Technical Meeting on Standards and Software Tools for Atomic and Molecular Databases
IAEA Headquarters, Vienna, Austria, 27 – 29 November 2019

Data activities of the Atomic and Molecular Data Unit

C. Hill, K. Heinola and L. Marian

IAEA
International Atomic Energy Agency
Atoms for Peace

Atomic and Molecular Data Unit,
Nuclear Data Section,
Department of Nuclear Sciences and Applications,
International Atomic Energy Agency

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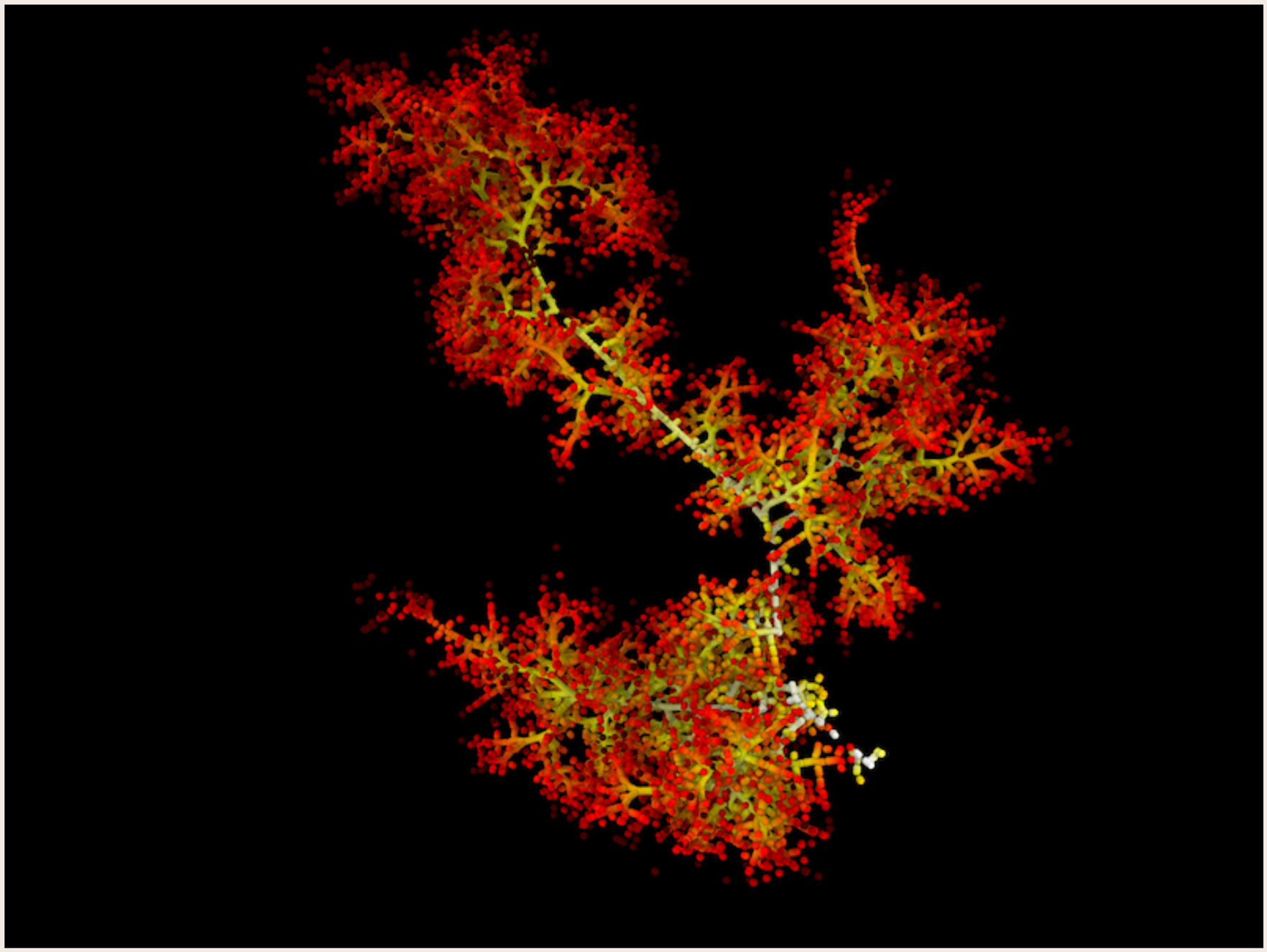
CascadesDB



CascadesDB

cascadesdb.org → cascadesdb.iaea.org

Data
1500+ simulations, 130 GB
plain old .xyz files

Metadata
relational database
output in XML (CDBML), text, HTML, JSON

CascadesDB

Author name: Sand

Publication DOI:

Material chemical formula:

e.g. W, Fe

Tmin K ≤ Initial temperature /K ≤ Tmax K

Emin keV ≤ Projectile / PKA energy /keV ≤ Emax keV

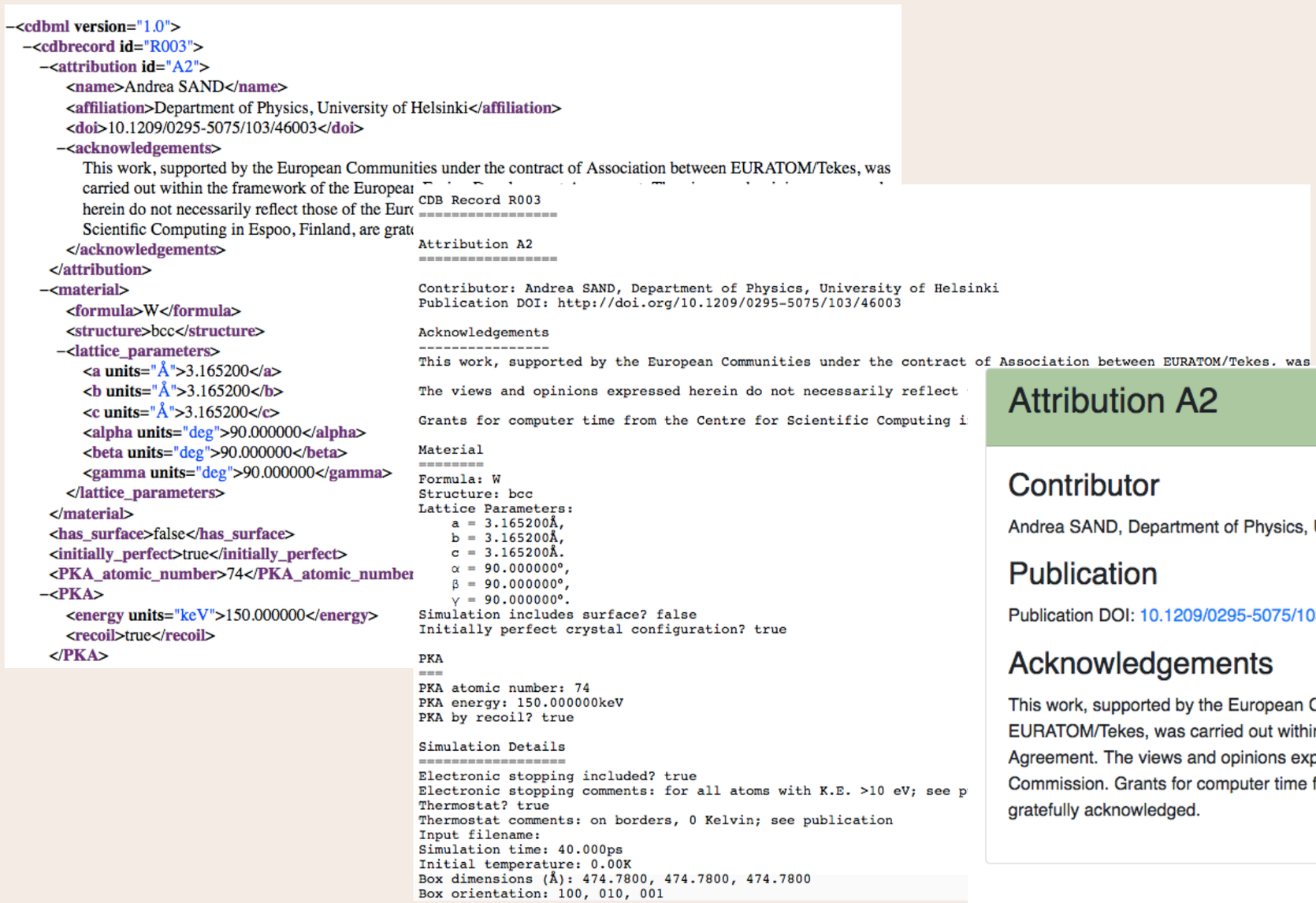
Archive name:

Search

Results

Attribution	Material	PKA energy /keV	Initial T /K	Simulation time /ps	Number of simulations	Metadata	Data	Source
Andrea SAND	W (bcc)	150.0	0.0	40.0	10	html | xml | txt	R003 (661.5 MB)	link | bibtex

CascadesDB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<name>Andrea SAND</name>
<affiliation>Department of Physics, University of Helsinki</affiliation>
<doi>10.1209/0295-5075/103/46003</doi>
−<acknowledgements>
This work, supported by the European Communities under the contract of Association between EURATOM/Tekes, was
carried out within the framework of the Europea
herein do not necessarily reflect those of the Eur
Scientific Computing in Espoo, Finland, are grat
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CDB Record R003
Attribution A2
Contributor: Andrea SAND, Department of Physics, University of Helsinki
Publication DOI: http://doi.org/10.1209/0295-5075/103/46003
Acknowledgements
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Grants for computer time from the Centre for Scientific Computing i
Material
Formula: W
Structure: bcc
Lattice Parameters:
a = 3.165200Å,
b = 3.165200Å,
c = 3.165200Å.
α = 90.000000°,
β = 90.000000°,
γ = 90.000000°.
Simulation includes surface? false
Initially perfect crystal configuration? true
PKA
PKA atomic number: 74
PKA energy: 150.000000keV
PKA by recoil? true
Simulation Details
Electronic stopping included? true
Electronic stopping comments: for all atoms with K.E. >10 eV; see p
Thermostat? true
Thermostat comments: on borders, 0 Kelvin; see publication
Input filename:
Simulation time: 40.000ps
Initial temperature: 0.00K
Box dimensions (Å): 474.7800, 474.7800, 474.7800
Box orientation: 100, 010, 001
Attribution A2
Contributor
Andrea SAND, Department of Physics, University of Helsinki
Publication
Publication DOI: 10.1209/0295-5075/103/46003
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Material
Formula: W
Structure: bcc
a = 3.165200 Å, b = 3.165200 Å, c = 3.165200 Å.

Identifying atomic and (small) molecular species

No widely-adopted standard exists, e.g.

- “W LXIV”
- “Na-like W”
- “W+63”
- “W63+”
- “W^{+63}”
- “W^{+63}”
- “W⁺⁶³”

Identifying atomic and (small) molecular species

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- Searching difficult or impossible
- Databases are incompatible
- Duplicates and errors
- Ambiguities:

“C2+” => C_2^+ or C^{2+}?

Identifying atomic and (small) molecular states

The situation is worse:

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° and (2pnd)^(1,3)P° Rydberg States of the be Atom via the Modified Atomic Orbital Theory

```
Infrared emission spectroscopy of the a$\prime$3$\{upSigma}$$
\mathplus$ -a3$\{upPi}$ band of {CS}
```

Possible solution: atomic and (small) molecular species

1. Adopt a standard for identifying species (e.g. in databases, journal article metadata, keywords, etc.)
2. Provide software libraries to parse, transform and validate the specification

Possible solution: atomic and (small) molecular species

Examples

W+63	W⁶³⁺ W^{63+} mass = 183.3 u charge = 63
C2H5OH	C₂H₅OH $\mathrm{C}_{2}\mathrm{H}_{5}\mathrm{O}\mathrm{H}$ mass = 46.068 u charge = 0 natoms = 9

Possible solution: atomic and (small) molecular states

Example

```
CO 1SIGMA+;v=0;J=2
        mass = 28.0101 u
charge = 0
states:
Molecular term symbol:
  <sup>1</sup>Σ<sup>+</sup>
  S=0, L=0, irrep=Σ+
Vibrational state:
  v=0
Rotational state:
  J=2
```

Possible solution: atomic and (small) molecular states

Example

```
Si+ [Ne].3s2.3p1; 2P_3/2
        mass = 28.0855 u
        charge = 1
        states:
        Atomic Configuration:
          [Ne]3s<sup>2</sup>3p<sup>1</sup>
          nelectrons = 13
          full_config = 1s2.2s2.2p6.3s2.3p1
        Atomic term symbol
          <sup>2</sup>P<sub>3/2</sub>
          L=1, S=0.5, J=1.5
```

Processes and Reactions

Example

```
O2 X(3SIGMA-g);v=0 + hv -> O2 a(1DELTAg);v=2
```

Validate charge, stoichiometry conversion

Translation to LaTeX and HTML, e.g.

$$O_2\ X(^3\Sigma^-_g);v=0 + h\nu \rightarrow O_2\ a(^1\Delta_g);v=2$$

Connect to database resource to retrieve ν / λ (and other data)

Processes and Reactions

Validation examples:

```
H2O + H+ -> H3O
```

Error: charge not conserved

```
H2O + H+ -> H3O+ + OH
```

Error: stoichiometry not conserved

```
H(35Cl) v=0 -> H(35Cl) v=2 + hv
```

Error: energy not conserved

Classification of Processes

Version 1.2 of standards:
D. Humbert, Yu. Ralchenko, P. Krstić, R. E. H. Clark (2003)

Electron-Heavy Particle Interactions
Recommended category code: **E**

SUBCATEGORY	IAEA	ORNL	GAPHYOR	DANSE	RECOMMENDED	PROCESS
General	GE	E01		**none**	**EGN**	
Angular Scattering	EG	E17	SC	**EAS**	**EAS**	
Bremsstrahlung	EB	E11	BS	**EBS**	**EBS**	e+A → e+A+hν
Deexcitation	ED	E07	DX	**EDX**	**EDX**	e+A* → e+A
Elastic Scattering	EE	E02	EL	**EEL**	**EEL**	e+A → e+A
Line Broadening, Shapes and Shifts	EL	E08		**ELB**	**ELB**	

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Electron-Heavy Particle Interactions

Recommended category code: **E**

ALADDIN
AMBDAS

SUBCATEGORY	IAEA	ORNL	GAPHYOR	DANSE	RECOMMENDED	PROCESS
General	GE	E01		**none**	**EGN**	
Angular Scattering	EG	E17	SC	**EAS**	**EAS**	
Bremsstrahlung	EB	E11	BS	**EBS**	**EBS**	e+A → e+A+hν
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Line Broadening, Shapes and Shifts	EL	E08		**ELB**	**ELB**	

Atoms and isotopes; ions

Supported species types

```
H, Ar, Zn
H+, H-, Nb+2, O-2
(1H), (2H), (40K)
(107Ag)+, (133Cs)+4, (35Cl)-, (81Br)-2
```

NB the parentheses are mandatory

Atoms and isotopes; ions

TODO

```
H+2 etc.: raise a validation error
Z > 104: Db, Sg, Bh, Hs, Mt, Ds, …, Og
Extend set of recognised isotopes
```

Molecules and isotopologues; ions

Supported species types

```
HCl, C2H5Br
CH3CH2OH
H(35Cl), (1H)(37Cl)
CO+, O2+2
(13C)(16O)-, (13C)H3+

i-C3H7OH = CH3CH(OH)CH3
o-C6H4(CH3)2 = ortho-C6H4(CH3)2 = 1,2-C6H4(CH3)2
D-CH3CH(NH2)COOH
1,1,2-C2H3Cl3
CH(CH3)3
β-H2NC3H6CH(NH2)CH2CO2H
```

Other recognised species types

Supported species types

```
hν = hν
M
e-
```

Atomic configurations

Supported strings

```
1s2
1s2.2s1
1s2.2s2.2p2
[Ne].3s2.3p1
[Xe].4f14.5d1.6s2

expands to:
1s2.2s2.2p6.3s2.3p6.3d10.4s2.4p6.4d10.5s2.5p6.4f1
4.5d1.6s2

NB separate orbitals by ‘.’, no ‘^’ characters
```

Atomic term symbols

Supported strings

```
1S_0
2P_1/2, 2P_3/2
1Po, 1Po_1          [parity]
3D_2

NB J subscript indicated with '_', half-odd
integer values written as 'x/2'
|L-S| <= J <= L+S is required
```

Molecular term symbols

Supported strings

1SIGMA+ = 1Σ+, 1SIGMA- = 1Σ-
6SIGMA+g = 6Σ+g, 6SIGMA-g = 6Σ-g
2Π_3/2 = 2PI_3/2
a(1DELTAg) = a(1Δg)
A’(3PHIg_2) = A’(3Φg_2), A”(3Φg_2)

NB Capitalised words or upper-case Greek letters can be used;
What about term labels like Ã?

Vibrational States, Rotational States

Supported strings

`v=0, v=1, …`
`v1 = ν1`
`2v2+v3 = 2ν2 + ν3`

`Diatomics vs polyatomics recognised`
`What about linear triatomics (e.g. CO2: v1v2`^{l_2}`v3)?`

`J = 0`
`J = 2`
`J = 3/2`

Key-value pairs: general quantum labels

Supported strings

```
N=1
F=3/2
Ka=3
Kc=4
sym=A
C=321
Omega=5/2, Ω=5/2

TODO: parse half-odd-integers?
```

Generic excited states

Supported strings

```
*
**
***
****
5*
10*
```

Multiple state specifications

Supported strings

```
(52Cr)(1H) X(6SIGMA+); J=5/2; N=0; F=3
CO2 v1+2v2;l2=2;J=4
```

Separate by ‘;’, with or without whitespace

Reactions, equilibria

Supported strings

```
e- + B -> e- + B 3D
O2 X(3SIGMA-g) + hv -> O2 a(1DELTAg)
e- + N2 v=0 → e- + N2 v=1
CH3CO2H + H2O <-> CH3CO2- + H3O+

NB '->' or '→' supported; also '<->' or '<=>'
Stoichiometry and charge must be conserved
```