to the stoichiometry of the elementary reaction. Currently the site contains 56 XML data files on the direct determination of 10 elementary reactions.

All combustion data are stored according to the ReSpecTh Kinetics Data Format Specification (RKDFS). A document containing the definition of the data format is available on the ReSpecTh site. This data format consists of a set of specifications, aiming to provide an unambiguous definition of the storage of combustion experimental data and rate coefficient measurements. RKDFS defines an XML data format to provide flexible data representation and allow for easy extension of the format specification.

RKDFS is directly based on the PrIMe experimental data format [16] and most of the specification is directly derived from the XML elements and attributes defined within PrIMe. In the PrIMe format some experimental setups are not defined unambiguously. The RKDFS format is unambiguous and therefore the corresponding data are uniquely interpretable by computer codes. Within RKDFS the PrIMe format was extended with new elements, like the definition of experimental detection of ignition. Due to the modifications and extensions of the PrIMe format, the PrIMe experimental data format files are not correct RKDFS files. Nevertheless, any PrIMe experimental datafile can easily be converted to the RKDFS format.

RKDFS provides a set of instructions for the interpretation of XML files. It defines XML elements and attributes, and how they must be interpreted within the RKDFS. RKDFS also defines the elements which must be present in an XML file to make it a complete data file. Other elements are not compulsory, but may carry important information. Finally, further XML nodes can be present in the file, which will not be interpreted within RKDFS but can be used to store auxiliary information.

The ReSpecTh site contains not only the documentation of the data specification and many data files, but also utility codes for the creation and interpretation of RKDFS data files. The data file creator program reads the data provided in text files and prints out the proper XML datafiles. The code checks the data for completeness (*e.g.*, whether all physical conditions are provided and whether the experiment is well defined) and contradictions (*e.g.*, whether the reaction temperature was defined multiple times). The XML data file interpreter program is capable of creating CHEMKIN-II [17] input files for the SENKIN, PRS, and PREMIX simulation codes. Since the source code of the program is provided, it can be easily modified, making it usable with any other combustion simulation code.

The aim of providing accurate data format specification and utility codes for the creation and interpretation of such files is that we want to support the long-term and laboratory-independent storage of experimental data. Also, we want to assist mechanism developers, making the testing ("validation") of reaction mechanisms considerably faster.

A collection of hydrogen and syngas combustion mechanisms was also made available on the ReSpecTh site. These mechanisms were investigated in the recent publications of Olm *et al.* on hydrogen combustion [14] (20 mechanisms) and syngas combustion [18] (16 mechanisms). The ELTE 2015 optimized hydrogen combustion mechanism [15] is also given. The ReSpecTh site contains the mechanisms in Chemkin format, together with the corresponding transport files and references to the origin of the mechanisms. The Leeds Methane Oxidation Mechanism [19], together with its various extensions and formats, was also transferred to ReSpecTh from the "Combustion Simulations in Budapest" website.

A series of utility programs developed in Budapest and relevant to the analysis of reaction kinetics models are available on the ReSpecTh site: KINALC, MECHMOD, FluxViewer, and SEM. KINALC is a postprocessor to Chemkin-based simulation programs, it performs the analysis of reaction mechanisms based on calculated concentrations, reaction rates and sensitivity coefficients. MECHMOD is a modification tool for Chemkin-format reaction mechanisms. It is capable of removing species and their reactions from a mechanism, or changing the units of the rate parameters. FluxViewer is a visualization tool for species fluxes at various space or time points during a simulation. SEM is a mechanism reduction code based on the method of simulation error minimization [20, 21]. These utility programs have been published on the "Combustion Simulations in Budapest" web site.

The next set of codes is related to newly published studies. Recently, Nagy *et al.* [22] published a methodology for the determination of the uncertainty domain of Arrhenius parameters from chemical kinetics literature data. The Matlab program *u-Limits* reads a text data file that contains all Arrhenius parameters published in review-type, experimental, or theoretical articles. This program calls UBAC for the determination of the uncertainty band of Arrhenius curves, and the code JPDAP for the calculation of the joint probability density of the Arrhenius parameters. Finally, the program SAMAP is able to generate random or quasi-random samples of Arrhenius parameter sets knowing the covariance matrix of Arrhenius parameters for uncertainty analysis or mechanism optimization purposes.

ReactionKinetics is a *Mathematica*-based package [23] that investigates reaction mechanisms using a selected set of structural and graph theoretical approaches as well as techniques which are related to the time evolution of the concentration sets obtained from the considered mechanisms. Results of the analyses by ReactionKinetics for all hydrogen and syngas reaction mechanisms given in ReSpecTh were published in a recent article [24].

High-resolution spectroscopy

It is generally accepted that almost all present-day knowledge about the structures and properties of molecules comes via studies of their spectra. Although laboratory measurements are usually considered to be the prime source for the relevant information, there are a number of occasions where theory has played, and will continue to play, a central role in the understanding of properties of molecules and their spectra.

Cutting-edge experimental studies in high-resolution molecular spectroscopy help to answer questions raised in the Introduction but also create new ones demanding new theoretical approaches. An important point is that even when laboratory spectra have been recorded for a particular species, the data are only partial and not sufficiently detailed for many modeling applications. One such situation, which is particularly common for unstable or reactive species, is that wavelengths can be measured to high accuracy but there is no or extremely limited information on transition probabilities and line strengths.

It must be realized that many modelling applications are particularly demanding on spectroscopic data. For example, to model the role of triatomic species, such as H_2O [25] or [H,C,N], which are important components of O-rich and C-rich cool stars, respectively, may require up to a billion vibration–rotation transitions. The laboratory measurement and analysis of a dataset of transitions of this size is completely impractical. Computational molecular spectroscopy, with its fourth-age quantum chemical techniques [1], comes to the rescue and allows the straightforward determination of huge molecular line-lists. Help is provided through computation of potential energy (PES) and property (like the dipole moment surface, DMS) hypersurfaces [26, 27], which can be obtained with modern techniques of electronic structure theory and then employed in sophisticated variational nuclear-motion computations. Generation, storage, and retrieval of such line-lists is a significant challenge requiring novel theoretical tools.

One such new approach allowing to deal with the huge and complex data generated by high-resolution spectroscopic experiments is the use of spectroscopic networks (SN) [28].

At present ReSpecTh contains all the data related to the high-resolution spectroscopy of nine major water isotopologues, as assembled by an IUPAC Task Group [29-33], the three main isotopologues of H_3^+ (H_3^+, H_2D^+, and D_2H^+) [34, 35], and the parent ketene molecule [36]. In the near future ReSpecTh will contain the same type of data of parent ammonia ($^{14}NH_3$). ReSpecTh includes both the energy levels of experimental accuracy and the validated measured transitions. The validation is performed by the well-documented MARVEL procedure and code [37-40]. The acronym MARVEL stands for measured active rotational-vibrational energy levels. MARVEL is based on the concept of spectroscopic networks [28, 39]. MARVEL is designed for critically evaluating and validating experimental transition wavenumbers and uncertainties collected from the literature as well as for inverting the wavenumber information in order to obtain the best possible energy levels with attached uncertainties in a highly efficient way. ReSpecTh contains a large number of properly referenced high-level first-principles spectroscopic data, augmenting and enhancing MARVEL analyses.

The ReSpecTh website also provides a search facility whereby the user can search either in articles, those that were used to construct the MARVEL databases, or in the measured energies and lines, those that the MARVEL datasets contain, or in computed spectroscopic data.

Thermochemistry

First-principles thermochemistry relies on advanced techniques of electronic structure theory to compute accurate thermochemical quantities, while for the determination of temperature-dependent, effective quantities one needs the techniques of nuclear motion theory. One of the key questions in electronic structure theory concerns the accuracy of the computed molecular quantities, including relative energies. The composite focal-point analysis (FPA) approach developed some two decades ago by us [41, 42] provides a clean way to determine the uncertainties of computed energetic quantities.

Another important area of the application of quantum chemistry in thermochemistry concerns the determination of accurate partition functions and related thermochemical data of small(er) molecules with well-defined uncertainties. The traditional approaches rely either on simple model assumptions or on effective Hamiltonians fitted to experimental data. Thus, they give poor results with unknown uncertainties especially at higher temperatures. Based on the joint use of the in-house MARVEL protocol and nuclear motion computations, the explicit summation technique based on accurate rovibrational energy levels with known uncertainties offers an accurate way to determine thermochemical quantities over a wide temperature range ($T < 6000$ K) which could be used in many scientific and engineering applications.

NEAT [43], standing for a "network of computed reaction enthalpies leading to atom-based thermochemistry", is a simple and fast, weighted, linear least-squares refinement protocol and code for inverting the information contained in a network of quantum chemically computed 0 K reaction enthalpies. This inversion yields internally consistent 0 K enthalpies of formation for the species of the network. The refinement takes advantage of the fact that the accuracy of computed enthalpies depends strongly on the quantum-chemical protocol employed for their determination. Different protocols suffer from different sources of error; thus, the reaction enthalpies computed by them have "random" residual errors. Since it is much more natural for quantum-chemical energy and enthalpy results, including reaction enthalpies, to be based on the electronic ground states of the atoms and not on the historically preferred elemental states, and since these two possible protocols can be converted into each other straightforwardly, it is proposed that first-principles thermochemistry should employ the ground electronic states of atoms. In this scheme, called atom-based thermochemistry (AT), the enthalpy of formation of a gaseous compound corresponds simply to the total atomization energy of the species; it is always positive, and it reflects the bonding strength within the molecule. The inversion protocol developed and based on AT is termed NEAT, which represents the fact that the protocol proceeds from a network of computed reaction enthalpies towards atom-based thermochemistry, most directly to atom-based enthalpies of formation.

The `ReSpecTh` site contains a mirror of Burcat's thermodynamic data collection [11]. This site has been mirrored in the Combustion Simulations in Budapest site [12]. Creation of the new mirror site allowed adding new services. This includes a species search capability, which allows a search for complete species names or parts of species names. The page also shows the c_p, ΔH_f and s_m values of the selected species at 298.15 K. Also, these thermodynamic properties are plotted as a function of temperature in the whole range of validity of the data.

Conclusions

In early 2015 we set up a new web site at http://respecth.hu/ containing information related to gas-phase reaction kinetics, high-resolution molecular spectroscopy, and chemical thermodynamics. We have added to this site several data files, documents and computer codes that have been published in several other web sites maintained by the authors. Also, we used the opportunity of setting up this web site to publish information that was related to our recently published articles. New content will be added regularly to `ReSpecTh`.

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