Electron scattering data classification and organization: contribution of LoKI

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The LisbOn KInetics (LoKI) simulation tool

(developed under MATLAB®)

LoKI-B

OPEN SOURCE

https://github.com/IST-Lisbon/LoKI

- solves the space independent form of the two-term electron Boltzmann equation, for DC/HF or time-dependent (non-oscillatory) electric fields.
- includes e-e collisions, CAR operator, and growth models for the electron density.

LoKI-C

- solves the system of 0D rate balance equations for the heavy particles.
- includes modules to describe
  (i) the collisional, radiative and transport mechanisms controlling the creation / destruction of species
  (ii) the thermal heating of the neutral gas

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The LisbOn KInetics Boltzmann solver (LoKI-B)

Focus on LoKI-B

(released as open-source code licensed under the GNU GPL3.0)
developed as a response to the need of having an electron Boltzmann solver easily addressing the simulation of the electron kinetics

- in **any** complex gas mixture (of atomic / molecular species)
- describing **first and second-kind** electron collisions
- with **any** target species (electronic, vibrational and rotational)
- characterized by **any** user-prescribed population

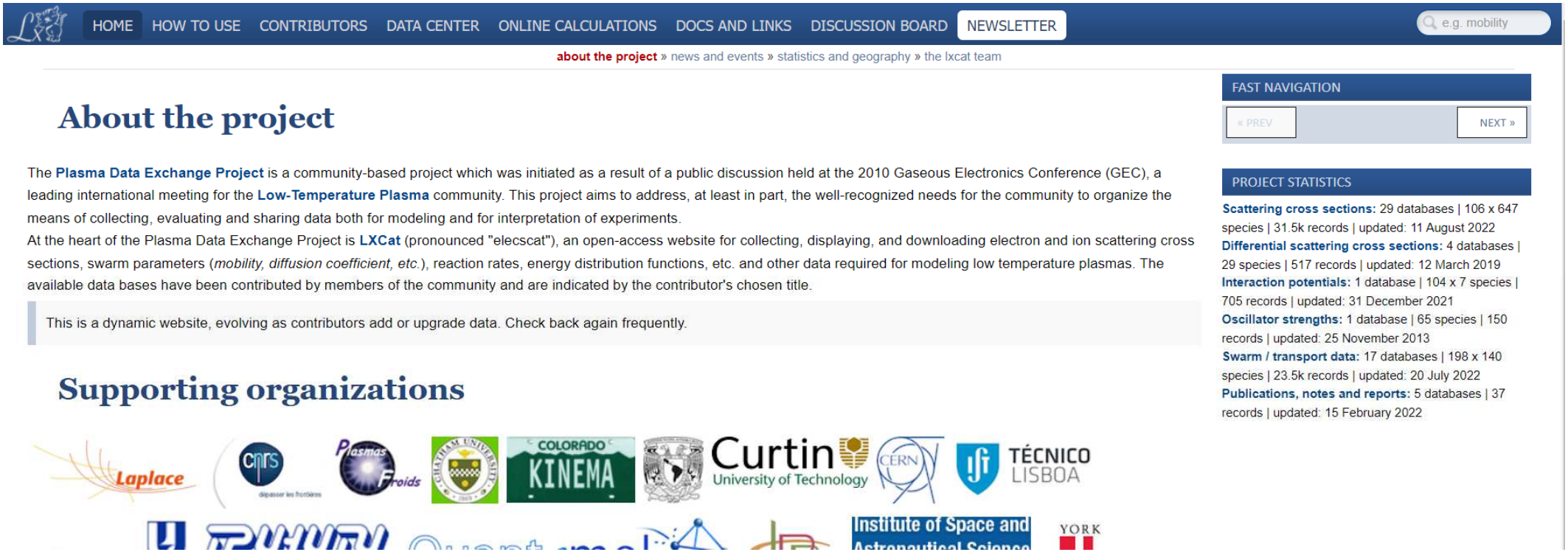
Focus on electron scattering data

LoKI-B is developed following a **clear ontology** in terms of data handling

- as **input**, it receives electron scattering cross sections, parsed adopting a format compliant with the open-access website **LXCat**
- as **output**, it provides the electron energy distribution function and the corresponding electron macroscopic parameters

A. Tejero-del Caz, et al. Plasma Sources Science and Technology, **28** (2019) 043001
A. Tejero-del Caz, et al. Plasma Sources Science and Technology, **30** (2021) 065008

The open-access website LXCat



publishing data in a public database is advantageous for both users and developers

- to **separate tools and data**
- to ensure the **open access** to data
- to promote using **validated** (recommended) data
- to encourage adopting a **standardized classification and organization** of data

Motivation / Outline

Contribution of LoKI to the classification and organization of electron scattering data

- **Organization of LXCat**
  - Databases in general
  - IST-Lisbon database
  - Possible ontologies for data classification & organization

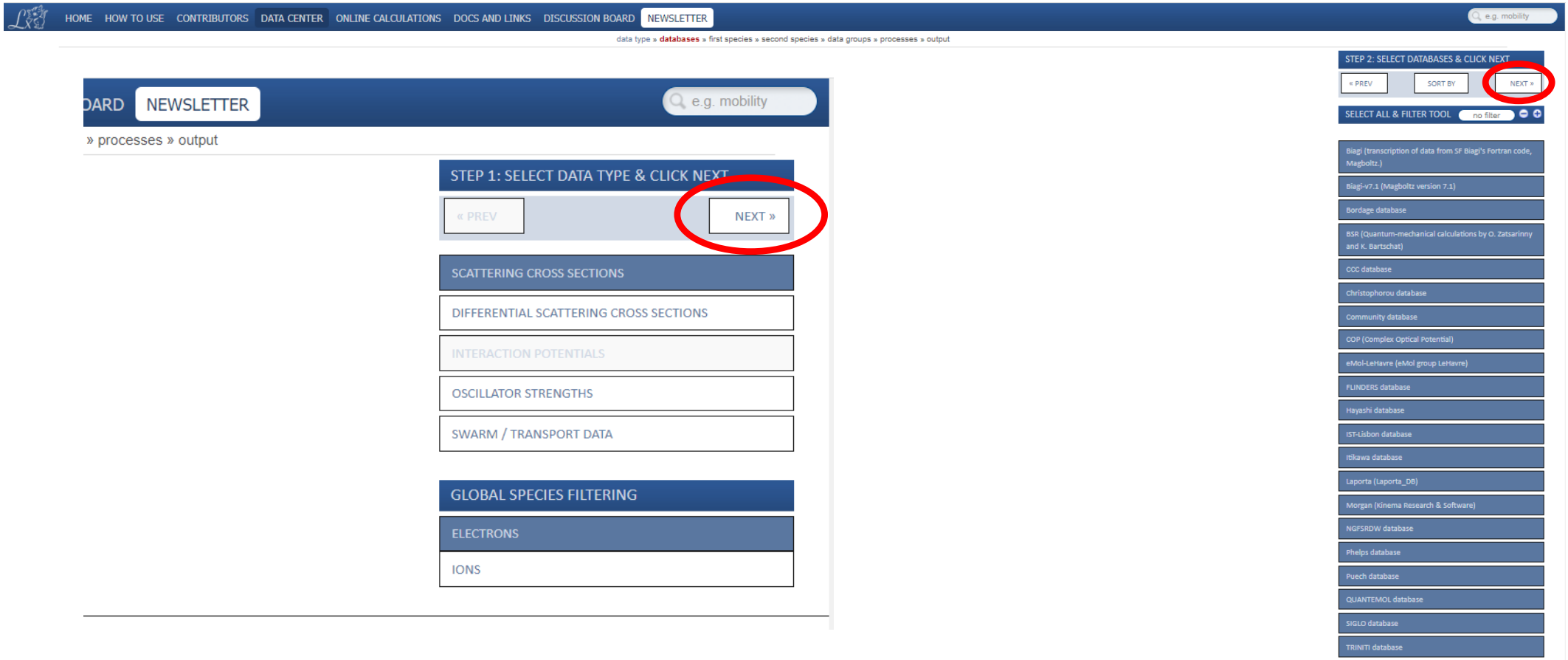
- **Organization of data in LoKI**
  - General ontology
  - Data input: chemistry and cross sections data
  - Parsing LXCat's metadata for LoKI

- **Proposal for organizing e-scattering data**

- **Final prospective remarks**

Organization of LXCat

Data and databases

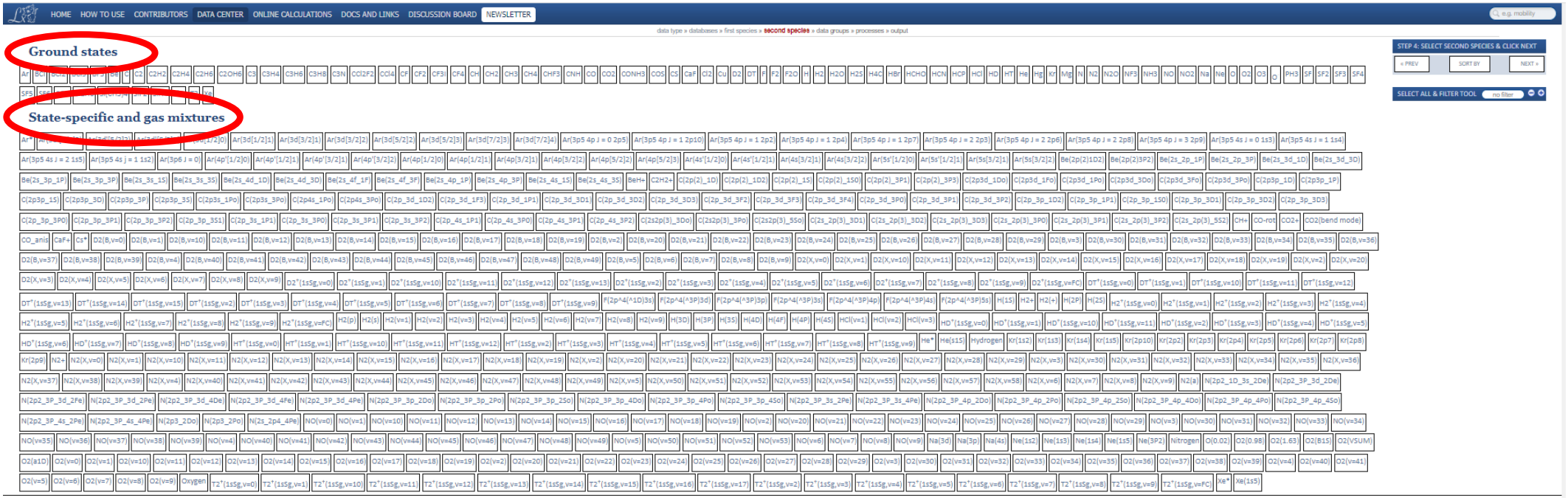


LXCat provides mainly **electron scattering cross sections** and **swarm parameters** "required for modelling low temperature plasmas".
For the purpose of a swarm analysis, the data are delivered in a simple effective way

The data is available from different databases

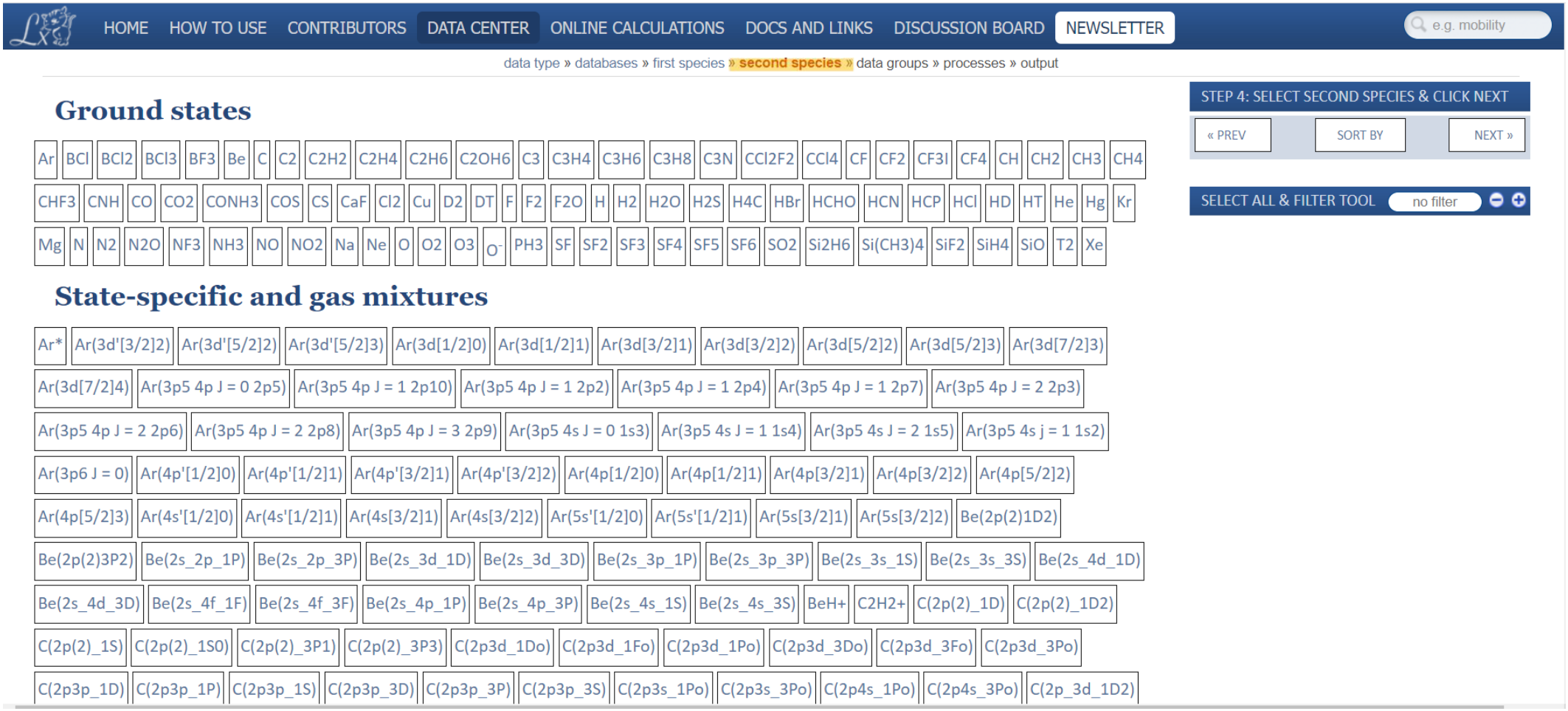
Organization of LXCat – ALL databases

Data for "Ground states" and for "State-specific and gas mixtures"



Organization of LXCat – ALL databases

Data for "Ground states" and for "State-specific and gas mixtures" - zoom



Cumbersome display of the data, due to a **reaction-oriented organization** focused mainly on swarm-analysis purposes

Organization of IST-Lisbon @ LXCat

Data for "Ground states" and for "State-specific and gas mixtures"

Ground states

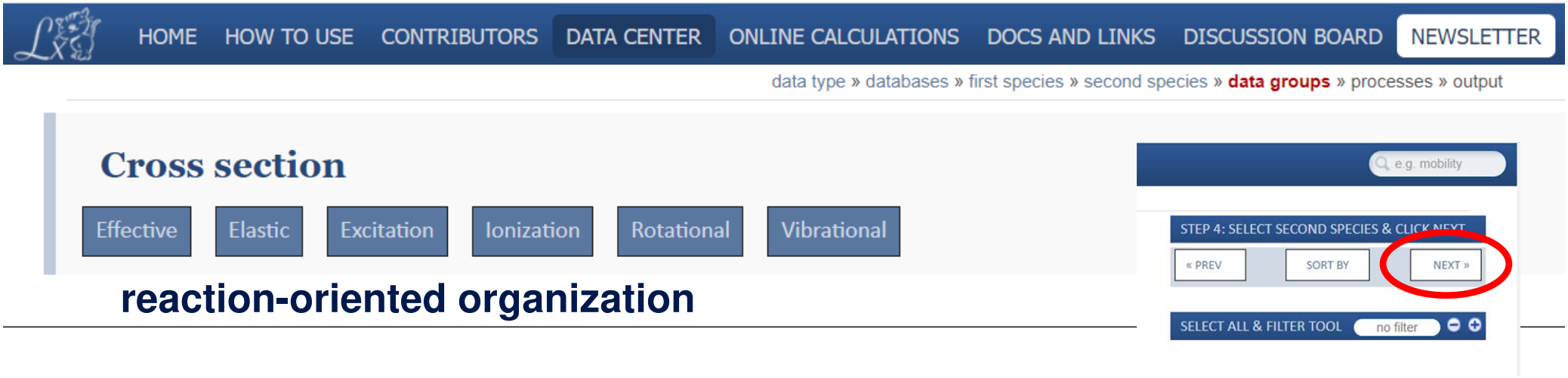
- e-cross sections for collisions with ground-states of atoms/molecules
- data corresponding to **complete sets of cross sections** for basic swarm analyses

State-specific and gas mixtures

- e-cross sections for collisions with "other" states
- the data are **automatically displayed by the repository under this "class"**, with no control by the contributors.

Organization of IST-Lisbon @ LXCat

Data for "Ground states" and for "State-specific and gas mixtures"



reaction-oriented organization

Note the unavailability of some cross section tags:
e.g. *Detachment*, *Recombination*, *Momentum-transfer*

Organization of IST-Lisbon @ LXCat

Data Groups: example for [N2] and [Nitrogen]

Definition of **five Data Groups,** for a tentative **species-oriented organization**

Organization of IST-Lisbon @ LXCat

Data Groups – description: : example for [N2] and [Nitrogen]

Ground states [N2]

[N2] … cross sections for collisions with ground-state $N_2(X,v=0)$

State-specific and gas mixtures [Nitrogen]

[N2-rot] … cross sections for collisions with rotational states $N_2(X,v=0,J)$

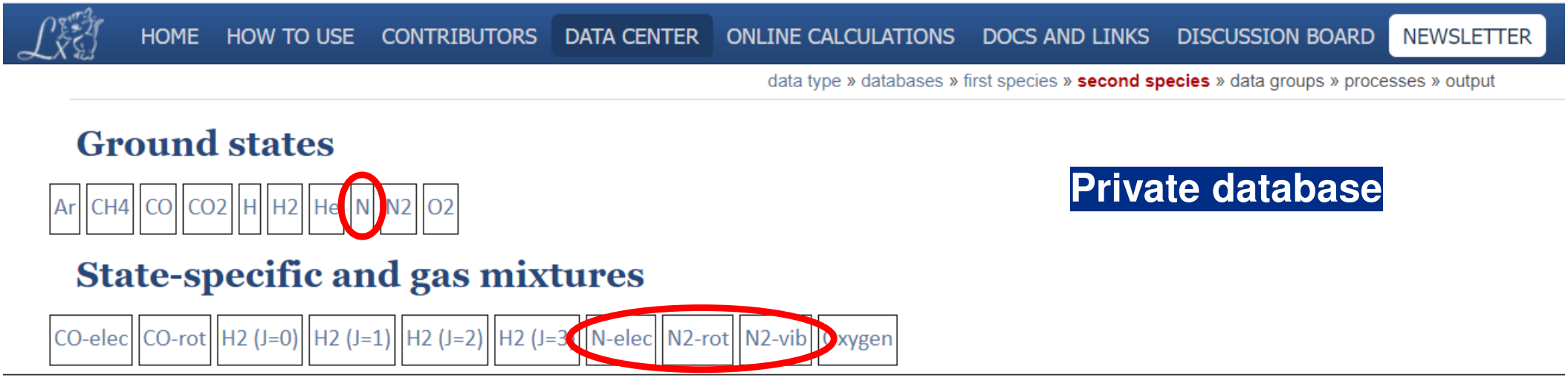
[N2-vib] … cross sections for collisions with vibrational states $N_2(X,v\neq0)$

[N] … cross sections for collisions with the ground-state $N(^4S)$

[N-elec] … cross sections for collisions with electronic excited states $N(^2D,^2P)$

Organization of LXCat : IST-Lisbon vs private database

Alternative ontologies

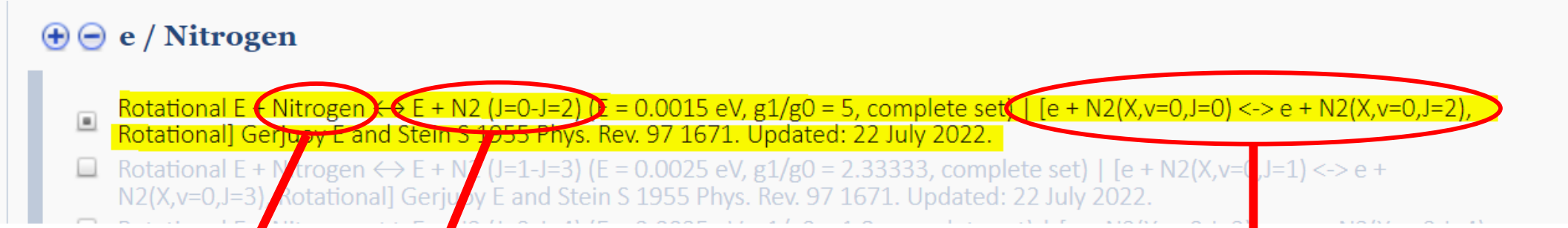


The **same data** can be displayed with **alternative ontologies** in different databases
Using the lower row to discriminate state-specific cross sections is cumbersome

Organization of IST-Lisbon @ LXCat

Description of the e-collisions: example for [N2-rot]

Data Group [N2-rot]: E. Gerjouy and S. Stein, "Rotational Excitation by Slow Electrons" 1955 Phys. Rev. 97 1671.
N2-rot is a set of rotational excitation cross sections by electron impact, for transitions N2(X,v=0,J) --> N2(X,v=0,J+2) (J=0,1,.,30), which complements the COMPLETE set of N2 cross sections, available in this database under group N2.



The name of the "State-specific and gas mixture" is **automatically assigned as *target species***
(⇒ which limits a detailed state-to-state description)

The ***final state*** **field is free**,
thus it is often used to provide state-to-state details
(⇒ which promotes a relaxed description of species)

The ***comment*** **field is free,**
and is used to parse
"metadata" for LoKI-B

Organization of data in LoKI

General ontology

The LoKI suite raises the bar in the classification and organization of data, **adopting a state-to-state description of kinetic mechanisms leveraging on a species-oriented organization of the data**

- requiring details on the internal structure (electronic / vibrational / rotational) of both target and product species
- extending the set of electron cross sections to the scattering by excited states
- unambiguously classifying every type of cross section (avoiding an over-clustering with tag *Excitation*)

Every target/product species is written with details of its internal structure

Organization of data in LoKI

Data input – chemistry: example for Nitrogen

The **reaction (chemistry) data** are retrieved from a .chem file (extract below)

```
%---- electron impact excitation/deexcitation ----
e + N2(X,v=0) <-> e + N2(A3Su+)                                  | eedf
e + N(4S) <-> e + N(2D)                                          | eedf

%---- e-V processes ----
e + N2(X,v=0) <-> e + N2(X,v=1)                                  | eedf
e + N2(X,v=1:9) -> e + N2(X,v=v+1)                               | nitrogenEVscaling

%---- electron impact dissociation ----
e + N2(X,v=0) -> e + 2N(4S)                                      | eedf

%---- electron impact ionization ----
e + N2(X,v=0) -> 2e + N2(+,X)                                    | eedf
e + N2(A3Su+) -> 2e + N2(+,X)                                    | eedf
e + N(4S) -> 2e + N(+,gnd)                                       | eedf

%---- electron recombination ----
e + N2(+,X) -> 2N(4S)                                            | powerElectronTemp

%---- heavy species collisions ----
N2(B3Pg) + N2(X) -> N2(A3Su+) + N2(X)                            | constantRateCoeff
N(2D) + N(4S) + N2(X) -> N2(B3Pg) + N2(X)                        | constantRateCoeff
N(2D) + N2(X) -> N(4S) + N2(X)                                   | arrheniusGasTemp
N2(+,X) + N2(X,v=0) + N2(X) -> N4(+,X) + N2(X)                   | powerGasTemp
N(4S) + N(4S) + N2(X) -> N2(a1Pg) + N2(X)                        | arrheniusGasTemp
N2(C3Pu) -> N2(B3Pg)                                             | constantRateCoeff

%---- V-V processes ----
N2(X,v=1:10) + N2(X,w=0:v-1) <-> N2(X,v=v-1) + N2(X,v=w+1)       | nitrogenMolecularVV
N2(X,v=1:10) + N2(X,v=10) -> N2(X,v=v-1) + 2N(4S)                | nitrogenMolecularVVDis

%---- Molecular V-T processes ----
N2(X,v=1:10) + N2(X) <-> N2(X,v=v-1) + N2(X)                     | nitrogenMolecularVT
N2(X,v=10) + N2(X) -> 2N(4S) + N2(X)                             | nitrogenMolecularVTDis

%---- Atomic V-T processes ----
N2(X,v=7:10) + N(4S) <-> N2(X,v=v-1) + N(4S)                     | nitrogenAtomicVT
```

A species-oriented organization

The LoKI suite

- identifies the various species
- writes the balance equation for each species, considering its gain/loss due to the various reactions

Organization of data in LoKI

Data input – cross sections: example for Nitrogen

The **cross section (electron kinetics) data** are retrieved from LXCat files (listed in an input file)

```
17  % --- configuration of the electron kinetics ---
18  electronKinetics:
19    isOn: true              % true or false (to activate of deactivate the electron Kinetics)
20    eedfType: boltzmann     % boltzmann or prescribedEedf (generalized expression Maxwellian/Druyvesteyn)
21  %   shapeParameter: 1       % prescribedEedf shape parameter from 1 (Maxwellian) to 2 (Druyvesteyn)
22    ionizationOperatorType: conservative % conservative, oneTakesAll, equalSharing or usingSDCS
23    growthModelType: temporal % temporal or spatial
24    includeEECollisions: false  % true or false (to include or not the effect of e-e collisions on the EEDF)
25    LXCatFiles:               % cross section files
26      - Nitrogen/N2_LXCat.txt
27      - Nitrogen/N2_vib_LXCat.txt
28      - Nitrogen/N2_rot_LXCat.txt
29      - Nitrogen/N_LXCat.txt
30    LXCatFilesExtra:
31      - Nitrogen/N2_LXCat_extra.txt
32      - Nitrogen/N_LXCat_extra.txt
```

Each LXCat file

- contains a selection of data
- is downloaded from the **IST-Lisbon@LXCat database**

How are LXCat data/metadata parsed to LoKI ?

Organization of data in LoKI

Data input – parsing metadata: example for rotational collision

```
74  ********************************************** Nitrogen **************************
75
76  ROTATIONAL
77  SPECIES: e / Nitrogen
78  PROCESS: E + Nitrogen <-> E + N2 (J=0-J=2), Rotational
79  PARAM.:  E = 0.0015 eV, g1/g0 = 5, complete set
80  COMMENT: [e + N2(X,v=0,J=0) <-> e + N2(X,v=0,J=2), Rotational] Gerjuoy E and Stein S 1955
81  COMMENT: Phys. Rev. 97 1671.
82  UPDATED: 2022-07-22 04:00:39
83  COLUMNS: Energy (eV) | Cross section (m2)
84  ----------------------------
85    1.500000e-3    0.000000e+0
86    1.501000e-3    9.585900e-23
```

File N2_rot_LXCat.txt (extract)

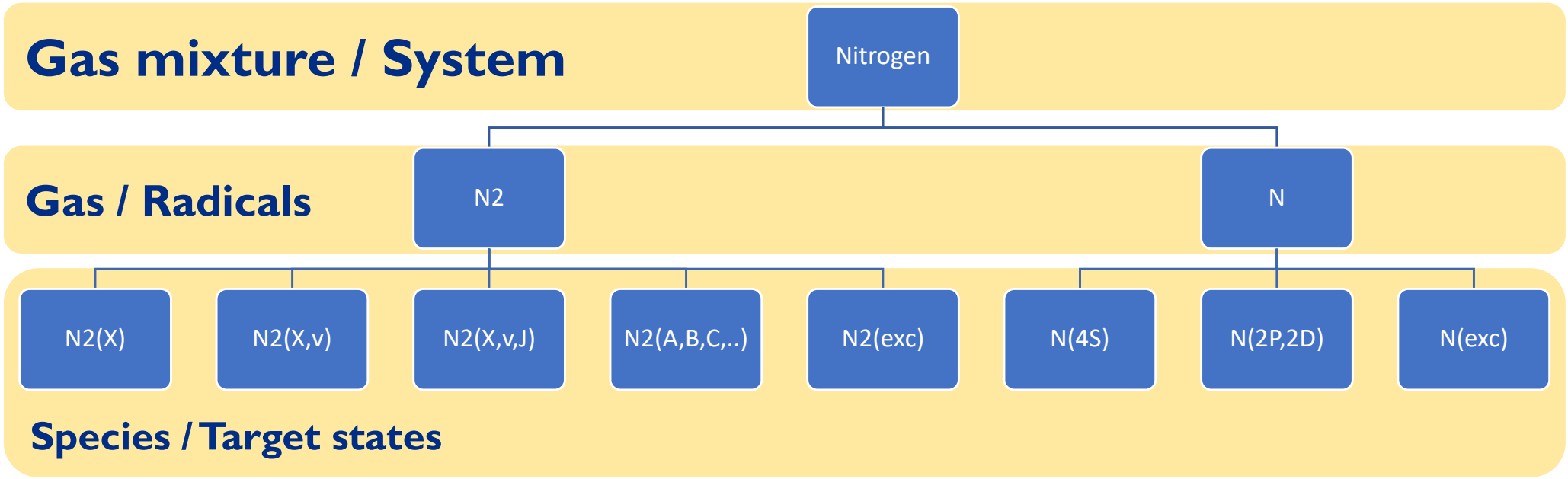
Workaround for parsing LXCat metadata: use of the free-field COMMENT in LXCat

The COMMENT field includes

- the reaction, with full AMO description of target/product species
- additional comments about the cross section
- the original reference from where the cross section was obtained

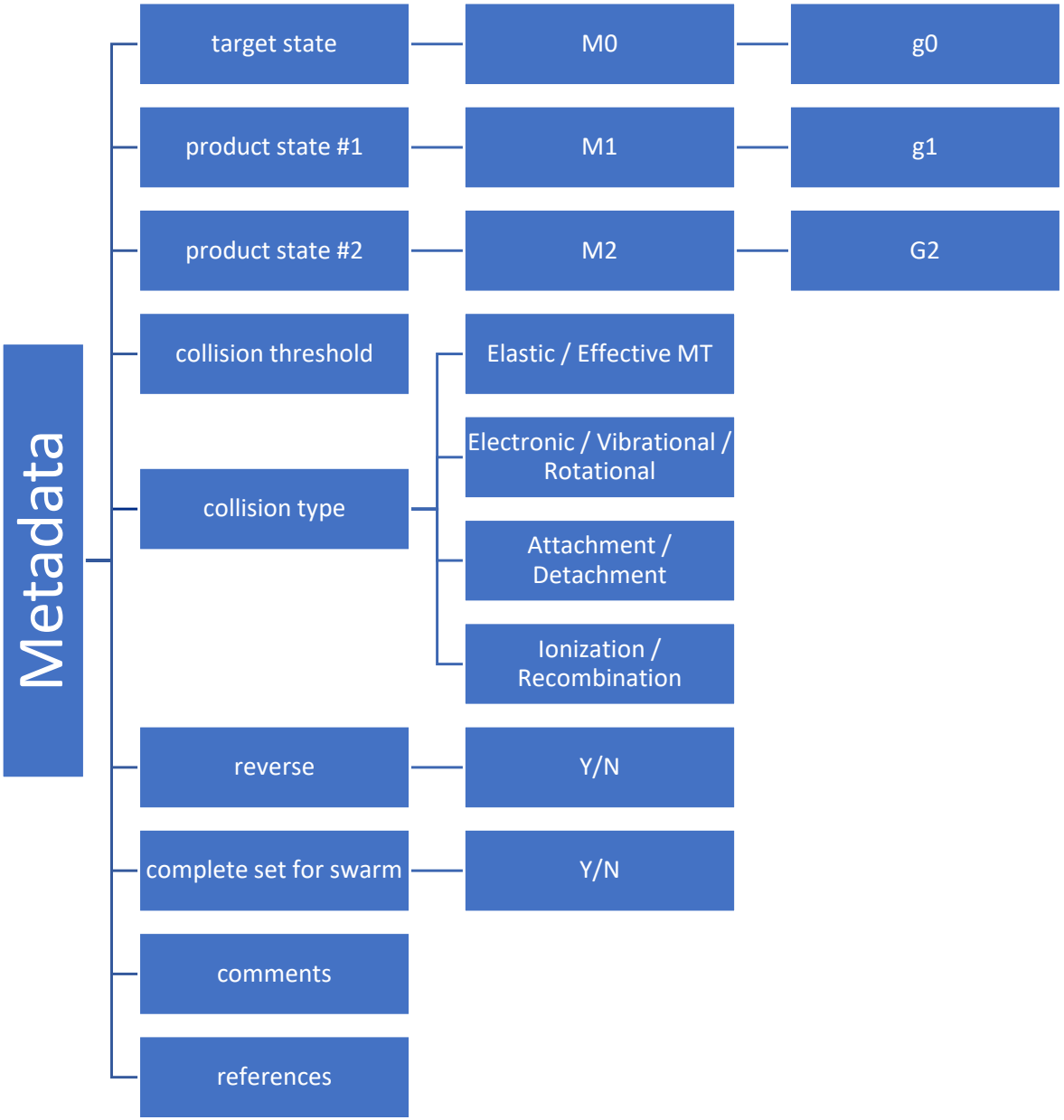
Organization of e-scattering data – proposal

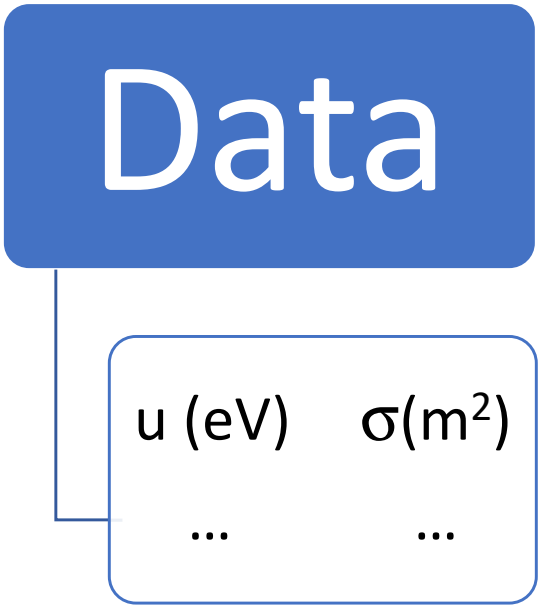
Classification of data using three levels



Organization of e-scattering data – proposal

Input of metadata and data





Final prospective remarks

Data classification and organization should

- preserve the separation between tools and data
- allow flexibility, within a well-defined policy
- ensure scientific rigor

Data handling should check data integrity

- by allowing direct communication of codes with databases (via APIs), or
- at least by providing checksums of downloaded datafiles.

The present work

- has highlighted limitations in the organization of LXCat data
- proposed solutions, leveraging on our experience during the conception and the development of the LisbOn Kinetics (LoKI) simulation tool
  Any evolution should **be inclusive** and should **preserve legacy**
  [See next talk by J van Dijk & Daan Boer]

Fostering these solutions will contribute to **improve the curation of data beyond electron scattering cross sections**, paving the way for new open-access databases for plasma-chemistry related data.

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