

INDC International Nuclear Data Committee

Technical Meeting on the Development of Software Programs and Database Tools for Modelling Edge Plasma Processes in Fusion Devices

Summary Report of the Meeting
IAEA Headquarters, Vienna, Austria
27 – 29 November 2019

Prepared by

C. Hill
Nuclear Data Section, International Atomic Energy Agency
Vienna, Austria

December 2019

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or to:

Nuclear Data Section
International Atomic Energy Agency
Vienna International Centre
PO Box 100
1400 Vienna
Austria

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ABSTRACT

A Technical Meeting formulating new and reviewing existing standards and software tools for representing, storing and classifying atomic and molecular species, states and plasma-relevant processes was held at IAEA Headquarters in Vienna from 27 – 29 November 2019. 12 IAEA staff and participants from 6 Member States attended the meeting. This report summarises their discussions and the meeting conclusions and includes drafts of the updated standards documents, which are freely-available on the website of the Atomic and Molecular Data Unit in their final form.

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1. Introduction

The accurate and unambiguous identification of atomic and molecular species, states and processes is essential to the effective description of data concerning them. Although many alternative standards have been proposed and implemented, none has been universally adopted by the plasma physics and spectroscopy community in their data services. This introduction will consider, in turn, the two broad areas of identifying species and their states, and of identifying the collisional and other processes that such species undergo, with a particular focus on plasma physics.

1.1 Atomic and molecular species

The two broad categories of identifiers for species are those which assign arbitrary numbers or strings to a species and those which attempt to encode the molecular structure into a single string. The former method, of course, requires the maintenance of a database in which to look up details concerning a species from its identifier. The most comprehensive such database may be the Chemical Abstracts Services (CAS) Registry, a catalogue of unique numerical identifiers for (as of November 2019) 156,000,000 organic and inorganic substances referenced in the scientific literature since the early 1800s[1]. ChemSpider[2] is a similar, free chemical structure database, containing information on more than 78,000,000 molecules, owned by the UK Royal Society of Chemistry.

Similar registries exist for the fields of organic chemistry (for example, the Beilstein database[3]), inorganic and organometallic chemistry (Gmelin[4]) bioinformatics (ChEBI[5], ChEMBL[6], PubChem[7]) and for regulatory purposes (EC Number[8], UN Number[9], CompTox Chemicals Dashboard[10]). These databases are much more limited in scope, since they are restricted to molecules of interest to specified research domains.

Of the standards that encode the molecular structure in their identifiers, the most widely-used are the XML-based Chemical Markup Language (CML)[11], the Simplified molecular-input line-entry system (SMILES)[12] and the International Chemical Identifier (InChI)[13].

For use in databases of processes for astrophysical, fusion and other plasma applications, no single standard currently provides an adequate method of unambiguously identifying species: common problems in the case of databases using arbitrary identifiers are incompleteness and ambiguity over the phase, isotopic composition and isomeric forms of molecules. The CML standard lacks software tools for parsing and validating identifiers (and has apparently not been updated since 2012), whilst SMILES and InChI can be cumbersome to use and struggle to reliably and unambiguously identify isotopologues (particularly those of inorganic compounds involving isotopes of hydrogen) and metal hydrides.

In the absence of any concise and easy-to-use convention in widespread use for the description of even simple systems such as atomic ions, where fully word-processed solution is not possible, a range of plain-text notations are used in the scientific literature. For example, the highly-charged tungsten ion conventionally written as W^{63+} is variously

indicated by the strings “W LXIV”, “Na-like W”, “W+63”, “W63+”, “W⁺⁶³”, and “W⁺⁶³”, (the last examples two (ab)using the syntax of LaTeX and HTML).

There are few, standards in use for the description of the internal states of atomic and molecular species. The XSAMS format, initially developed at the IAEA in 2001 and subsequently developed within Virtual Atomic and Molecular Data Centre (VAMDC) Consortium[14] provides a comprehensive XML-based standard for describing atomic and molecular states, but typically requires several nested XML elements per state and is intended to be machine- rather than human-readable. In the absence of any simple standard for the specification of such states, authors in the scientific literature have resorted to images, un-rendered mark-up or verbose description in their titles and article metadata. Some representative examples are given below.

```
Infrared emission spectroscopy of the a $\prime$ 3 $\sigma$ +
 $\pi$ - band of {CS}
```

PAPER

Isotope shifts of the $1s^2 2s 2p(J) - 1s^2 2s^2$ transition energies in Be-like thorium and uranium

Calculations of the High Lying $(2pns)^{(1,3)}P^{\circ}$ and $(2pnd)^{(1,3)}P^{\circ}$ Rydberg States of the Be Atom via the Modified Atomic Orbital Theory

The lack of a easy-to-use standard in this area means that such articles are hard to search for and are not easily transcribed into a bibliography.

1.2 Collisional processes in plasmas

The IAEA published a document in 2003 attempting to classify collisional and other processes and to assign each a recommended 3-letter code for use in databases [15]. This document received input from experts from the IAEA, the US National Institute of Standards and Technology (NIST) and the Controlled Fusion Atomic Data Center (CFADC) at Oak Ridge National Laboratory (ORNL), in Tennessee, US. The standards referred to three main databases, the CFADC database at Oak Ridge, GAPHYOR (“GAZ-PHYsics-ORSay”) at Université Paris-Sud, France, and AMBDAS (“Atomic and Molecular Bibliographic Data System”) at the IAEA. Only the last of these databases is still extant.

The meeting reported here has updated this document and released Version 2.0 of the recommended classifications[16] with the redundant information removed and an extended set of plasma and other processes considered.

[1] <https://www.cas.org/about/cas-content>

[2] <http://www.chemspider.com/>

[3] Access to the Beilstein database is through the Reaxys web-based tool, which is licensed by the Elsevier publishing company <https://www.reaxys.com/>

[4] Based originally on Leopold Gmelin's *Handbook of Inorganic Chemistry*, published in 1817, this database is also now searchable through Reaxys.

[5] Chemical Entities of Biological Interest: <https://www.ebi.ac.uk/chebi/>

[6] Chemical database of bioactive molecules: <https://www.ebi.ac.uk/chembl/>

[7] <https://pubchem.ncbi.nlm.nih.gov/>

[8] The European Community Number: https://echa.europa.eu/documents/10162/23036412/substance_id_en.pdf

[9] UN numbers (United Nations numbers) are four-digit numbers that identify hazardous materials with a focus on their transport: <http://www.unece.org/trans/danger/danger.html>

[10] The CompTox Chemicals Dashboard is an online database maintained by the US Environmental Protection Agency (EPA) for regulatory purposes.

[11] <http://www.xml-cml.org/documentation/index.html>

[12] <https://www.daylight.com/dayhtml/doc/theory/theory.smiles.html>

[13] <https://iupac.org/who-we-are/divisions/division-details/inchi/>

[14] M.-L. Dubernet et al., "The Virtual Atomic and Molecular Data Centre (VAMDC) Consortium for Astrophysics", *Journal of Physics B: Atomic, Molecular and Optical Physics* **49**, 074003 (2016)

[15] D. Humbert, Yu. Ralchenko, P. Krstic, R. E. H. Clark, "Classification of Processes, Version 1.2", Nuclear Data Centre, International Atomic Energy Agency Publication (2003)

[16] Classification of Processes, Version 2.0: <https://amdis.iaea.org/databases/processes>

2. Proceedings

The Meeting was opened by the Head of the Atomic and Molecular Data Unit, C. Hill. After the welcoming address and some administrative formalities, participants introduced

themselves and the Agenda was adopted. As meeting convener, C. Hill outlined the scope and background to the meeting, and described previous relevant publications and standards in the area of atomic and molecular physics.

Grzegorz KARWASZ (Nicolaus Copernicus University, Toruń, Poland) described his research group's work on the production of total and partial electron scattering cross sections for fusion and other applications. The particular difficulty of measuring accurate electronic excitation (as opposed to elastic scattering or ionization) cross sections was highlighted.

Bratislav MARINKOVIĆ (Laboratory for Atomic Collision Processes, Institute of Physics Belgrade, Serbia) gave a detailed account of elastic electron scattering differential cross section data in the Belgrade Electron-Atom/Molecule DataBase (BEAMDB)[1]; the need for a set of standards for codifying atomic and molecular species and states to facilitate interoperability with other databases was emphasised.

Carlo Maria ZWÖLF (Paris Observatory, France), on behalf of colleagues Marie-Lise DUBERNET and Nicolas MOREAU, presented an account of the present status of the Virtual Atomic and Molecular Data Centre[2, 3], an interoperable e-infrastructure providing a portal to query and retrieve atomic and molecular data from around 30 online databases in a standard format, XSAMS. An important recent development is the ability for this portal to archive user queries in a "Query Store" and to deposit the corresponding XSAMS documents in the Zenodo repository[4] operated by CERN, where they can be assigned Digital Object Identifiers (DOIs). The VAMDC have also been working with the Research Data Alliance[5] and Scholix initiative[6] to promote Open Data based on the FAIR principle[7]: that research data should be Findable, Accessible, Interoperable and Reusable.

Sebastian MOHR (Quantemol LTD, UK) described the approach taken by Quantemol and University College London to the production of plasma chemistries: assemblies of plasma reactions (collisional processes) for modelling the behaviours of plasmas of a given composition for industrial and other purposes. The QuantemolDB[8] data model and implementation was outlined, and the internal standards used to specify atomic and molecular species and states described.

Christian ENDRES (Max Planck Institute for Extraterrestrial Physics, Germany) gave an account of the current status of the Cologne Database for Molecular Spectroscopy (CDMS) [9], a catalogue of microwave spectroscopic data used by astrophysicists in research concerning the interstellar medium (ISM) and circumstellar envelopes.

Thomas MARQUART (Uppsala University, Sweden) described the Vienna Atomic Line Database (VALD)[10], a catalogue of data concerning atomic (and diatomic) transitions significantly contributing to absorption in stellar spectra. VALD contains data for a wide variety of atom and ion systems whose electronic states can only be accurately specified using one of several angular momentum coupling schemes (LS-, JJ-, JK-, LK-coupling). The VALD developers have formulated a comprehensive notation for the description of such states[11].

Christian HILL (Atomic and Molecular Data Unit, International Atomic Energy Agency), summarised the Unit's ongoing activities in support of fundamental data for fusion applications and gave illustrative examples of the need for new standards for the description of atomic and molecular species and states in this and other, related fields.

Ludmila MARIAN (Nuclear Data Section, International Atomic Energy Agency) gave an account of the available software tools for conducting Open Science, with a particular focus on those provided by CERN: the Zenodo repository[4], the CERN Document Server (CDS) [12] and reproducible research data analysis with the REANA tool[13].

The meeting then split into two groups to work on the recommendation of standards in (a) collisional processes, with a view to the drafting of version 2.0 of a document classifying such processes; and (b) the description of atomic and molecular species and states. A summary of these recommendations is given in Section 4 of this report.

The remainder of the meeting was spent in discussions reviewing currently-active databases in fundamental atomic and molecular physics, the need and prospects for databases and workflows to promote open data methodologies and exchange. The meeting participants collectively assessed and evaluated a draft of the recommendations to be made, and future work and collaborations were planned.

[1] <http://servo.aob.rs/emol/>

[2] M.-L. Dubernet et al., "The Virtual Atomic and Molecular Data Centre (VAMDC) Consortium for Astrophysics", *Journal of Physics B: Atomic, Molecular and Optical Physics* **49**, 074003 (2016)

[3] <http://www.vamdc.org/>

[4] <https://zenodo.org/>

[5] <https://www.rd-alliance.org/>

[6] <http://www.scholix.org/>

[7] M. D. Wilkinson et al., "The FAIR Guiding Principles for scientific data management and stewardship", *Scientific Data* **3**, 160018 (2016)

[8] <https://quantemoldb.com>

[9] <https://cdms.astro.uni-koeln.de/>

[10] <http://www.astro.uu.se/valdwiki/FrontPage>

[11] <http://www.astro.uu.se/valdwiki/AtomicLevel>

[12] <http://cds.cern.ch/?ln=en>

[13] <http://reanahub.io/>

3. Discussions

3.1 Currently-active data resources for atomic and molecular physics

The following is a non-exhaustive list of databases of fundamental atomic and molecular data for collisional and spectroscopic processes known to be active (that is, currently maintained and updated in the last five years).

ADAMANT

<http://www.adamant.tfai.vu.lt/>

An online, open-access database containing theoretical high-precision spectroscopic parameters and electron/photon interaction with ion parameters for the complex atoms and multicharged ions developed at Vilnius University, Lithuania.

Continuously updated.

ADAS

<http://www.adas.ac.uk/index.php>

The Atomic Data and Analysis Structure (ADAS) is an interconnected set of computer codes and data collections for modelling the radiating properties of ions and atoms in plasmas. Its applications are in plasmas in the interstellar medium, and stellar atmospheres, industrial processes, and experimental thermonuclear fusion devices.

Continuously updated.

ALADDIN

<https://www-amdis.iaea.org/ALADDIN/>

ALADDIN (A Labelled Atomic Data INterface) is a database of evaluated and recommended atomic, molecular and plasma-surface interaction data for fusion applications maintained by the International Atomic Energy Agency.

Continuously updated.

AMBDAS

<https://www-amdis.iaea.org/AMBDAS/>

The Atomic and Molecular Bibliographic Data System (AMBDAS) is a bibliographic database of literature on fundamental atomic and molecular processes for fusion applications maintained by the International Atomic Energy Agency.

Continuously updated.

BASECOL

<https://basecol.vamdc.eu/>

A database devoted to collisional ro-vibrational excitation of molecules by colliders including atoms, ions, molecules, and electrons.

Continuously updated.

BEAMDB

<http://servo.aob.rs/emol/>

Electron interaction cross sections for elastic scattering, electron excitation, ionization and total scattering.

Continuously updated.

CDMS

<https://cdms.astro.uni-koeln.de/>

The Cologne Database for Molecular Spectroscopy is a database of microwave spectroscopic data concerning 900+ species in the interstellar medium (ISM) and circumstellar envelopes.

Continuously updated (2–3 updates per month).

CDSO

<ftp://ftp.iao.ru/pub/CDSO-4000/>

A high-temperature line list for CO₂, produced by the V.E. Zuev Institute of Atmospheric Optics, Tomsk Russia, in 2011: S. A. Tashkun and V. I. Perevalov, *Journal of Quantitative Spectroscopy and Radiative Transfer* **112**, 1403 (2011).

Fixed at the 2011 version, but continues to be available at the IAO FTP site.

CHIANTI

https://www.chiantidatabase.org/chianti_linelist.html

An atomic database for spectroscopic diagnostics of astrophysical plasmas. The supporting Python software library, ChiantiPy (<https://github.com/chianti-atomic/ChiantiPy/>) seems to be actively maintained.

Last updated: 2015 (version 8.0).

ECaSDa, GeCaSDa, MeCaSDa, RuCaSDa, SHeCaSDa, TFMeCaSDa

<http://vamdc.icb.cnrs.fr/PHP/>

A suite of “Calculated Spectroscopic Databases (CaSDa)” for the individual molecules: C₂H₄ (ECaSDa), GeH₄ (GeCaSDa), CH₄ (MeCaSDa), RuO₄ (RuCaSDa), SF₆ (SHeCaSDa), CF₄ (TFMeCaSDa).

Updated as new calculations are completed.

Electron Scattering Cross Sections at UMK

<http://dydaktyka.fizyka.umk.pl/ESCS/index.html>

A database of electron-atom and electron-molecule scattering cross sections maintained by the group of Grzegorz Karwasz at Nicolaus Copernicus University in Toruń (Uniwersytet Mikołaja Kopernika w Toruniu, UMK).

Continuously updated.

ExoMol

<http://exomol.com/>

A database of molecular line lists that can be used for spectral characterisation and simulation of exoplanet and cool star atmospheres. Since some line lists in this collection are extremely large (up to 10^{14} lines), a service to produce absorption cross section data at a user-defined resolution is provided.

Continuously updated.

GEISA

<http://cds-espri.ipsl.upmc.fr/geisa/>

A spectroscopic line list database for atmospheric applications with an interactive interface.

Continuously updated.

Grotrian

<http://grotrian.nsu.ru/en/>

The “Grotrian” Electronic Structure of Atoms Information System is a collection of experimental and theoretical data on energy levels and transitions in atoms and ions with an interactive interface maintained by researchers at Novosibirsk State University in Russia.

Continuously updated.

HITRAN

<https://hitran.org/>

HITRAN (High-resolution TRANsmission) is a compilation of spectroscopic parameters that a variety of computer codes use to predict and simulate the transmission and emission of light in planetary atmospheres.

Continuously updated, with major releases every four years.

IDEADB

<http://ideadb.uibk.ac.at/>

A database of cross sections for dissociative electron attachment to molecules.

Apparently no longer updated, but the web service is still useable.

JPL Molecular Spectroscopy Database

<https://spec.jpl.nasa.gov/ftp/pub/catalog/catform.html>

A companion database to the CDMS catalogue, this is a compilation of rotational transition frequencies and intensities of molecules of astrophysical interest.

Continuously updated.

KIDA

<http://kida.astrophy.u-bordeaux.fr/>

The Kinetic Database for Astrochemistry is a database of kinetic data of interest for astrochemical (interstellar medium and planetary atmospheres) studies.

Continuously updated.

LXCat

https://fr.lxcat.net/data/set_type.php

A database of electron- and ion-scattering cross sections, swarm parameters, reaction rates, energy distribution functions and other data required for modelling low-temperature plasmas initiated in 2010 by researchers at Laboratoire des Plasmas et Conversion d'Énergie (LAPLACE), a laboratory operated jointly by the CNRS, the University of Toulouse and the Institut Polytechnique of Toulouse.

Continuously updated.

Mold

<http://servo.aob.rs/mold/>

A database of photodissociation cross sections with an interactive interface, run by the Institute of Physics Belgrade and Astronomical Observatory Belgrade.

Continuously updated.

NIFS Databases

<https://dbshino.nifs.ac.jp/nifsdb/>

A suite of databases of fundamental atomic and molecular data for fusion applications developed and maintained by the Atomic and Molecular Research Center at the National Institute for Fusion Science, Japan.

Continuously updated.

NIST Atomic Spectra Database (ASD)

https://physics.nist.gov/PhysRefData/ASD/lines_form.html

A database of radiative transitions and energy levels in atoms and atomic ions managed by the US National Institute of Standards and Technology.

Continuously updated.

PEARL

<http://pearl.kaeri.re.kr/pearl/>

The Photonic Electronic Atomic Reaction Library (PEARL) is a database of photoionization/ electron-impact ionization and dielectronic recombination cross sections and rate coefficients maintained by the Atomic Data Center of the Korea Atomic Energy Research Institute (KAERI).

Continuously updated.

QuantemolDB

<https://www.quantemoldb.com/>

A commercial database (with separate licensing terms for academic use) of plasma collisional processes and chemistries for industrial, astrophysical and fusion applications.

Continuously updated.

SPECTR-W³

<http://spectr-w3.snz.ru/index.phtml>

A database of spectroscopic properties of atoms and ions, including ionization potentials, energy levels, transition frequencies and intensities, and collisional data). Managed by the Joint Institute for High Temperatures (JIHT) of the Russian Academy of Sciences (RAS) and the All-Russian Scientific Research Institute Of Technical Physics (VNIITF).

Last updated: since January 2014.

STARK-B

<https://stark-b.obspm.fr/>

A database for "Stark" broadening of isolated lines of atoms and ions in the impact approximation.

Last updated: February 2017.

TipTopbase

<https://tiptopbase.obspm.fr/>

Two databases: TIPbase, containing fine-structure atomic data computed for ions of astrophysical interest; and TOPbase, an online atomic database created as part of the Opacity Project (<http://cdsweb.u-strasbg.fr/topbase/publi.html>).

Last updated: although the database itself may not have been updated for some time (2009?), the data service itself continues to run effectively.

UMIST RATE2012

<http://udfa.ajmarkwick.net/>

The UMIST Database for Astrochemistry contains reaction rate coefficient data for species of astrophysical interest, with a particular emphasis on hydrocarbons and their ions.

Last updated: 2012.

VALD

<http://vald.astro.uu.se/>

The Vienna Atomic Line Database (VALD) is a collection of atomic and molecular transition parameters of astronomical interest. Now identifying as VALD3, it is provided by mirrored servers in Uppsala, Sweden, Vienna, Austria, and Moscow, Russia.

Continuously updated.

3.2 Considerations and scope of the recommended standards

3.2.1 Collisional processes in plasmas

In drafting a update to the “Classification of Processes”, it was noted that of the databases and data services referred to in Version 1.2 (2003) of this document, only the AMBDAS database still exists. Version 2.0 will therefore remove the historical reference to codes used by the CFADC and GAPHYOR databases.

In order to ensure backwards-compatibility, no process code definitions will be changed; where clarity is needed, new codes will be assigned. Older codes no longer recommended will be deprecated but their definitions still listed.

As a general principle, all processes categorised should be associated with a generic example, in which electrons are represented by ‘e-’ and atoms by ‘A’, ‘B’, ‘C’, ...

The recommended classifications will be available at the Atomic and Molecular Data Unit’s website, <https://amdis.iaea.org/databases/> and in the form of a downloadable PDF document. A draft version is presented in Appendix 4 of this report.

3.2.2 Atomic and molecular species and states

The goal of the standards proposed for the description of atomic and molecular species and states at this Meeting is to provide a simple, plain-text based notation for unambiguously identifying atoms and ions, and their isotopes; small molecules, molecular ions, and their isotopologues; and the internal (electronic, vibrational, rotational) states of such species. Because of the wide variety of molecular structures possible for molecules with even a few atoms, “small” is left deliberately undefined: simple structures with many atoms, such as linear hydrocarbons without substituents, may easily be described by the proposed format, the notation may be cumbersome or impossible for cyclic or highly-branched species. The goal of the project is not the comprehensive description of all species, but the practical and

effective description of a large proportion of the species actually considered in plasma science and spectroscopy.

It was noted that any standard proposed in this area has a much better chance of becoming adopted if it is (a) associated with full documentation, including examples; (b) implemented on as many as possible “seed” databases which are widely used by the community; and (c) associated with software tools and libraries (including online applications) to assist in resolving and validating identifiers.

After some discussion, it was decided to build on the existing free, open-source PyValem tool, written in the Python programming language to define a vocabulary and grammar that can be used to specify species and states within the domain of interest here. A draft version of the PyValem tool, describing the syntax used is presented in Appendix 5 of this report; the document available at <https://amdis.iaea.org/databases/> should be considered normative.

3.3 Miscellaneous comments

- The FOSTER Plus initiative[1], a two-year European Union-funded project to promote Open Science in research was noted.
- The following conferences to be held in 2020 were identified as relevant events at which to connect with communities likely to find the proposed standards useful:
 - ASA-HITRAN 2020[2]
 - International Symposium on the Physics of Ionized Gases (SPIG-2020)[3]
 - International Conference on Matter and Radiation at Extremes (ICMRE 2020)[4]
 - International Conference on the Physics of Highly Charged Ions (HCI-2020)[5]
- The standards are seen as complementary to the existing XML-based XSAMS format: the XSAMS Schema can be extended to include new collisional process codes and the “OrdinaryStructuralFormula” element is the obvious location for strings conforming to the standardised description of atomic and molecular species.
- It was noted that by creating standardised descriptive strings from existing XSAMS documents (including those deposited with the Zenodo repository), a database connecting publications (identified by DOI) with species (identified by standardised strings) could be constructed.
- The project to write a draft “manifesto” on Open Data principles initiated by the Open Data Libraries Workshop at the IEEE Nuclear and Plasma Sciences Society’s Nuclear Science Symposium (NSS) and Medical Imaging Conference (MIC), held in Manchester, UK on 27 October 2019 was noted. This document is likely to focus on nuclear physics and at the time of writing is at a relatively early stage of preparation.

- [1] <https://www.fosteropenscience.eu/>
- [2] To be held in Reims, France, 26 – 28 August 2020: <https://www.univ-reims.fr/asa-hitran/home/asa-hitran-2020,18642,32042.html>
- [3] To be held in Šabac, Serbia, 24 – 28 August 2020: <http://www.spig2020.ipb.ac.rs/>
- [4] To be held in Xi'an, China, August 2020
- [5] To be held in Matsue, Japan, 7 – 11 September 2020: <http://yebisu.ils.uec.ac.jp/hci2020/>

4. Summary and Recommendations

A draft document, version 2.0 of the “Classification of Processes” publication will be circulated amongst the meeting participants and subsequently to the broader plasma physics community, including members of the Data Centres Network[1].

The new classification codes will be incorporated into the next release of the ALADDIN and AMBDAS databases at the IAEA[2, 3].

After review by the VAMDC Consortium, the new process codes may be incorporated into the XSAMS Schema, and used in the VAMDC Species Store[4].

The recommended standards for describing atomic and molecular species and states will be described in a separate document, to be placed on the AMD Unit’s website at <https://amdis.iaea.org/databases/> and an online service parsing and validating standardised strings will be implemented at a suitable location on the same server.

Subject to review and, potentially, modification or extension of the standards, the notation may be used on the VALD, CDMS, BASECOL, and BEAMDB databases, with a view to demonstrating its usage for further database services.

- [1] <https://amdis.iaea.org/DCN/>
- [2] <https://amdis.iaea.org/ALADDIN/>
- [3] <https://amdis.iaea.org/AMBDAS/>
- [4] <https://species.vamdc.eu/>

Appendix 1: Participants

Marie-Lise DUBERNET, Observatoire de Paris, 61 Avenue de L'Observatoire, 75014
PARIS, FRANCE

Christian ENDRES, Max Planck Institute for Extraterrestrial Physics, Gießenbachstrasse 1, 85748 GARCHING, GERMANY

Kalle HEINOLA, IAEA Division of Physical and Chemical Sciences, Nuclear Data Section, Vienna International Centre, A-1400 VIENNA, AUSTRIA

Christian HILL, IAEA Division of Physical and Chemical Sciences, Nuclear Data Section, Vienna International Centre, A-1400 VIENNA, AUSTRIA

Grzegorz KARWASZ, University Nicolaus Copernicus, Institute of Physics, ul. Grudziadzka 5-7, 87100 TORUN, POLAND

Ludmila MARIAN, IAEA Division of Physical and Chemical Sciences, Nuclear Data Section, Vienna International Centre, A-1400 VIENNA, AUSTRIA

Bratislav MARINKOVIĆ, Laboratory for Atomic Collision Processes, Institute of Physics Belgrade, 11080 BELGRADE, SERBIA

Thomas MARQUART, Department of Physics and Astronomy, Uppsala University, Box 516, 75120 UPPSALA, SWEDEN

Sebastian MOHR, Quantemol LTD, 320 Angel, 320 City Road, EC1V 2NZ LONDON, UK

Carlo Maria ZWÖLF, Observatoire de Paris, 61 Avenue de L'Observatoire, 75014 PARIS, FRANCE

Appendix 2: Meeting Agenda

Wednesday, 27 November 2019

09:30 – 10:00 **Christian HILL** and **Kalle HEINOLA**: Welcome, introduction of the participants, adoption of the agenda

Session 1: Collisional Processes

Chair: Christian HILL

10:00 – 10:25 **Grzegorz KARWASZ**, *Nicolaus Copernicus University, Toruń, Poland*
Total and partial cross sections for electron scattering on atoms and molecules

10:25 – 10:50 **Bratislav MARINKOVIĆ**, *Laboratory for Atomic Collision Processes, Institute of Physics Belgrade, Serbia*
Elastic electron scattering by atomic particles and cross section representation in the Belgrade Electron-Atom/Molecule DataBase: BEAMDB

10:50 – 11:20 Coffee Break

11:20 – 12:10 **Marie-Lise DUBERNET**, *Paris Observatory, France*

12:10 – 12:35 **Sebastian MOHR**, *Quantemol LTD, United Kingdom*
Quantemol-DB: A species and reaction database for plasma applications

12:35 – 14:00 Lunch

Session 2: Atomic and Molecular Spectroscopy

Chair: Marie-Lise DUBERNET

14:00 – 14:30 **Christian ENDRES**, *Max Planck Institute for Extraterrestrial Physics, Germany*
The Cologne Database for Molecular Spectroscopy, CDMS: spectroscopic data for Astrochemists and Astrophysicists

14:30 – 15:00 **Thomas MARQUART**, *Uppsala University, Sweden*

15:00 – 15:30 Coffee Break

Session 3: Databases and Data Services at the IAEA

Chair: Kalle HEINOLA

15:30 – 17:00 **Christian HILL**, *IAEA, Austria*
Data activities of the Atomic and Molecular Data Unit

Thursday, 28 November 2019

Session 4: Databases and Data Services at the IAEA

Chair: Kalle HEINOLA

09:00 – 09:25 **Ludmila MARIAN**, *IAEA, Austria*
Open Science Tools

Session 5: Discussion: Atomic and Molecular Species and States

09:25 – 11:00 Discussion (all): Recommendations for identifying, classifying and representing atoms, molecules, ions and their states

11:00 – 11:30 Coffee Break

11:30 – 12:30 Discussion (all): Surfaces and plasma-surface interactions: description and representation

12:30 – 14:00 Lunch

Session 6: Discussion: Collisional Process Description and Classification

14:00 – 15:30 Discussion (all): Recommendations for classifying and exemplifying collisional processes

15:30 – 16:00 Coffee Break

16:00 – 17:30 Drafting of recommendations report; summary of discussions

19:00 – 21:30 Social Dinner

Friday, 29 November 2019

Session 7: Discussion: Database Implementation, Maintenance and Interoperability

- 09:00 – 11:00 Discussion (all): Structures for storage and querying of atomic and molecular data; Database implementations and sustainability
- 11:00 – 11:30 Coffee Break
- 11:30 – 13:00 Discussion (all): Facilitating interoperability between databases; Software tools for comparison and interconversion between data formats; Units
- 13:00 – 14:00 Lunch

Session 8: Discussion: Recommendations and Draft Report

- 14:00 – 16:00 Drafting of recommendations report; Summary of meeting
- 16:00 – 16:30 Concluding remarks; Close of meeting

Appendix 3: Abstracts

From Species to publications by going through data: the VAMDC species database and Query Store

*Marie-Lise DUBERNET, Carlo Maria ZWOLF and Nicolas MOREAU
Paris Observatory, France*

After recalling the functioning of the VAMDC species database and the Query Store, we will highlight the related main features of these services and will sketch possible future development for directly link species to publications.

The Cologne Database for Molecular Spectroscopy, CDMS: spectroscopic data for Astrochemists and Astrophysicists

Christian P. Endres

Max Planck Institute for Extraterrestrial Physics, Germany

The interpretation and analysis of astronomical observations crucially depends on the knowledge and availability of accurate rest frequencies and intensity information. Such information is usually generated from laboratory data for rest frequencies and complemented by quantum chemical calculations for intensity information.

The CDMS was founded in the year 1998 to provide such information for atoms and molecules of astrophysical and atmospheric interest to the astronomical and spectroscopical community in a standardized way. At present, the catalog covers mostly rotational transitions from the radio-frequency to the terahertz region and lower mid-infrared region. Its entries, together with those in the JPL catalog, cover a large fraction of more than 200 molecules detected in the interstellar medium (ISM) or in circumstellar envelopes (CSEs) of late type stars. Both databases are accessible through the Virtual Atomic and Molecular Data Centre.

Radio astronomical spectra are often analyzed under the assumption of local thermodynamic equilibrium (LTE), but deviations from LTE may be considerable at lower temperatures, especially in the diffuse ISM. In these cases it is often necessary to take into account collisional processes with H₂, He and/or with H and electrons. This task, to access and combine spectroscopic data together with collisional data, has been greatly simplified thanks to the infrastructure and tools developed by VAMDC.

Total and partial cross sections for electron scattering on atoms and molecules

Grzegorz Karwasz

Nicolaus Copernicus University, Institute of Physics, 87100 Toruń, Poland

Total and partial cross sections for electron scattering on atoms and molecules will be presented in a possibly wide (0.001 – 1000 eV) energy range. Total scattering and elastic cross sections are based mainly on experimental data, corrected whenever some systematical errors related to a specific technique used are suspected. Ionization total and partial cross sections are based on experiments; ionization total are further checked against Born-Bethe binary-encounter model [1]. Data for electronic excitation are poor: experiments may suffer from incorrect attribution of states and from normalization errors: the case of H₂O and N₂O will be discussed. For CH₄ the theory (R-matrix) will be shown. Vibrational excitation have little direct experiments but one can deduce cross sections from Born approximation and (in resonances) from differences between total and elastic. Rotational will be based on R-matrix calculations. Comprehensive sets of data will be shown [2].

[1] G.P. Karwasz, P. Możejko, Mi-Young Song, “Electron-impact ionization of fluoromethanes – review of experiments and binary-encounter models”, *Int. J. Mass Spectrom.*, **365/366** (2014) 232-237.

[2] M-Y. Song, J. Yoon, H. Cho, G. Karwasz, V. Kokoouline, Y. Nakamura, J. R. Hamilton, and J. Tennyson, “Cross Sections for Electron Collisions with NF₃”, *Journal of Physical and Chemical Reference Data* **46** (2017) 043104.

Elastic electron scattering by atomic particles and cross section representation in the Belgrade Electron-Atom/Molecule DataBase -BEAMDB

Bratislav P. Marinković

Laboratory for Atomic Collision Processes, Institute of Physics Belgrade, Serbia

Elastic electron scattering by an atomic particle (atom/molecule/ion) we define as a scattering process that conserves the kinetic energy of the colliding particles. Elastic cross sections are usually measured for unpolarised beams of electrons and atomic particles at specific energies and angles and they are defined as differential cross sections (DCS). DCS represents the ratio between number of scattered particles in unit time and unit solid angle and the incoming current density. In the crossed-beam scattering experiments DCSs are determined through a rather complex expression involving geometrical and instrumental functions, averaging over the angular and energy resolution [1]. In the Belgrade Laboratory for Atomic Collisional Processes, many data have been experimentally obtained on electron scattering cross section for metal atomic particles (see for e.g. [2,3]) or data for reference gases (such as Ar [4]). Such type of collisional data, among the other (excitation, ionization, etc. cross sections), are presented in the Belgrade Electron-Atom/Molecule DataBase (BEAMDB) [5]. Representing the atomic/molecular states as a single string data within the current database, we faced with certain challenges that need to be overcome by codifying a set of standards.

[1] R T Brinkmann and S Trajmar, “Effective path length corrections in beam-beam scattering experiments”, *J. Phys. E: Sci. Instrum.*, **14** (1981) 245-255.

[2] B. P. Marinković, V. Pejčev, D. M. Filipović, D. Šević, S. Milisavljević, B. Predojević, “Electron collisions by metal atom vapours”, *Rad. Phys. Chem.* **76** (2007) 455-460.

[3] B. P. Marinković, R. Panajotović, D. Šević, R. P. McEachran, G. García, F. Blanco, and M. J. Brunger, “Experimental and theoretical cross sections for elastic electron scattering from zinc”, *Phys. Rev. A* **99** (2019) 062702.

[4] M. Lj. Ranković, J. B. Maljković, K. Tökési, and B. P. Marinković, “Elastic electron differential cross sections for argon atom in the intermediate energy range from 40 eV to 300 eV”, *Eur. Phys. J.D* **72** (2018) 30.

[5] B. P. Marinković, V. A. Srečković, V. Vujčić, S. Ivanović, N. Uskoković, M. Nešić, Lj. M. Ignjatović, D. Jevremović, M. S. Dimitrijević, and N. J. Mason, “BEAMDB and MOLD – Databases at the Serbian Virtual Observatory for collisional and radiative processes”, *Atoms*, **7** (2019) 11.

Quantemol-DB: A species and reaction database for plasma applications

*Sebastian Mohr,
Quantemol LTD, UK*

The importance of computer simulations for the understanding of plasmas and the design of reactions is ever growing. However, accurate results can only be obtained with detailed knowledge about the chemical reactions both between electrons and heavy particles and between different heavy particles. This information is often scattered over several publications, so assembling a chemistry set for a given problem is an arduous task. To assist with a fast assembly of reaction sets from reliable sources, Quantemol started the Quantemol-DB project, an online database of species and reactions related to plasma applications.

The Quantemol-DB comprises a large collection of species and reactions along with either cross sections or reaction rate coefficients. It is currently primarily aimed at low temperature plasma applications but can easily be extended to other fields such as fusion plasmas. The database is complemented by some additional functionalities such as pre-assembled chemistry sets and a tool to assemble custom chemistry sets from the database. The assembled data can be downloaded in formats compatible with common simulation programmes such as COMSOL.

This presentation will give an overview over the underlying data model, with an emphasis on the classification of excited species and reactions, and a demonstration of the website interface.

Appendix 4: Classification of Processes in Plasma Physics (Draft Version 2.0)

Electron-Heavy Particle Interactions

EAE	Auger Electron Ejection	Electron-impact induced Auger electron ejection	$e^- + A \rightarrow A^{***} + 2e^-$; $A^{***} \rightarrow A^{*2+} + e^-$
EAS	Angular Scattering	Differential electron-scattering cross sections, usually as a function of energy and angle.	
EBS	Bremsstrahlung	The emission of electromagnetic radiation by a charged particle as it is decelerated through Coulomb interactions with other charges; "free-free" radiation in the context of plasma physics.	$e^- + A \rightarrow e^- + A + h\nu$
EDA	Dissociative Attachment	Dissociative attachment	$e^- + AB \rightarrow A + B^-$
EDC	Dielectronic Capture	Dielectronic capture	$e^- + A^+ \rightarrow A^{**}$
EDE	Dissociative Excitation	Electron-impact dissociative excitation	$e^- + AB \rightarrow A^* + B + e^-$
EDI	Dissociative Ionization	Electron-impact dissociative ionization	$e^- + AB \rightarrow A^+ + B + 2e^-$
EDP	Depolarization, Change of Polarization	Electron-impact change of polarization, including depolarization	
EDR	Dissociative Recombination	Electron-impact dissociative recombination	$e^- + AB^+ \rightarrow A + B$
EDS	Dissociation	Electron-impact dissociation	$e^- + AB \rightarrow A + B + e^-$
EDT	Electron Detachment	Electron-impact detachment	$e^- + A^- \rightarrow A + 2e^-$
EDX	De-excitation	Generic inelastic collisional processes in which a scattered electron gains energy from the target particle.	$e^- + A^* \rightarrow e^- + A$
EEL	Elastic Scattering	Scattering of an electron with no change in energy.	$e^- + A \rightarrow e^- + A$
EEX	Excitation	Electron-impact excitation	$e^- + A \rightarrow e^- + A^*$
EEX	Change of Excitation	Electron-impact change of excitation. <i>Deprecated: Use EEX: Excitation or EDX: De-excitation instead.</i>	$e^- + A^* \rightarrow e^- + A^{**}$
EFL	Fluorescence (Optical Emission)	Total optical emission following electron-impact events	
EGN	General	General electron-impact processes that do not fall into any more specific category.	
EHT	Transport	Transport cross sections: momentum, viscosity and higher-order.	

EIN	Ionization	Electron impact ionization	$e^- + A \rightarrow A^+ + 2e^-$
EIP	Ion-Pair Formation	Electron-impact induced formation of a (positive, negative) ion pair	$e^- + AB^+ \rightarrow A^+ + B^-$
ELB	Line Broadening, Shapes and Shifts	Data relating to the line shapes and positions of radiative transitions	
EMI	Multiple Ionization	Electron-impact ionization to a charge state greater than +1	$e^- + A \rightarrow A^{n+} + (n+1)e^-$
EMT	Momentum Transfer	Electron impact momentum transfer	
ENI	Negative Ion Formation	Electron-impact formation of negative ion (attachment)	$e^- + A \rightarrow A^-$
ERC	Recombination	Electron-impact recombination	$e^- + A^{n+} \rightarrow A^{(n-1)+}$
ERD	Dielectronic Recombination	Electron-impact dielectronic recombination	$e^- + A^+ \rightarrow A^{**} \rightarrow A^* + h\nu$
ERO	Electron-Ion-Other Recombination	Electron-ion recombination involving a third body other than an electron	$e^- + A^+ + B \rightarrow A + B$
ERR	Radiative Recombination	Electron-impact recombination with radiative emission	$e^- + A^+ \rightarrow A + h\nu$
ERT	Three-Body Recombination	Electron-impact three-body recombination	$e^- + e^- + A^+ \rightarrow A + e^-$
ERV	Rovibrational Excitation	Electron-impact rovibrational excitation	$e^- + AB \rightarrow e^- + AB$ ($v=*; J=*$)
ESF	Spin-Flip	Electron-impact change of spin state	$e^- + [S]A \rightarrow e^- + [S']A$
ETS	Total Scattering	Total electron scattering cross sections	
EUP	Unknown Products	Electron-impact collision with unknown products. <i>Deprecated: use EGN (General) instead.</i>	
EXE	Electronic Excitation	Electron-impact electronic excitation	$e^- + AB \rightarrow e^- + AB^*$
EXR	Rotational Excitation	Electron-impact rotational excitation	$e^- + AB \rightarrow e^- + AB$ ($J=*$)
EXV	Vibrational Excitation	Electron-impact vibrational excitation	$e^- + AB \rightarrow e^- + AB$ ($v=*$)

Photon-Particle and Field-Particle Interactions

PAD	Scattering	Photon scattering (angular diffusion)	
PAE	Auger Electron Ejection	Photon-induced Auger electron ejection	$A + h\nu \rightarrow A^{***} + e^-$; $A^{***} \rightarrow A^{*2+} + e^-$
PCS	Compton Scattering	Inelastic scattering of a photon by a charged particle that decreases the photon energy.	
PDP	Depolarization, Change of Polarization	Photon-induced change of polarization, including depolarization	

PDS	Photodissociation	Photodissociation of a molecule	$h\nu + AB \rightarrow A + B$
PDT	Photodetachment	Absorption of a photon inducing the removal of an electron from an anion to form a neutral species.	$h\nu + A^- \rightarrow A + e^-$
PEA	Effective Absorption, Total Diffusion	Effective Absorption, Total Diffusion of photons	
PED	Elastic Diffusion	Photon elastic diffusion processes (Thomson scattering, Rayleigh scattering)	
PES	Elastic Scattering	Scattering of a photon with no change in energy.	$h\nu + A \rightarrow h\nu + A$
PEX	Photoexcitation	Photon absorption leading to excitation	$h\nu + A \rightarrow A^*$
PPF	Inverse Bremsstrahlung	Acceleration of a charged particle by a photon absorption process mediated by an electron-particle Coulomb interaction; "free-free absorption" in the context of plasma physics.	$e^- + A + h\nu \rightarrow A + e^-$
PFL	Fluorescence	Fluorescence	$A^* \rightarrow A + h\nu$
PGF	General Electromagnetic Field	Miscellaneous effects induced by an electromagnetic field	
PGN	General	General photon-particle interaction processes which do not fall into any more specific category	
PIN	Photoionization	Photon-induced ionization	$h\nu + A \rightarrow A^+ + e^-$
PIP	Ion-Pair Formation	Photon-induced formation of a (positive, negative) ion pair	$AB + h\nu \rightarrow A^+ + B^-$
PMA	Multiphoton Excitation	Absorption of more than one photon, leaving to excited and/or charged products	$n h\nu + A \rightarrow A^+/A^*/A^{*+}$
PNL	Non-Linear Effects	Non-linear radiative effects	
PRV	Rovibrational Excitation	Photon-induced rovibrational excitation	$BC + h\nu \rightarrow BC$ ($v=*$; $J=*$)
PSE	Stark Effect	Spectral line-splitting caused by an external electric field	
PTA	True Absorption	True Absorption of a photon	
PTF	Interaction with Time-Varying Fields	General interactions with time-varying fields	
PTS	Total Absorption, Total Scattering	Total photon absorption or scattering cross sections.	
PXE	Electronic Excitation	Photon-induced electronic excitation	$BC + h\nu \rightarrow BC^*$
PXR	Rotational Excitation	Photon-induced rotational excitation	$BC + h\nu \rightarrow BC$ ($J=*$)

PXV	Vibrational Excitation	Photon-induced vibrational excitation	$BC + h\nu \rightarrow BC$ ($v=*$)
PZE	Zeeman Effect	Spectral line-splitting caused by a static magnetic field	

Heavy Particle-Heavy Particle Interactions

HAS	Association	Heavy-particle collision leading to association (i.e. bond formation)	$A + B \rightarrow AB$
HAS	Angular Scattering	Heavy-particle differential scattering cross sections, usually as a function of energy and angle.	
HAT	Attenuation	Attenuation	
HCX	Charge Transfer	Heavy-particle impact leading to charge-transfer.	$A^+ + B \rightarrow A + B^+$; $A^- + B \rightarrow A + B^-$
HDC	Dissociative Charge Transfer	Heavy-particle dissociative charge transfer	$A^+ + BC \rightarrow A + B^+ + C$
HDS	Dissociation	Heavy-particle impact leading to dissociation (bond-breaking)	$A + BC \rightarrow A + B + C$
HDT	Detachment	Heavy-particle collisions leading to electronic detachment.	$A + B^- \rightarrow A + B + e^-$
HDX	De-excitation	Heavy-particle impact leading to de-excitation (decrease of total internal energy).	$A^* + B \rightarrow A + B$
HEL	Inelastic Energy Losses	Heavy-particle collisions leading to inelastic energy loss.	
HES	Elastic Scattering	Scattering of heavy particles with no change in energy.	$A + B \rightarrow A + B$
HET	Energy Transfer	Heavy-particle collisions with energy transfer between the particles.	
HEX	Excitation	Heavy-particle impact leading to excitation (increase of total internal energy).	$A + B \rightarrow A^* + B$
HFL	Fluorescence	Heavy particle collisional excitation followed by radiative decay.	$A + B \rightarrow A^* + B$; $A^* \rightarrow A + h\nu$
HGN	General	General heavy-particle collisional processes which do not fall into any more specific category	
HIN	Ionization	Heavy-particle collisions leading to ionization	$A + B \rightarrow A + B^+ + e^-$
HIP	Interaction Potentials	Interaction potentials between heavy particles.	
HIR	Interchange Reactions	Heavy-particle interchange reactions	$A + BC \rightarrow AB + C$

HLB	Line Broadening, Shapes and Shifts	Data relating to line shapes and positions determined by heavy-particle collisions.	
HMN	Mutual Ion-Ion Neutralization	Neutralization of heavy-particle ions.	$A^+ + B^- \rightarrow A + B$
HPN	Penning Ionization	Ionization through collision of an internally-excited heavy-particle with another heavy particle.	$A^* + B \rightarrow A + B^+ + e^-$
HRC	Recombination	Heavy-particle collisions with recombination	
HRV	Rovibrational Excitation	Heavy particle impact rovibrational excitation	$A + BC \rightarrow A + BC$ ($v=*; J=*$)
HST	Electron-Stripping	Ionization of the projectile in a heavy-particle collision.	$A + B \rightarrow A^+ + B + e^-$
HTI	Transfer Ionization	Transfer of an electron from an atom to an ion, followed by further ionization.	$A + B^+ \rightarrow A^{2+} + B + e^-$
HTS	Total Scattering	Total heavy particle scattering cross sections	
HUP	Unknown Products	Heavy-particle collisions/reactions with unknown products.	$A + B \rightarrow ?$
HXE	Electronic Excitation	Heavy particle impact electronic excitation	$A + BC \rightarrow A + BC^*$
HXF	Fine-Level Excitation	Heavy particle impact fine-level excitation	$A + B \rightarrow A + B$ ($J=*$)
HXH	Hyperfine Excitation	Heavy particle impact hyperfine-level excitation	$e^- + AB \rightarrow e^- + AB$ ($F=*$)
HXR	Rotational Excitation	Heavy particle impact rotational excitation	$A + BC \rightarrow A + BC$ ($J=*$)
HXT	Excitation Transfer	Transfer of internal excitation in a heavy-particle collision.	$A^* + B \rightarrow A + B^*$
HXV	Vibrational Excitation	Heavy particle impact vibrational excitation	$A + BC \rightarrow A + BC$ ($v=*$)

Structure and Spectra

SAD	Autodetachment	Autodetachment in atoms and molecules
SAI	Autoionization	Autoionization processes in atoms and molecules.
SDP	Dynamic Polarizability	Dynamic polarizability of atoms and molecules
SDS	Autodissociation	Autodissociation in atoms and molecules
SEW	Energy Levels and Wavelengths	Energy levels and transition frequencies / wavelengths of atoms and molecules.
SFT	Forbidden Transitions	Forbidden transitions in atoms and molecules
SGN	General	General spectral processes and structural properties that do not fall into any more specific category
SHF	Hyperfine Structure	Hyperfine structure of atoms and molecules

SIA	Interatomic Potentials	Interatomic Potentials as they relate to the spectral or structural properties of atoms or molecules.
SIE	Isoelectronic sequences	Isoelectronic sequences of atoms
SIP	Ionization Potentials	Ionization potentials of atoms and molecules.
SIR	Infrared Spectra	Infrared spectra of atoms and molecules
SLS	Line Broadening, Shapes and Shifts	Data relating to line shapes and positions with a focus on spectroscopy or atomic/molecular structure.
SMM	Magnetic Moments	Magnetic moments (dipolar, quadrupolar, etc.) of atoms and molecules.
SPM	Polarizabilities, Electric Moments	Polarizabilities and electric moments (dipolar, quadrupolar, etc.) of atoms and molecules.
SQE	QED Effects	QED effects in atoms and molecules
SRA	Raman spectroscopy	Raman spectroscopy of atoms and molecules.
SRP	Relaxation Processes	Relaxation processes in atoms and molecules.
SRS	Rotational Spectra	Rotational spectra of molecules
SRY	Rydberg States	Rydberg states of atoms and molecules.
SSM	Potential Curves and Structure of Molecules	Potential energy curves/surfaces and molecular structure data.
STP	Transition Probabilities and Oscillator Strengths	Transition probabilities (Einstein A-factors), oscillator strengths and line intensities of radiative transitions in atoms and molecules.
SUV	UV/VUV/XUV Spectra	UV spectra of atoms and molecules from ~10 nm (extreme ultraviolet) to ~400 nm (near ultraviolet).
SVS	Visible Spectra	Visible spectra of atoms and molecules
SVS	Vibrational Spectra	Vibrational spectra of molecules
SXR	X-Ray Spectra	X-Ray spectra of atoms and molecules

Particle-Matter Interactions

MAC	Accommodation	Accommodation
MA D	Adsorption	Adsorption on a surface
MBS	Backscattering	Backscattering from a surface
MCP	Charge State Population	Charge state population of condensed materials.
MCR	Chemical Reactions	Chemical reactions at a surface
MCS	Chemical Sputtering	Chemical sputtering of surfaces.
MDE	Desorption	Desorption from a surface.
MDP	Deposition	Deposition on a surface.
MEL	Energy Loss and Stopping Power	Energy loss and stopping power of materials with respect to a flux of particles.

MEP	Excited State Population	Excited state population of condensed materials.
MER	Erosion	Erosion of a surface (over a longer timescale than sputtering)
MGN	General	General particle-matter interaction processes that do not fall into any more specific category.
MIR	Particle-Impact Induced Radiation	Radiation induced by particle impact on surfaces.
MM S	Multiple Scattering	Multiple scattering of particles within a material.
MNE	Neutralization, Ionization, Dissociation	Neutralization, ionization or dissociation at a surface.
MPE	Photoelectric Ejection of Electrons	Ejection of electrons due to incoming radiation (the photoelectric effect).
MP M	Permeation	Permeation of particles through a solid
MPR	Particle Range	Data relating to the particle transmission through a material.
MPS	Physical Sputtering	Physical sputtering of surfaces.
MRE	Reemission	Re-emission of accommodated particles at a surface
MRF	Reflection	Reflection of particles from a surface.
MRH	Reflection of Heavy Particles from Surfaces	Reflection of heavy particles from surfaces
MRL	Reflection of Electrons from Surfaces	Reflection of electrons from surfaces
MRS	Radiation-Enhanced Sublimation	Radiation-enhanced sublimation of solids.
MSD	Surface Damage	Surface damage of a surface due to impinging particles over a short timescale.
MSE	Secondary Electron Emission	Secondary electron emission from a surface.
MSI	Surface Interactions	Interactions at surfaces.
MSP	Sputtering	Sputtering of surface material by impinging particles
MTD	Trapping, Detrapping	Trapping and detrapping of accommodated particles in a solid.
MTR	Transmutation	Transmutation of nuclei in solid material by impact of subatomic particles.
MVP	Vapour Formation and Properties	Formation and properties of vapour in front of a surface; in the context of plasma physics, vapour shielding phenomena.

Data Compilations

DEH	Electron-Heavy Particle Interactions	Data compilations concerning electron-heavy particle interactions.
DGN	General	General data compilations that do not fall into any more specific category.

DHH	Heavy Particle-Heavy Particle Interactions	Data compilations concerning heavy particle-heavy particle interactions.
DPF	Photon-Particle and Field-Particle Interactions	Data compilations concerning photon-particle and field-particle interactions.
DPM	Particle-Matter Interactions	Data compilations concerning particle-matter interactions.
DSS	Structure and Spectra	Data compilations concerning atomic and molecular structure and spectra.
DTP	Transport Properties	Data compilations concerning transport properties.

Bibliographic Resources

BEH	Electron-Heavy Particle Interactions	Bibliographic data resources concerning electron-heavy particle interactions.
BGN	General	General bibliographic data resources that do not fall into any more specific category.
BHH	Heavy Particle-Heavy Particle Interactions	Bibliographic data resources concerning heavy particle-heavy particle interactions.
BPF	Photon-Particle and Field-Particle Interactions	Bibliographic data resources concerning photon-particle and field-particle interactions.
BSS	Structure and Spectra	Bibliographic data resources concerning atomic and molecular structure and spectra.
BTP	Transport Properties	Bibliographic data resources concerning transport properties.

Appendix 5: Draft Standards for the Representation of Atomic and Molecular Species and States in Databases

pyvalem

Release 2.0

Christian Hill

Mar 25, 2020

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INTRODUCTION TO PYVALEM

PyValem is a Python package for parsing, validating, manipulating and interpreting the chemical formulas, quantum states and labels of atoms, ions and small molecules.

Species and states are specified as strings using a simple and flexible syntax, and may be compared, output in different formats and manipulated using a variety of predefined Python methods.

1.1 Installation

For now:

```
python setup.py install
```

1.2 Examples

The basic (state-less) chemical formula class is `Formula`. A `Formula` object can be created by passing its constructor a valid string. This object contains attributes for producing its plain text, HTML and LaTeX representations, and for calculating its molar mass:

```
In [1]: from pyvalem.formula import Formula

In [2]: f = Formula('C2H5OH')

In [3]: print(f)
C2H5OH

In [4]: print(f.html)
C<sub>2</sub>H<sub>5</sub>OH

In [5]: print(f.latex)
 $\mathrm{C}_2\mathrm{H}_5\mathrm{O}\mathrm{H}$ 

In [6]: print(f.rmm)      # g.mol-1
46.069
```

Note that there is no underscore character (`_`) before between the element symbol and its stoichiometry. Isotopes are specified with the mass number placed before the element symbol, with both surrounded by parentheses. Do not use a caret (`^`) to indicate a superscript:

```
In [7]: f = Formula('(14C)')

In [8]: print(f.html)
<sup>14</sup>C

In [9]: print(f.rmm)
14.0032419884

In [10]: f = Formula('H2(18O)')

In [11]: print(f.rmm)
20.015159612799998
```

For isotopically-pure compounds, the mass returned is the atomic mass.

Charges are specified as +n or -n, where n may be omitted if it is 1. Do not use a caret (^) to indicate a superscript:

```
In [12]: f = Formula('H3O+')
In [13]: print(f.charge)
1

In [14]: print(f.html)
H<sub>3</sub>O<sup>+</sup>

In [15]: f = Formula('Co(H2O)6+2')
In [16]: print(f.charge)
2

In [17]: print(f.html)
Co(H<sub>2</sub>O)<sub>6</sub><sup>2+</sup>
```

“Stateful” species are formulas which consist of a valid Formula string, followed by whitespace, followed by a semicolon-delimited sequence of valid quantum state or label specifications. Stateful species know which states they possess and can render these states in different ways. For example:

```
In [18]: from pyvalem.stateful_species import StatefulSpecies
In [19]: ss1 = StatefulSpecies('Ne+ 1s2.2s2.2p5; 2P_1/2')
In [20]: ss1.states
Out[21]: [1s2.2s2.2p5, 2P_1/2]

In [22]: ss1.states[1].__class__
Out[22]: pyvalem.atomic_term_symbol.AtomicTermSymbol

In [23]: ss1.html
Out[23]: 'Ne<sup>+</sup> 1s<sup>2</sup>2s<sup>2</sup>2p<sup>5</sup>; <sup>2</sup>P<sub>1/2</sub>'
```

This HTML renders as:

Ne⁺ 1s²2s²2p⁵; ²P_{1/2}

Another example:

```
In [24]: ss2 = StatefulSpecies('(52Cr) (1H) 1σ2.2σ1.1δ2.1π2; 6Σ+; v=0; J=2')
In [25]: ss2.html
<sup>52</sup>Cr<sup>1</sup>H 1σ<sup>2</sup>.2σ<sup>1</sup>.1δ<sup>2</sup>.1π<sup>2</sup><sup>+</sup>; <sup>6</sup>Σ<sup>+</sup>; v=0; J=2
```

which produces:

$^{52}\text{Cr}^1\text{H } 1\sigma^2.2\sigma^1.1\delta^2.1\pi^2; {}^6\Sigma^+; v = 0; J = 2$

The syntax for writing different types of quantum state are described in later pages of this documentation.

FORMULA

A `Formula` object instance represents the chemical formula of an atom, isotope, ion, molecule, molecular ion, or certain sorts of other particle. The `Formula` class has methods for producing representations of the formula in HTML, LaTeX and plain text.

`Formula` objects are not supposed to be unique (different `Formula` objects can represent the same formula); nor is their syntax or this library designed to be applied to large or complex molecules. `PyValem` is intended as a lightweight, easy-to-use library with an expressive syntax for representing many common small atoms and molecules and their isotopes, states and reactions.

Furthermore, whilst some validation functionality is built into the library, `PyValem` does not attempt to verify that a provided formula is chemically plausible. In particular, it knows nothing about valence or oxidation state.

2.1 Instantiation

A `Formula` object may be instantiated by passing a valid string, conforming to the following grammar:

- Single atoms, with atomic weights given by a default natural isotopic abundance are specified with their element symbol, e.g. `H`, `Be`, `Fr`.
- Isotopes are specified in parentheses (round brackets) with the isotope mass number preceding the element symbol, e.g. `(12C)`, `(35Cl)`, `(235U)`. Note that no caret (^) is used to indicate a superscript.
- Charged species are specified with the charge following the formula in the format `+n` or `-n`, where `n` may be omitted if it is 1. Do not use a caret (^) to indicate a superscript. For example, `He+`, `C+2`, `W-`, `(79Br)-2`.
- Molecular formulas are written as a sequence of element symbols (which may be repeated for clarity over the structure), with their stoichiometries specified as an integer following the symbol. No underscore (_) character is used. For example, `H2O`, `(1H)2(16O)`, `C2H6OH`, `CH3CH2OH`, `NH+`, `CO3+2`.
- Moieties within formula can be bracketed for clarity, for example `CH3C(CH3)2CH3`.
- A limited number of formula prefixes are supported, for example `L-CH3CH(NH2)CO2H`, `cis-CH3CHCHCH3`, `ortho-C6H4(CH3)2`
- **There are some special species:**
 - `e-` is the electron;
 - `e+` is the positron;
 - `M` is a generic third-body with no specific identity (and no defined mass or charge);
 - `hν` (or `hν`) is the photon.

2.2 Output as HTML, LaTeX and slugs

The `Formula` attributes `html` and `latex` return strings representing the formula in HTML and LaTeX respectively. The attribute `slug` returns a URL-safe slug which uniquely identifies the formula's plain text string. For example:

```
In [1]: from pyvalem.formula import Formula

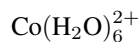
In [2]: f = Formula('')
In [3]: print(f.formula)      # or simply print(f)
Co(H2O)6+2

In [4]: print(f.html)
Co(H<sub>2</sub>O) <sub>6</sub><sup>2+</sup>

In [5]: print(f.latex)
\mathrm{Co}(\mathrm{H}_{2}\mathrm{O})_{6}^{2+}

In [6]: print(f.slug)
Co-_1_H2O_r_6_p2
```

The HTML and LaTeX representations render as:



2.3 Formula Attributes

`Formula` objects can count atoms, calculate masses and record the total species charge:

```
In [7]: f = Formula('CO3-2')
In [8]: print(f.natoms)
4
In [9]: print(f.rmm)
60.008

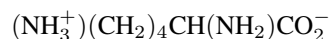
In [10]: print(f.charge)
-2

In [11]: lys = Formula('(NH3+) (CH2)4CH(NH2)CO2-')
In [12]: print(lys.natoms)
24

In [13]: print(lys.rmm)      # relative molecular mass
146.19

In [14]: print(lys.charge)
0
```

This last example is the Lysine zwitterion,



The same applies to isotopes and isotopically-pure molecules, in which case the exact mass is held by the `mass` attribute:

```
In [15]: f = formula('(1H) (35Cl)+')
In [16]: print(f.mass)
35.9766777262
```

The stoichiometric formula can be output either in order of increasing atomic number (the default) or in alphabetical order:

```
In [17]: print(lys.stoichiometric_formula())  
H14C6N2O2  
  
In [18]: print(lys.stoichiometric_formula('alphabetical'))  
C6H14N2O2
```


STATES

PyValem recognises several different kinds of quantum states and labels and is able to deduce the state type, parse quantum numbers and symmetries from provided strings, and do some validation.

States of different types can be instantiated directly from their class or associated with a species formula as a `StatefulSpecies` object.

3.1 GenericExcitedState

A “generic excited state” is simply an unspecified excitation of the species above its ground state: it may represent excitation of a single species to an unspecified quantum level or the general excitation of an ensemble of such species to a range of levels under equilibrium or non-equilibrium conditions.

A `GenericExcitedState` object is instantiated as a string of 1-4 asterisks or as a number preceding a single asterisk. For example:

```
In [1]: from pyvalem.generic_excited_state import GenericExcitedState
In [2]: x0 = GenericExcitedState('*')
In [3]: x1 = GenericExcitedState('****')
In [4]: x2 = GenericExcitedState('5*')
```

3.2 AtomicConfiguration

The electronic configuration of atoms, ions and isotopes is represented by the `AtomicConfiguration` class. The string representation provided to instantiate an `AtomicConfiguration` object is a sequence of orbital specifiers, separated by a full stop (period, `.`). An atomic orbital is represented by its principal quantum number, n , the azimuthal quantum number, l written as the letter `s`, `p`, `d`, ..., and the an occupancy (number of electrons, 1 or 2). For example:

```
In [1]: from pyvalem.atomic_configuration import AtomicConfiguration
In [2]: c0 = AtomicConfiguration('1s2')
In [3]: c1 = AtomicConfiguration('1s2.2s2.2p6')
In [4]: c2 = AtomicConfiguration('1s2.2s2.2p6.3s2.3d10')
```

The closed-shell part of an atomic configuration can be specified by providing the corresponding noble gas element symbol in square brackets:

```
In [5]: c2 = AtomicConfiguration('[Ne].3s2.3d10')
```

The HTML representation of the atomic configuration is returned by the `html` attribute:

```
In [5]: print(c2)
[Ne]3s<sup>2</sup>3d<sup>10</sup>
```

which renders as:

$$[\text{Ne}]3s^23d^{10}$$

If the same atomic orbital appears more than once or an orbital is specified as being occupied by more than the number of electrons allowed by the Pauli exclusion principle, an `AtomicConfigurationError` is raised:

```
In [6]: c3 = AtomicConfiguration('[Ar].3s2')
...
AtomicConfigurationError: Repeated subshell in [Ar].3s2

In [7]: c3 = AtomicConfiguration('1s2.2s2.2p7')
...
AtomicConfigurationError: Too many electrons in atomic orbital: 2p7
```

3.3 AtomicTermSymbol

The `AtomicTermSymbol` class represents an atomic electronic term symbol in the LS-coupling (Russell–Saunders coupling) notation. The total electronic spin quantum number, S , is specified by a multiplicity, $2S+1$, followed by the total electronic orbital angular momentum quantum number, L , as a letter, S, P, D, \dots for $L = 0, 1, 2, \dots$; there may optionally follow a parity label, o (for odd-parity states), and a total (spin-orbit coupled) electronic angular momentum quantum number, J after an underscore character ($_$). Half (odd)-integers are specified as fractions: $1/2, 3/2, 5/2$, etc.

Examples:

```
In [1]: from pyvalem.atomic_term_symbol import AtomicTermSymbol
In [2]: a0 = AtomicTermSymbol('3P_1/2')
In [3]: a1 = AtomicTermSymbol('4D')
In [4]: a2 = AtomicTermSymbol('2Po_1/2')
```

`AtomicTermSymbol` objects know about their quantum numbers, where defined:

```
In [5]: a0.S, a0.L, a0.J
Out[5]: (1.0, 1, 0.5)

In [6]: a1.S, a1.L, a1.J
Out[6]: (1.5, 2, None)

In [7]: a2.S, a2.L, a2.J, a2.parity
Out[7]: (0.5, 1, 0.5, 'o')
```

As with other states, the `html` attribute returns the HTML representation:

```
In [8]: print(a2.html)
<sup>2</sup>P<sup>o</sup><sub>1/2</sub>
```

which renders as:

$${}^2P_{1/2}^o$$

J must satisfy the “triangle rule” ($|L-S| \leq J \leq L+S$); if this test fails, an `AtomicTermSymbolError` is raised:

```
In [9]: a3 = AtomicTermSymbol('3P_3')
...
AtomicTermSymbolError: Invalid atomic term symbol: 3P_3 |L-S| <= J <= L+S must be_
↳satisfied.
```

3.4 DiatomicMolecularConfiguration

The electronic configuration of diatomic molecules, molecular ions and their isotopologues is represented by the `DiatomicMolecularConfiguration` class. This class is instantiated with a string consisting of a sequence of numbered molecular orbitals, separated by a full stop (period, `.`). Each orbital is denoted with a counting number (which increments for each orbital of the same symmetry), an orbital symmetry label, and an electron occupancy number.

The valid symmetry labels are the lower case greek letters, σ , π , and δ , with an optional letter, `u` or `g` denoting the inversion symmetry for centrosymmetric molecules. For convenience, the identifiers `sigma`, `pi`, `delta` may be used as identifiers instead of the greek labels.

Examples:

```
In [1]: from pyvalem.diatomic_molecular_configuration import_
↳DiatomicMolecularConfiguration
In [2]: c1 = DiatomicMolecularConfiguration('1σ')
In [3]: c2 = DiatomicMolecularConfiguration('1σu2')
In [3]: c3 = DiatomicMolecularConfiguration('1πu4.1πg3')
In [4]: c4 = DiatomicMolecularConfiguration('1σg2.1σu2.2σg2.2σu2.1πu4.3σg2')
```

An HTML representation of the configuration is held in the `html` attribute:

```
In [5]: print(c3.html)
1π<sub>u</sub><sup>4</sup>.1π<sub>g</sub><sup>3</sup>
In [6]: print(c4.html)
1σ<sub>g</sub><sup>2</sup>.1σ<sub>u</sub><sup>2</sup>.2σ<sub>g</sub><sup>2</sup>.2σ<sub>u</sub><sup>2</sup>
↳<sub>u</sub><sup>2</sup>.1π<sub>u</sub><sup>4</sup>.3σ<sub>g</sub><sup>2</sup>
```

These render as:

$1\pi_u^4 1\pi_g^3$ and $1\sigma_g^2 1\sigma_u^2 2\sigma_g^2 2\sigma_u^2 1\pi_u^4 3\sigma_g^2$

An attempt to fill an orbital with too many electrons raises a `DiatomicMolecularConfigurationError`, as does repeating an orbital:

```
In [7]: c5 = DiatomicMolecularConfiguration('1σ2.2σ2.3σ3')
...
DiatomicMolecularConfigurationError: Only two electrons allowed in σ orbital, but_
↳received 3
In [8]: c6 = DiatomicMolecularConfiguration('1σ2.2σ2.2σ1')
...
DiatomicMolecularConfigurationError: Repeated orbitals in 1σ2.2σ2.2σ1
```

3.5 MolecularTermSymbol

The `MolecularTermSymbol` class represents a molecular electronic term symbol. It is instantiated with a string providing the spin multiplicity ($2S+1$), electronic orbital angular momentum symmetry label and (optionally) the quantum number Ω in the Hund's case (a) formulation.

Symmetry labels are specified as an appropriate letter combination representing the irreducible representation of the electronic orbital wavefunction. For molecules with a centre of symmetry, the *u/g* label comes last, preceded by any $+/-$ label denoting the reflection symmetry of the wavefunction. Do not use a caret (^) or underscore (_) character to indicate superscripts or subscripts. For linear molecules, the irrep symbols Σ , Π , Δ and Φ may be replaced with `SIGMA`, `PI`, `DELTA`, and `PHI`.

If a term symbol has a label, this is given before the term symbol itself, which should be enclosed with parentheses.

Examples:

```
In [1]: from pyvalem.molecular_term_symbol import MolecularTermSymbol
In [2]: c1 = MolecularTermSymbol('1Σ-')
In [3]: c2 = MolecularTermSymbol('1SIGMA-')
In [4]: c3 = MolecularTermSymbol('3Σ+g')
In [5]: c4 = MolecularTermSymbol('3SIGMA+g')
In [7]: c5 = MolecularTermSymbol('b(4Π-3/2)')
In [8]: c6 = MolecularTermSymbol("A'(1A1g_0)")
In [9]: c7 = MolecularTermSymbol('A(1A"')
```

The `html` attribute returns the HTML representation of the molecular term symbol. The examples above are represented by:

```
1Σ-
1Σ-
3Σ+
3Σ+g
b(4Π-3/2)
A'(1A1g0)
A(1A"')
```

`MolecularTermSymbol` objects know about their total spin angular momentum quantum number, S , the electronic orbital angular momentum wavefunction irrep, the projection of the total angular momentum along the symmetry axis, Ω , and the term label. For example:

```
In [10]: c6 = MolecularTermSymbol('X(4Πu-3/2)')
In [11]: c6.S, c6.term_label, c6.irrep, c6.Omega
Out[11]: (1.5, 'X', 'Πu', -1.5)
```

3.6 VibrationalState

Molecular vibrational states of diatomic and polyatomic molecules are represented by the `VibrationalState` class. For diatomic molecules, this class is instantiated with a string of the form $v=n$ for $n=0, 1, 2, \dots$. Polyatomic vibrational states are initialised with a string giving the number of quanta in each labelled normal mode. Unspecified vibrational excitation is denoted $v=*$. For example:

```
In [1]: from pyvalem.vibrational_state import VibrationalState
In [2]: v0 = VibrationalState('v=0')
In [3]: v1 = VibrationalState('v=*')
```

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```
In [4]: v2 = VibrationalState('3v2+v3')
In [5]: v3 = VibrationalState('v1+v2')
In [6]: v4 = VibrationalState('2v1 + 3v4')
In [7]: v5 = VibrationalState('2v1+1v2+v3')
```

The attribute `html` holds an HTML representation of the vibrational state:

```
In [8]: print(v5.html)
2v<sub>1</sub> + v<sub>2</sub> + v<sub>3</sub>
```

This renders as:

$$2\nu_1 + \nu_2 + \nu_3$$

3.7 RotationalState

A single class, `RotationalState`, represents the total rotational angular momentum (excluding nuclear spin) quantum number, J , for both atoms and molecules. It is instantiated with a string, $J=n$, where n is an integer or half integer (expressed as a fraction or in decimal notation). Three different levels of unspecified rotation excitation may alternatively be specified by providing n as one to three asterisks. The parsed value of J is available as an attribute with that name.

Examples:

```
In [1]: from pyvalem.rotational_state import RotationalState
In [2]: r0 = RotationalState('J=0')
In [3]: r1 = RotationalState('J=3/2')
In [4]: r2 = RotationalState('J=1.5')
In [5]: r3 = RotationalState('J=*')
In [6]: print(r1.J)
1.5
```

3.8 KeyValuePair

The `KeyValuePair` class represents an arbitrary quantum number or symmetry provided as a (key, value) pair. It is instantiated with a string of the form `key=value`. For example:

```
In [1]: from pyvalem.key_value_pair import KeyValuePair
In [2]: kv1 = KeyValuePair('n=1')
In [3]: kv2 = KeyValuePair('C = 45a#')
```


STATEFUL SPECIES

A *stateful species* is a species identified by a chemical formula which is associated with one or more quantum states of labels, and can be represented by an instance of the `StatefulSpecies` class.

A `StatefulSpecies` object can be instantiated by providing a string consisting of the formula (which can be parsed into a `Formula` object), followed by whitespace and a semicolon delimited sequence of strings that can be parsed by one of the `State` classes described previously. The state type is deduced from the format of the string.

Examples:

```
In [1]: from pyvale.stateful_species import StatefulSpecies
In [2]: ss1 = StatefulSpecies('HCl v=2;J=0')
In [3]: ss2 = StatefulSpecies('NCO v2+3v1;J=10.5;a(2E-g)')
In [4]: ss3 = StatefulSpecies('Ar+ 1s2.2s2.2p5; 2P_3/2')
In [5]: ss4 = StatefulSpecies('CrH 1sigma2.2sigma1.1pi4.3sigma1; 6SIGMA+')
```

An HTML representation is accessible through the `html` attribute:

```
In [6]: print(ss4.html)
CrH 1σ<sup>2</sup>.2σ<sup>1</sup>.1π<sup>4</sup>.3σ<sup>1</sup>; <sup>6</sup>Σ<sup>+</sup>
↪sup>
```

This example renders as:

CrH $1\sigma^2 2\sigma^1 1\pi^4 3\sigma^1; {}^6\Sigma^+$

The `Formula` object and a list of the parse `State` objects are returned by the `formula` and `states` attributes:

```
In [7]: print(ss4.formula)
CrH

In [8]: print(ss4.states)
[1σ2.2σ1.1π4.3σ1, 6Σ+]
```

Two `StatefulSpecies` are considered the same (equal) if they have equal `Formula` objects and matching states:

```
In [9]: ss5 = StatefulSpecies('CO2 v2+3v1; J=2')
In [10]: ss6 = StatefulSpecies('CO2 J=2; v2+3v1')
In [11]: ss5 == ss6
Out[11]: True
```

Some `State` types cannot be repeated within a `StatefulSpecies` object (e.g. it doesn't make sense for a molecule to have two rotational quantum numbers, J). This is checked for:


```
In [12]: StatefulSpecies('N2 J=0;J=1')
...
StatefulSpeciesError: Multiple states of type RotationalState specified for N2 J=0;J=1

In [13]: StatefulSpecies('Li 1s2.2s1; 1s2.2p1')
...
StatefulSpeciesError: Multiple states of type AtomicConfiguration specified for Li
↪1s2.2s1;1s2.2p1
```

REACTION

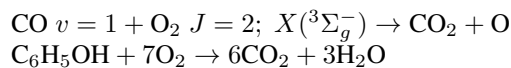
A Reaction object is a collection of reactants and a collection of products, each of which is represented by a StatefulSpecies (though an individual species need not be associated with a specified state). It is instantiated using a string consisting of reactant and product StatefulSpecies, each separated by a plus sign surrounded by whitespace: ' + '. Reactants and products are separated by any of the following strings: ' → ', ' = ', ' ⇌ ', ' -> ', ' <-> ', ' <=> '. Examples:

```
In [1]: from pyvalem.reaction import Reaction
In [2]: r1 = Reaction('CO + O2 → CO2 + O')
In [3]: r2 = Reaction('CO v=1 + O2 J=2;X(3SIGMA-g) → CO2 + O')
In [4]: r3 = Reaction('HCl + hv -> H+ + Cl + e-')
In [5]: r4 = Reaction('C6H5OH + 7O2 → 6CO2 + 3H2O')
```

An HTML representation of the reaction is returned by the html attribute:

```
In [6] print(r2.html)
CO v=1 + O<sub>2</sub> J=2; X(<sup>3</sup>Σ<sup>-</sup><sub>g</sub>) → CO<sub>2</sub> + O
↳+ O
In [7] print(r4.html)
C<sub>6</sub>H<sub>5</sub>OH + 7O<sub>2</sub> → 6CO<sub>2</sub> + 3H<sub>2</sub>O
```

These examples render as:



Reaction objects are validated to ensure that the charge and stoichiometry are conserved:

```
In [8]: Reaction('BeH+ + I2 ⇌ BeI + HI')
...
ReactionChargeError: Charge not preserved for reaction: BeH+ + I2 ⇌ BeI + HI

In [9]: Reaction('BeH + I2 ⇌ BeI')
...
ReactionStoichiometryError: Stoichiometry not preserved for reaction: BeH + I2 ⇌ BeI
```


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Nuclear Data Section

International Atomic Energy Agency
Vienna International Centre, P.O. Box 100
A-1400 Vienna, Austria

E-mail: nds.contact-point@iaea.org

Fax: (43-1) 26007

Telephone: (43-1) 2600 21725

Web: <http://nds.iaea.org>
