



VAMDC databases and partners

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VAMDC-USA Workshop - U. Heiter



VAMDC databases



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e-infrastructure



VAMDC databases – Atoms and Molecules

Uppsala/Moscow/Vienna	VALD database
Cologne	CDMS - Cologne Database for Molecular Spectroscopy
Pasadena	JPL Submillimeter, millimeter, and microwave spectral line catalog
Paris	SESAM - SpEctroScopy of Atoms and Molecules
Belgrade	Belgrade electron/Atom(Molecule) database
Vienna	ALADDIN (electron and heavy-particle collisions)
Belfast	VAMDC species database



VAMDC databases – Molecules

Cambridge (USA) + London	HITRAN
Paris	BASECOL
Bordeaux	KIDA - Kinetic Database for Astrochemistry
Belfast	UMIST Database for Astrochemistry
Reims	Ozone, methane, and ethylene calculated line lists
Dijon	Methane, carbon tetrafluoride, and sulfur hexafluoride calculated spectroscopic databases
Tomsk	Carbon dioxide and water spectroscopic databases
Caen	RADAM - Database for radiation damage of molecules of biological interest
Innsbruck	IDEADB - Innsbruck Dissociative Electron Attachment Database



VAMDC databases – Atoms

Cambridge (UK) + USA	Chianti
Paris + Belgrade	STARK-B
France, Venezuela, USA	TIPbase and TOPbase computed data (Iron Project and Opacity Project)
Moscow	D.E.S.I.R.E. (Lanthanides database)
Snezhinsk	Spectr-W3 atomic database
Gaithersburg	NIST Atomic Spectra Database (will be implemented soon)

Solids

Grenoble	GhoSST database (Solid Spectroscopy and Thermodynamics laboratory data)
Catania	Ices laboratory data



Chianti database (Landi et al. 2013)

- **Goal:** to include the best available calculations of atomic parameters for analyzing **astrophysical emission line spectra** (X-ray and UV), e.g. solar spectra
- **Contains** atomic energy levels, wavelengths, radiative rates, electron excitation, ionization, recombination rates for almost all **ions** of elements up to Zn
- Includes **routines** to calculate theoretical line intensities and optically thin synthetic spectra
- Data are **evaluated by comparison to solar spectra**
- Data are **included in several codes** such as XSTAR, CLOUDY, and in standard software of major solar missions



H I
He II

Li
Be

B

C I II III IV V VI
N I II III IV V VI VII
O I II III IV V VI VII VIII

F

Ne II III IV V VI VII VIII IX X

Na III IV V VI VII VIII IX X XI

Mg II IV V VI VII VIII IX X XI XII XII

Al II III V VI VII VIII IX X XI XII XIII

Si II III IV V VI VII VIII IX X XI XII XIII XIV

P V VII VIII IX X XI XII XIII XIV XV

S II III IV V VI VII VIII IX X XI XII XIII XIV XV XVI

Cl II III IV X XI XII XIV XVI XVII

Ar III IV V VII VIII IX X XI XII XIII XIV XV XVI XVII XVIII

K V VI IX XI XII XIII XIV XV XVI XVII XVIII XIX

Ca I V VI VII VIII IX X XI XII XIII XIV XV XVI XVII XVIII XIX XX

Sc

Ti XI XII XIV XV XVI XVII XVIII XIX XX

V

Cr VII VIII IX XIII XIV XVI XVII XVIII XIX XX XXI XXII

Mn VIII IX X XV XVII XVIII XIX XX XXI XXII XXIII

Fe II IV V VI VII VIII IX X XI XII XIII XIV XV XVI XVII XVIII XIX XX XXI XXII XXIII XXIV XXV XXVI

Co XI XII XIII XIV XV XVI XVII XVIII XIX XX XXI XXII XXIII XXIV XXV

Ni II XI XII XIII XIV XV XVI XVII XVIII XIX XX XXI XXII XXIII XXIV XXV XXVI XXVII XXVIII

Cu

XX XXIII XXIV XXV XXVII XXVIII

Chianti chart of ions

STARK-B database (Sahal-Bréchot et al. 2014)

- **Purpose:** to provide Stark broadening data for accurate spectroscopic diagnostics and modeling of stellar atmospheres and envelopes, laboratory plasmas, inertial fusion plasma, laser equipments, and technological plasmas
- **Contains line widths and shifts** of isolated lines of atoms and ions **due to collisions** with electrons, protons and different ions for a wide range of temperatures and perturber densities
- Data are based on **calculations using semiclassical-perturbation method** by Sahal-Bréchot, Dimitrijević et al.
- **Accuracy:** 20% for simpler spectra, worse for complex spectra



STARK-B ions

Choose an element and a ionization degree

- O I
- O II
- O III
- O IV
- O V
- O VI
- O VII

H																	He
Li	Be																
Na	Mg																Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
Fr	Ra	Ac															



JPL Submillimeter, millimeter, and microwave catalog (Pickett et al. 1998)

- **Purpose:** to be used as a planning guide or as an aid in the identification and analysis of observed **spectral lines in the interstellar medium, the Earth's atmosphere, and the atmospheres of other planets**
- **Contains** frequency (+error), intensity, lower state energy, and quantum number assignment for almost 400 species and over 4 million transitions
- Data are **calculated from least-squares fits of theoretical to observed frequencies** and predictions from molecular models
- **Errors** are estimated from covariance of fit parameters



KIDA (V. Wakelam et al.)

- Purpose: to provide **kinetic data relevant for astrochemistry** in Interstellar Medium or (exo-) planetary atmospheres (computing abundances from kinetic rates of reaction)
- **Contents**
 - ◆ for **species** (>400): polarizability, dipole moment, enthalpy of formation
 - ◆ for **reactions** (>6000): rate parameters, uncertainty, temperature range, reference, expert recommendation and comments
- **Reactions:** e.g. photo-processes, bimolecular reactions, radiative associations
- Data can be added by users (web interface) and is **evaluated by system of ~30 experts**



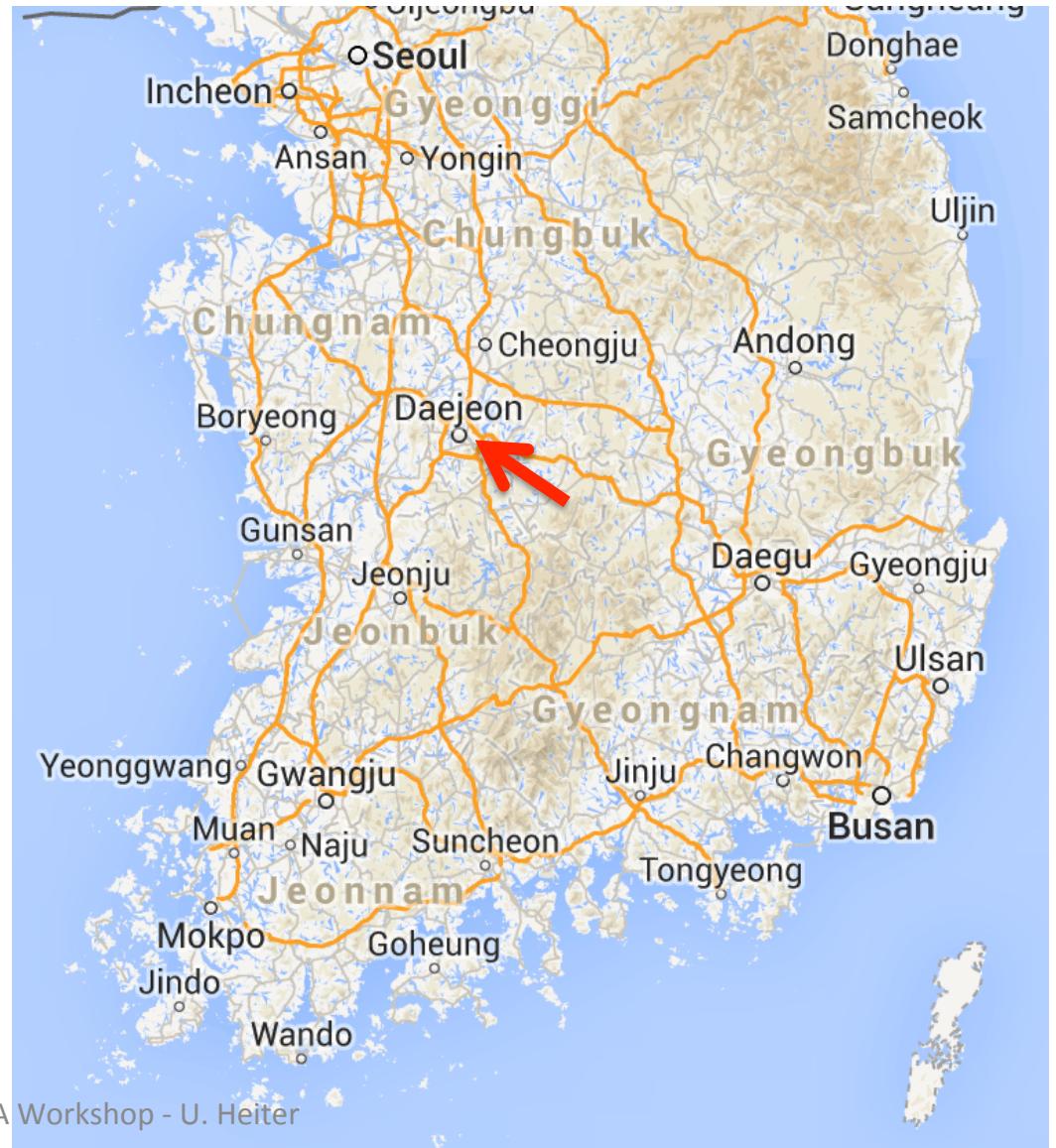
SUP-VAMDC partner: India

- **Tata Institute of Fundamental Research**, Mumbai, India
 - E Krishnakumar
- VAMDC-India workshops
- e-Atom/Molecule Database in Anand is being implemented as VAMDC node
- Discussions of data evaluation



SUP-VAMDC partner: Korea

- **Korea Atomic Energy Research Institute, Daejeon, South Korea – Yong-Joo Rhee**
- Interaction with A+M data users in Korea, and AMODS database



SUP-VAMDC partner: South Africa

- University of South Africa, Pretoria – Derck Smits
- Promotion of VAMDC in SA (conferences and articles)



SUP-VAMDC partner: Brazil



- Universidade Federal do Paraná, Curitiba – Milton Fujimoto
- Promotion of VAMDC in Brazil through presentations and tutorials at conferences



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