

# Electron scattering data classification and organization: contribution of LoKI

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<http://www.ipfn.ist.utl.pt>

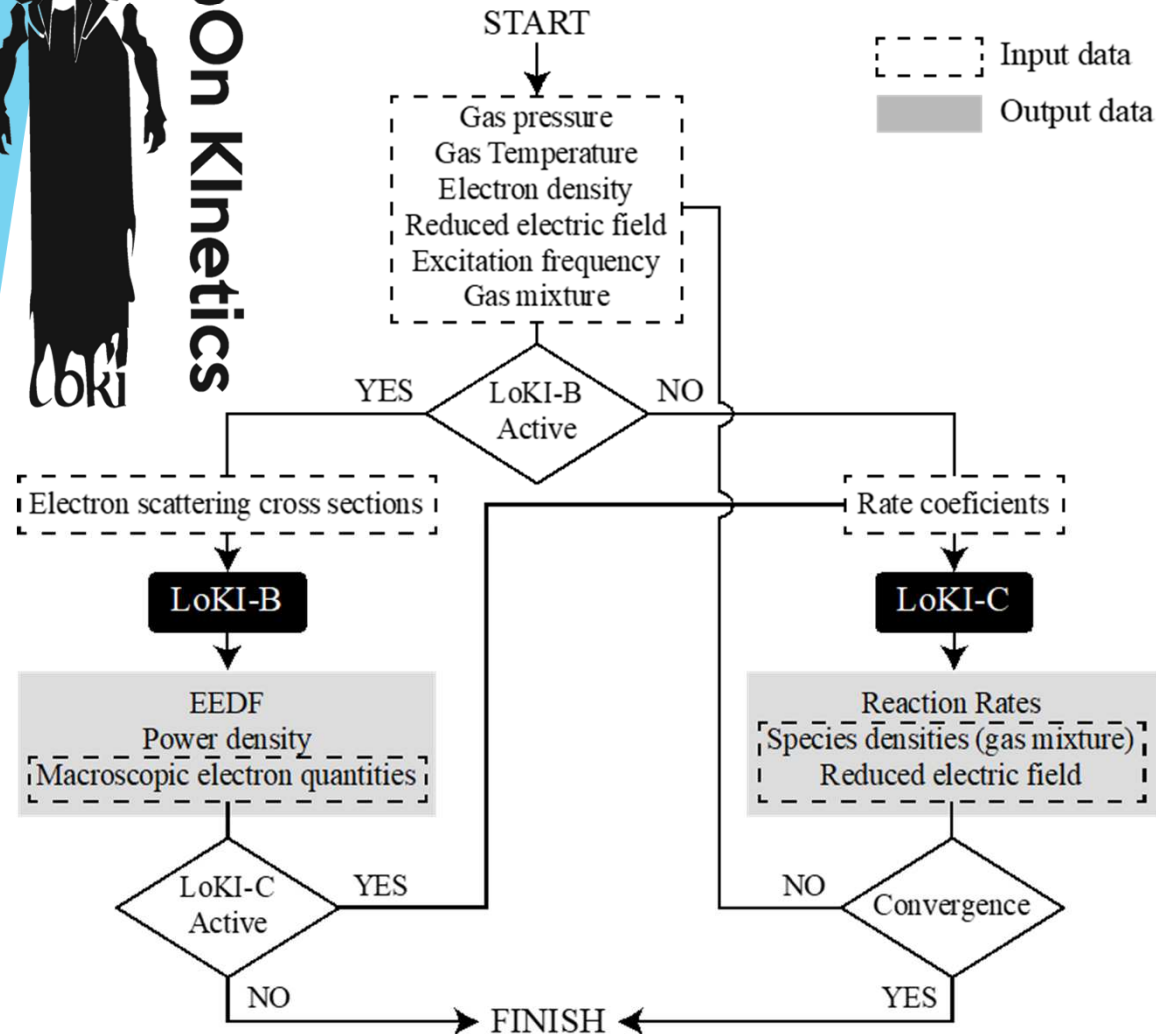
<https://www.ipfn.tecnico.ulisboa.pt/nprime/>

# The LisbOn Kinetics (LoKI) simulation tool

(developed under MATLAB®)



LisbOn Kinetics



**OPEN SOURCE**

## LoKI-B

<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

# The LisOn 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

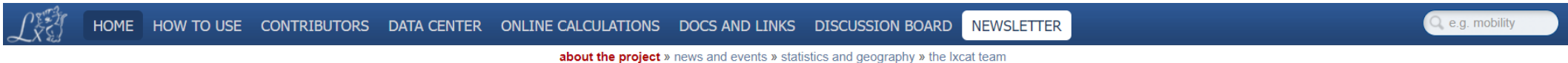
LoKI-B is developed following a **clear ontology** in terms of data handling

- 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



## About the project

The **Plasma Data Exchange Project** is a community-based project which was initiated as a result of a public discussion held at the 2010 Gaseous Electronics Conference (GEC), a leading international meeting for the **Low-Temperature Plasma** community. This project aims to address, at least in part, the well-recognized needs for the community to organize the means of collecting, evaluating and sharing data both for modeling and for interpretation of experiments.

At the heart of the Plasma Data Exchange Project is **LXCat** (pronounced "elecscat"), an open-access website for collecting, displaying, and downloading electron and ion scattering cross sections, swarm parameters (*mobility, diffusion coefficient, etc.*), reaction rates, energy distribution functions, etc. and other data required for modeling low temperature plasmas. The available data bases have been contributed by members of the community and are indicated by the contributor's chosen title.

This is a dynamic website, evolving as contributors add or upgrade data. Check back again frequently.

## Supporting organizations



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

### FAST NAVIGATION

« PREV

NEXT »

### PROJECT STATISTICS

**Scattering cross sections:** 29 databases | 106 x 647 species | 31.5k records | updated: 11 August 2022

**Differential scattering cross sections:** 4 databases | 29 species | 517 records | updated: 12 March 2019

**Interaction potentials:** 1 database | 104 x 7 species | 705 records | updated: 31 December 2021

**Oscillator strengths:** 1 database | 65 species | 150 records | updated: 25 November 2013

**Swarm / transport data:** 17 databases | 198 x 140 species | 23.5k records | updated: 20 July 2022

**Publications, notes and reports:** 5 databases | 37 records | updated: 15 February 2022

## 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

data type » **databases** » first species » second species » data groups » processes » output

STEP 1: SELECT DATA TYPE & CLICK NEXT

« PREV NEXT »

SCATTERING CROSS SECTIONS

DIFFERENTIAL SCATTERING CROSS SECTIONS

INTERACTION POTENTIALS

OSCILLATOR STRENGTHS

SWARM / TRANSPORT DATA

GLOBAL SPECIES FILTERING

ELECTRONS

IONS

STEP 2: SELECT DATABASES & CLICK NEXT

« PREV SORT BY NEXT »

SELECT ALL & FILTER TOOL no filter

Biagi (transcription of data from SF Biagi's Fortran code, Magboltz.)

Biagi-v7.1 (Magboltz version 7.1)

Bordage database

BSR (Quantum-mechanical calculations by O. Zatsarinny and K. Bartschat)

COC database

Christophorou database

Community database

COP (Complex Optical Potential)

eMol-Lehavre (eMol group Lehavre)

FLINDERS database

Hayashi database

IST-Lisbon database

Itikawa database

Laporta (Laporta\_DB)

Morgan (Kinema Research & software)

NGFSRDW database

Phelps database

Puech database

QUANTEMOL database

SIGLO database

TRINITY database

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” - zoom



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Q e.g. mobility

data type » databases » first species » **second species** » data groups » processes » output

## Ground states

Ar	BCl	BCl2	BCl3	BF3	Be	C	C2	C2H2	C2H4	C2H6	C2OH6	C3	C3H4	C3H6	C3H8	C3N	CCl2F2	CCl4	CF	CF2	CF3	CF4	CH	CH2	CH3	CH4			
CHF3	CNH	CO	CO2	CONH3	COS	CS	CaF	Cl2	Cu	D2	DT	F	F2	F2O	H	H2	H2O	H2S	H4C	HBr	HCHO	HCN	HCP	HCl	HD	HT	He	Hg	Kr
Mg	N	N2	N2O	NF3	NH3	NO	NO2	Na	Ne	O	O2	O3	O-	PH3	SF	SF2	SF3	SF4	SF5	SF6	SO2	Si2H6	Si(CH3)4	SiF2	SiH4	SiO	T2	Xe	

## State-specific and gas mixtures

Ar*	Ar(3d'[3/2]2)	Ar(3d'[5/2]2)	Ar(3d'[5/2]3)	Ar(3d[1/2]0)	Ar(3d[1/2]1)	Ar(3d[3/2]1)	Ar(3d[3/2]2)	Ar(3d[5/2]2)	Ar(3d[5/2]3)	Ar(3d[7/2]3)
Ar(3d[7/2]4)	Ar(3p5 4p J = 0 2p5)	Ar(3p5 4p J = 1 2p10)	Ar(3p5 4p J = 1 2p2)	Ar(3p5 4p J = 1 2p4)	Ar(3p5 4p J = 1 2p7)	Ar(3p5 4p J = 2 2p3)				
Ar(3p5 4p J = 2 2p6)	Ar(3p5 4p J = 2 2p8)	Ar(3p5 4p J = 3 2p9)	Ar(3p5 4s J = 0 1s3)	Ar(3p5 4s J = 1 1s4)	Ar(3p5 4s J = 2 1s5)	Ar(3p5 4s j = 1 1s2)				
Ar(3p6 J = 0)	Ar(4p'[1/2]0)	Ar(4p'[1/2]1)	Ar(4p'[3/2]1)	Ar(4p'[3/2]2)	Ar(4p[1/2]0)	Ar(4p[1/2]1)	Ar(4p[3/2]1)	Ar(4p[3/2]2)	Ar(4p[5/2]2)	
Ar(4p[5/2]3)	Ar(4s'[1/2]0)	Ar(4s'[1/2]1)	Ar(4s[3/2]1)	Ar(4s[3/2]2)	Ar(5s'[1/2]0)	Ar(5s'[1/2]1)	Ar(5s[3/2]1)	Ar(5s[3/2]2)	Be(2p(2)1D2)	
Be(2p(2)3P2)	Be(2s_2p_1P)	Be(2s_2p_3P)	Be(2s_3d_1D)	Be(2s_3d_3D)	Be(2s_3p_1P)	Be(2s_3p_3P)	Be(2s_3s_1S)	Be(2s_3s_3S)	Be(2s_4d_1D)	
Be(2s_4d_3D)	Be(2s_4f_1F)	Be(2s_4f_3F)	Be(2s_4p_1P)	Be(2s_4p_3P)	Be(2s_4s_1S)	Be(2s_4s_3S)	BeH+	C2H2+	C(2p(2)_1D)	C(2p(2)_1D2)
C(2p(2)_1S)	C(2p(2)_1S0)	C(2p(2)_3P1)	C(2p(2)_3P3)	C(2p3d_1Do)	C(2p3d_1Fo)	C(2p3d_1Po)	C(2p3d_3Do)	C(2p3d_3Fo)	C(2p3d_3Po)	
C(2p3p_1D)	C(2p3p_1P)	C(2p3p_1S)	C(2p3p_3D)	C(2p3p_3P)	C(2p3p_3S)	C(2p3s_1Po)	C(2p3s_3Po)	C(2p4s_1Po)	C(2p4s_3Po)	C(2p_3d_1D2)

STEP 4: SELECT SECOND SPECIES & CLICK NEXT

« PREV

SORT BY

NEXT »

SELECT ALL & FILTER TOOL

no filter



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”

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[data type](#) » [databases](#) » [first species](#) » **[second species](#)** » [data groups](#) » [processes](#) » [output](#)

## Ground states

Ar CH4 CO CO2 H2 He N2 O2

## State-specific and gas mixtures

CO-rot CO\_anis Hydrogen Nitrogen Oxygen

## 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”

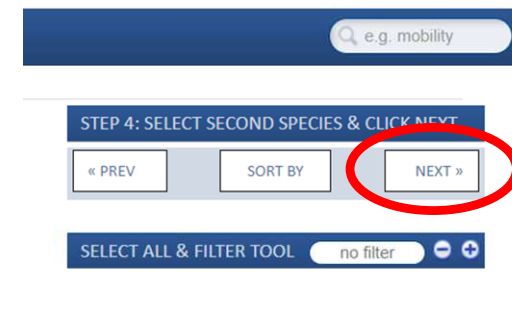


data type » databases » first species » **second species** » data groups » processes » output

## Ground states

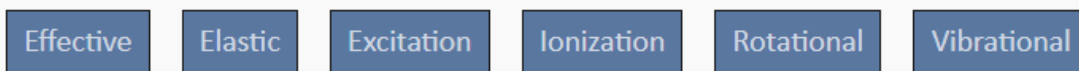


## State-specific and gas mixtures

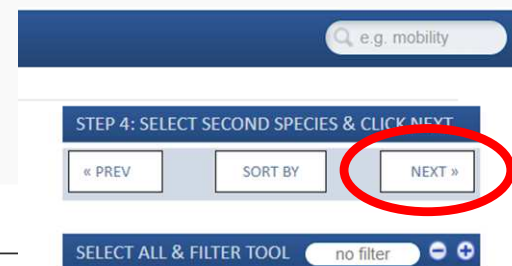


data type » databases » first species » second species » **data groups** » processes » output

## Cross section



**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]



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data type » databases » first species » second species » data groups » processes » output

### IST-Lisbon database

**Data Group [N]:** P. Coche, V. Guerra and L.L. Alves, "Microwave air plasmas in capillaries at low pressure I. Self-consistent modeling" 2016 J. Phys. D: Appl. Phys. 49 235207. The cross section set was obtained from Y. Wang, O. Zatsarinny and K. Bartschat 2014 Phys. Rev. A 89 062714, and it was extended to 1 keV using logarithmic extrapolation. These data, for the electron collisions with atomic nitrogen, complement the COMPLETE set of N<sub>2</sub> cross sections (available in this database under group N<sub>2</sub>) for use in a chemistry scheme. Here, N(2D) and N(2P) are also targets (in the superelastic collisions e+N(2D,2P) → e+N(4S)). Thus, when adopting this cross section set in Boltzmann calculations, one should also take the elastic momentum-transfer cross section for N(2D) and N(2P) (available in this database under group N-elec).

**Data Group [N<sub>2</sub>]:** J. Loureiro and C.M. Ferreira, "Coupled electron energy and vibrational distribution functions in stationary N<sub>2</sub> discharges" 1986 J. Phys. D 19 17. The complete cross sections set was compiled mostly from L.C. Pitchford and A.V. Phelps 1982 Bull. Am. Phys. Soc. 27 109 and K. Tachibana and A.V. Phelps 1979 J. Chem. Phys. 71 3544. The cross sections were originally limited to 40 eV kinetic energy, and were later extended to 1 keV using information from the databases BIAGI-v8.9 and PHELPS. The thresholds of vibrational cross sections for transitions from ground-state, N<sub>2</sub>(X,v=0) → N<sub>2</sub>(X,v') (1 ≤ v' ≤ 10), correspond to an anharmonic distribution of energy levels, close to the one obtained by assuming a Morse potential. When this complete set is used in a two-term Boltzmann solver (choosing a linear interpolation scheme), it yields calculated swarm parameters in good agreement with measurements for E/N values between 1 and 1000 Td. For E/N < 1 Td, the set must be further completed to include rotational excitation mechanisms (see below), in order to reproduce measured swarm data.  
**IMPORTANT NOTICE ABOUT ROTATIONAL TRANSITIONS**  
This set is to be completed with the rotational cross sections for transitions N<sub>2</sub>(X,v=0,J) → N<sub>2</sub>(X,v=0,J+2) (J=0,1,...,30), available in this database under group Nitrogen > N<sub>2</sub>-rot (see N<sub>2</sub>-rot description for more details). When the full cross section set for N<sub>2</sub> (containing momentum-transfer, and electronic excitation and ionization from ground-state) and N<sub>2</sub>-rot (including the rotational excitation / deexcitation to/from the N<sub>2</sub>(J=0), N<sub>2</sub>(J=1),..., N<sub>2</sub>(J=32) states) are used in a two-term Boltzmann solver, one obtains calculated swarm parameters in good agreement with measurements over a large range of E/N values (1e-4 to 1000 Td).

**Data Group [N<sub>2</sub>-rot]:** E. Gerjouy and S. Stein, "Rotational Excitation by Slow Electrons" 1955 Phys. Rev. 97 1671. N<sub>2</sub>-rot is a set of rotational excitation cross sections by electron impact, for transitions N<sub>2</sub>(X,v=0,J) → N<sub>2</sub>(X,v=0,J+2) (J=0,1,...,30), which complements the COMPLETE set of N<sub>2</sub> cross sections, available in this database under group N<sub>2</sub>. Calculations using these cross sections should include inelastic-stepwise and superelastic transitions between rotational states N<sub>2</sub>(J=0), N<sub>2</sub>(J=1),..., N<sub>2</sub>(J=32), assuming a Boltzmann distribution for their populations:  
 $n_J/N = (g_J/P_{rot}) \exp[-E_J/(k_B T_g)]$  with  $P_{rot} = \sum_{J=0}^{30} g_J \exp[-E_J/(k_B T_g)]$  [cf. L.S. Frost and A.V. Phelps 1962 Phys. Rev. 127 1621]. At T<sub>g</sub>=300K, these populations are n<sub>0</sub>/N=1.29E-02 n<sub>1</sub>/N=1.89E-02 n<sub>2</sub>/N=6.07E-02 n<sub>3</sub>/N=4.01E-02 n<sub>4</sub>/N=9.54E-02 n<sub>5</sub>/N=5.29E-02 n<sub>6</sub>/N=1.11E-01 n<sub>7</sub>/N=5.61E-02 n<sub>8</sub>/N=1.09E-01 n<sub>9</sub>/N=5.11E-02 n<sub>10</sub>/N=9.32E-02 n<sub>11</sub>/N=4.12E-02 n<sub>12</sub>/N=7.11E-02 n<sub>13</sub>/N=2.98E-02 n<sub>14</sub>/N=4.89E-02 n<sub>15</sub>/N=1.96E-02 n<sub>16</sub>/N=3.05E-02 n<sub>17</sub>/N=1.17E-02 n<sub>18</sub>/N=1.74E-02 n<sub>19</sub>/N=6.35E-03 n<sub>20</sub>/N=9.07E-03 n<sub>21</sub>/N=3.17E-03 n<sub>22</sub>/N=4.33E-03 n<sub>23</sub>/N=1.45E-03 n<sub>24</sub>/N=1.90E-03 n<sub>25</sub>/N=6.09E-04 n<sub>26</sub>/N=7.66E-04 n<sub>27</sub>/N=2.36E-04 n<sub>28</sub>/N=2.84E-04 n<sub>29</sub>/N=8.39E-05 n<sub>30</sub>/N=9.72E-05 n<sub>31</sub>/N=2.75E-05 n<sub>32</sub>/N=3.06E-05.

**Data Group [N<sub>2</sub>-vib]:** J. Loureiro and C.M. Ferreira, "Coupled electron energy and vibrational distribution functions in stationary N<sub>2</sub> discharges" 1986 J. Phys. D 19 17. N<sub>2</sub>-vib is a set of vibrational excitation cross sections by electron impact, for transitions N<sub>2</sub>(X,v) → N<sub>2</sub>(X,v') (1 ≤ v < v' ≤ 10), which complements the COMPLETE set of N<sub>2</sub> cross sections (available in this database under group N<sub>2</sub>) for use in a chemistry scheme. These cross sections were obtained by applying a threshold shift to the excitation cross sections for transitions from ground-state N<sub>2</sub>(X,v=0) → N<sub>2</sub>(X,v') (1 ≤ v' ≤ 10) (see group N<sub>2</sub> in this database). The cross sections are intended for use in electron kinetic calculations, e.g. when solving the electron Boltzmann equation. As recommended in Bourdon A and Vervisch P 2000 J. Thermophys. Heat Transfer 14 489 and in Colonna G et al 2015 Plasma Sources Sci. Technol. 24 035004, electron-vibrational mechanisms can be described in a chemistry model by using electron rate coefficients satisfying the scaling law  
 $k_{v,v+v'} = k_{0,v'} / (1 + 0.15^{v'})$  (1 ≤ v' ≤ 10; 0 ≤ v ≤ 49)  
where k<sub>0,v'</sub> are the rate coefficients for transitions from ground-state N<sub>2</sub>(X,v=0) → N<sub>2</sub>(X,v') (1 ≤ v' ≤ 10), that can be calculated from the corresponding electron cross sections (see group N<sub>2</sub> in this database).

**Data Group [N-elec]:** P. Coche, V. Guerra and L.L. Alves, "Microwave air plasmas in capillaries at low pressure I. Self-consistent modeling" 2016 J. Phys. D: Appl. Phys. 49 235207. The cross section set was obtained from Y. Wang, O. Zatsarinny and K. Bartschat 2014 Phys. Rev. A 89 062714, and it was extended to 1 keV using logarithmic extrapolation. These data, for electron collisions with the electronic excited states N(2D) and N(2P) of atomic nitrogen, complement the COMPLETE set of N<sub>2</sub> cross sections (available in this database under group N<sub>2</sub>) for use in a chemistry scheme.

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

### 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  $N_2(X,v\neq 0)$

**[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

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data type » databases » first species » **second species** » data groups » processes » output


### Ground states

Ar CH4 CO CO2 H2 He N2 O2

IST-Lisbon

### State-specific and gas mixtures

CO-rot CO\_anis Hydroge Nitrogen Oxygen

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data type » databases » first species » **second species** » data groups » processes » output

### Ground states

Ar CH4 CO CO2 H H2 He N N2 O2

Private database

### State-specific and gas mixtures

CO-elec CO-rot H2 (J=0) H2 (J=1) H2 (J=2) H2 (J=3) N-elec N2-rot N2-vib Oxygen

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  $N_2(X,v=0,J) \rightarrow N_2(X,v=0,J+2)$  ( $J=0,1,\dots,30$ ), which complements the COMPLETE set of N2 cross sections, available in this database under group N2.

⊕ ⊖ e / Nitrogen

- Rotational E + Nitrogen  $\leftrightarrow$  E + N2 (J=0-J=2) (E = 0.0015 eV, g1/g0 = 5, complete set) | [e + N2(X,v=0,J=0)  $\leftrightarrow$  e + N2(X,v=0,J=2), Rotational] Gerjouy E and Stein S 1955 Phys. Rev. 97 1671. Updated: 22 July 2022.
- Rotational E + Nitrogen  $\leftrightarrow$  E + N2 (J=1-J=3) (E = 0.0025 eV, g1/g0 = 2.33333, complete set) | [e + N2(X,v=0,J=1)  $\leftrightarrow$  e + N2(X,v=0,J=3), Rotational] Gerjouy E and Stein S 1955 Phys. Rev. 97 1671. Updated: 22 July 2022.

The name of the "State-specific and gas mixture" is **automatically assigned as *target species*** ( $\Rightarrow$  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 ( $\Rightarrow$  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)

```
1 %---- electron impact excitation/deexcitation ----
2 e + N2(X,v=0) <-> e + N2(A3Su+) | eedf
3 e + N(4S) <-> e + N(2D) | eedf
4
5 %---- e-V processes ----
6 e + N2(X,v=0) <-> e + N2(X,v=1) | eedf
7 e + N2(X,v=1:9) -> e + N2(X,v=v+1) | nitrogenEVscaling
8
9 %---- electron impact dissociation ----
10 e + N2(X,v=0) -> e + 2N(4S) | eedf
11
12 %---- electron impact ionization ----
13 e + N2(X,v=0) -> 2e + N2(+,X) | eedf
14 e + N2(A3Su+) -> 2e + N2(+,X) | eedf
15 e + N(4S) -> 2e + N(+,gnd) | eedf
16
17 %---- electron recombination ----
18 e + N2(+,X) -> 2N(4S) | powerElectronTemp
19
20 %---- heavy species collisions ----
21 N2(B3Pg) + N2(X) -> N2(A3Su+) + N2(X) | constantRateCoeff
22 N(2D) + N(4S) + N2(X) -> N2(B3Pg) + N2(X) | constantRateCoeff
23 N(2D) + N2(X) -> N(4S) + N2(X) | arrheniusGasTemp
24 N2(+,X) + N2(X,v=0) + N2(X) -> N4(+,X) + N2(X) | powerGasTemp
25 N(4S) + N(4S) + N2(X) -> N2(a1Pg) + N2(X) | arrheniusGasTemp
26 N2(C3Pu) -> N2(B3Pg) | constantRateCoeff
27
28 %---- V-V processes ----
29 N2(X,v=1:10) + N2(X,w=0:v-1) <-> N2(X,v=v-1) + N2(X,v=w+1) | nitrogenMolecularVV
30 N2(X,v=1:10) + N2(X,v=10) -> N2(X,v=v-1) + 2N(4S) | nitrogenMolecularVDis
31
32 %---- Molecular V-T processes ----
33 N2(X,v=1:10) + N2(X) <-> N2(X,v=v-1) + N2(X) | nitrogenMolecularVT
34 N2(X,v=10) + N2(X) -> 2N(4S) + N2(X) | nitrogenMolecularVTDis
35
36 %---- Atomic V-T processes ----
37 N2(X,v=7:10) + N(4S) <-> N2(X,v=v-1) + N(4S) | nitrogenAtomicVT
38
```

## 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 or 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)

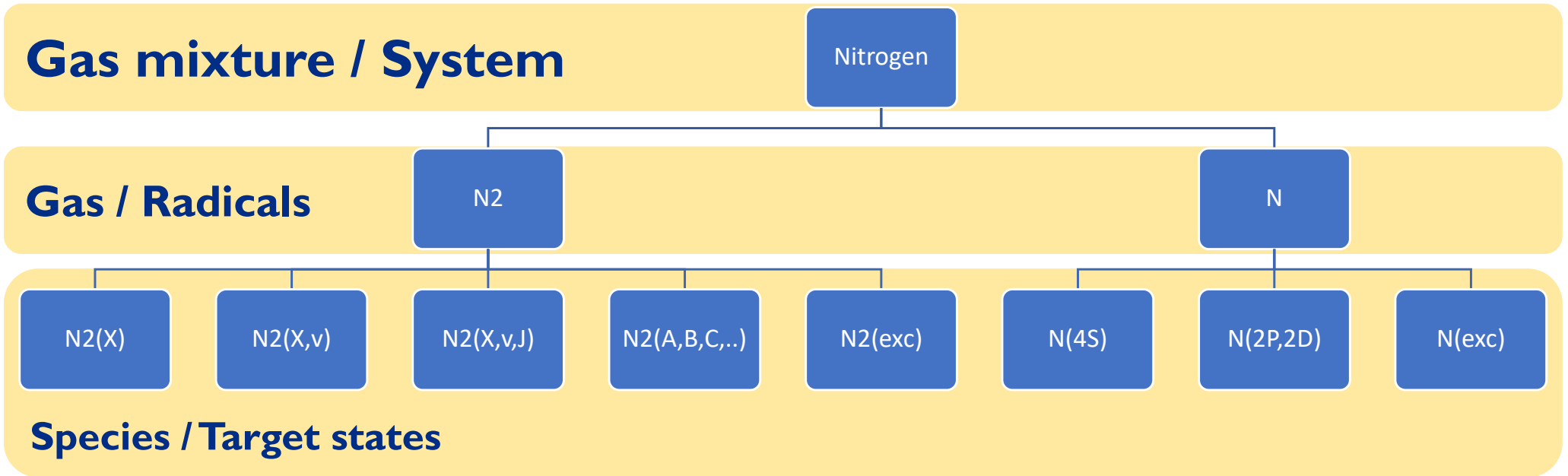
**Workaround** for parsing LXCat metadata: use of the free-field COMMENT in LXCat

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

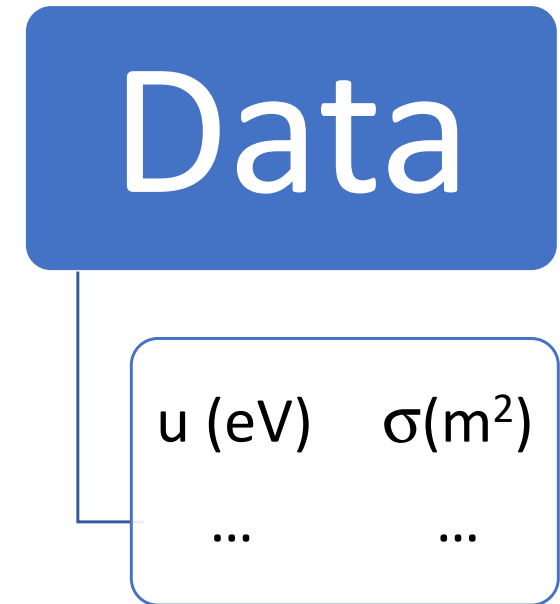
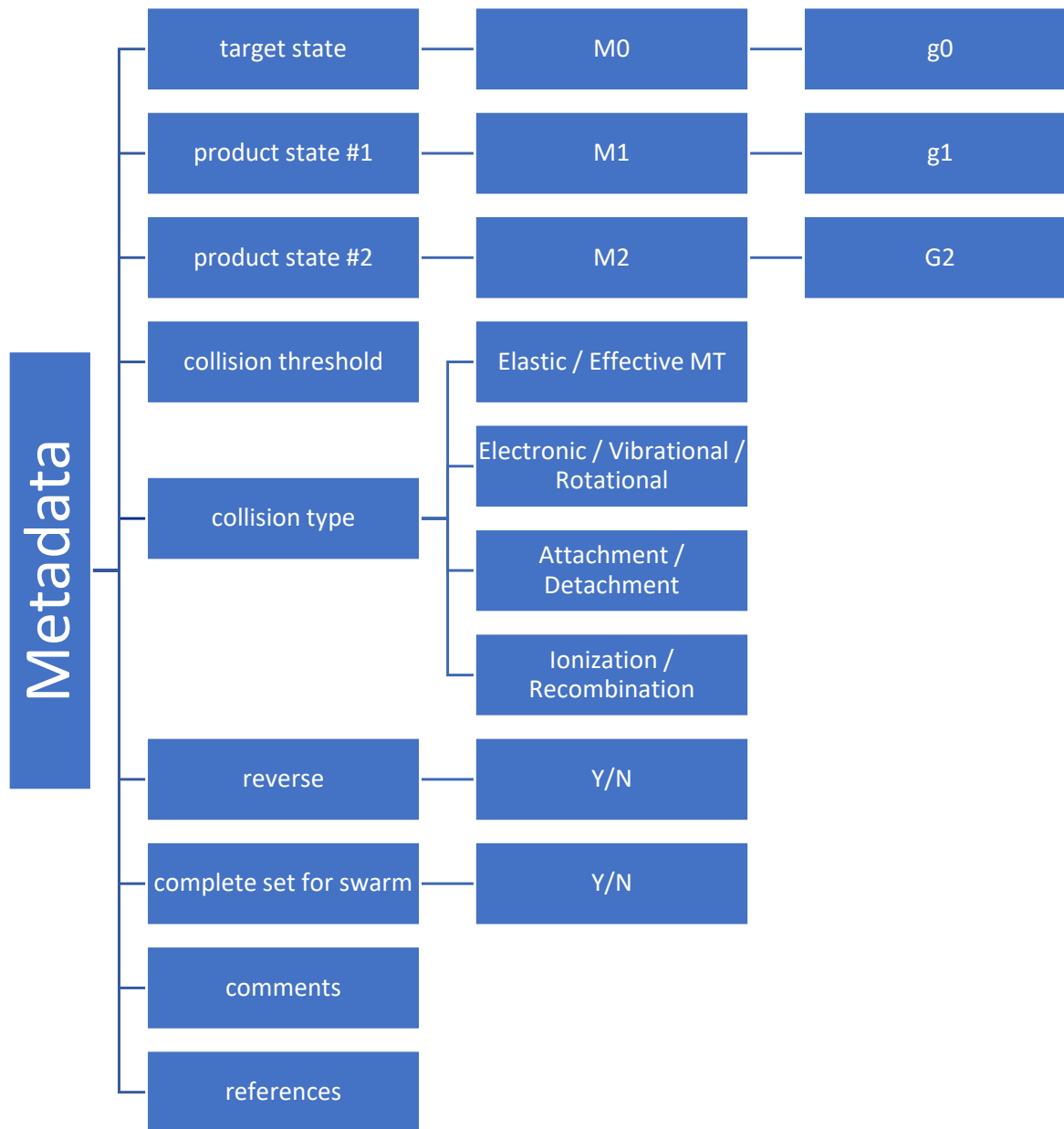
# Organization of e-scattering data – proposal

## 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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