

GAPHYOR Data Center

<http://gaphyor.lpgp.u-psud.fr>

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The GAPHYOR Data Center produces a Database on the properties of atoms, molecules and neutral or ionized gases, including Chemical Reactions, with about 500,000 entries.

1 Structure of a GAPHYOR record

The structure of a GAPHYOR entry was originally conceived to describe collisions/reactions in gases. It now describes also simpler (energy levels, ...) or more complex (gas-surface interactions, clusters, ...) phenomena. Every GAPHYOR entry includes the following fields:

/se/M1,M2,M3/pr/M4,M5,M6/
/info/enva/val/rem/
/an/jo,vo,page/au1,au2,...au10/nastci/

2 Initial and Final state: M1 M2 M3 - M5 M6 M7

Atomic and molecular reactants: /n form ix/s/

- **form** *Chemical formula:* Example /**H1C3N1O2**/.
1 to 4 elements, no more than 8 atoms in the molecule.
- **i** Index of ionization, **x** Index of excitation, **s** Index of internal structure.
- **n** Multiplicity of the Reactant (e.g. 2 **H** atoms in initial state).

Electrons, photons, fields, particles.

Special Reactants:

- Iso-electronic series. Example: **Aa(He)Z(02 - 12)**
- Clusters. Examples: **He(H2O)3/+**, **(C)60**
- Surface reactants (solid/liquid walls, adsorbed atoms/molecules).

3 Sections SE and Processes PR

GAPHYOR is a “broad band” Database organized into 5 Sections:

- 1 Properties of isolated atoms and molecules
- 2 Photonic Collisions
- 3 Electronic Collisions
- 4 Collisions between atoms or molecules
- 5 Macroscopic properties of Gases

| | Struct. | $h\nu$ coll. | e coll. | At.mol.coll. | Mac.prop. | Σ |
|-----------|---------|--------------|-----------|--------------|-----------|----------|
| Fact.Data | 267178 | 26941 | 29743 | 124753 | 32006 | 480621 |
| Num.Data | 6642 | 347 | 1650 | 9010 | 734 | 18383 |
| Σ | 272730 | 27244 | 30810 | 132107 | 32642 | 495533 |

Table 1: Statistics of Data (June 15th, 1997)

The list of Processes (PR) included in every Section (SE) is given in Appendix 1.

4 Additional information INFO

- Type of Data: **S** Total and transport cross sections, **R** Reaction rate constants, ...
- Nature of Data: **T** Theoretical data, **E** Experimental data, ...
- Energy domains: **L** Thermal, **J** Medium, **H** High energies
- Special information: **8** Clusters, / Gas-surface interactions, ...

5 Numerical Data

- **ENVA** gives the energy, or energy range covered by the Data. Example: 10 - 50 - 100 eV
- **VAL** gives the values them-selves (cross-sections, ...). Example: 3.5 - 12.2 - 6.4 E-16 cm²
- **REM** gives additional information (e.g. spectroscopic notations).

Note that the general idea is to give *simple information* (eg. lifetimes, reaction rates), or some *orders of magnitude*.

6 Internet server

GAPHYOR WWW server is now well developed and user-friendly. Its main features are:

- **Query forms.** Two query forms (simple and advanced search) are offered.
- **Intermediate report.** This gives a sketch of the first results of a search and offers some specific additional choices to the user.

- **Data displays.** Two displays are offered: a full display of all the found entries (possibly selecting the most recent ones), or, for large Data sets, a tabular display obtained by downloading a postscript file, which can then be printed locally.

Simplified statistics on User Locations are shown below.

| na | data sets | org.na | data sets |
|----------|-----------|-------------------|-----------|
| fr | 6098 | u-psud.fr | 1099 |
| ?? | 2293 | uni-heidelberg.de | 857 |
| de | 1194 | cnrs-immn.fr | 597 |
| ru | 1151 | univ-lille1.fr | 580 |
| us | 993 | cea.fr | 535 |
| jp | 530 | onera.fr | 337 |
| ... | ... | ... | ... |
| Σ | 14 885 | | 14 885 |

Table 2: Nations and Organizations using GAPHYOR

7 GAPHYOR Handbook

GAPHYOR is going to publish a new (fully redesigned) version of the HANDBOOK. The Volumes will be grouped in two Series:

- **Chemical Volumes** (17) describing the properties of a given group of Chemical systems.
- **Thematic Volumes** (9) describing a given group of Processes for all Chemical Systems.

The publication timing will be a function of the various orders from users for one or several specific Volumes. The sizes are small, so as to make it easy for every user to order only the Volumes covering their own field of interest.

The orders (see form in the Web) will be satisfied within a period of one month after receipt of payment.

| Chemical Volumes | | Selection | Pages | Price \$ |
|-------------------------|---|-----------|-------|----------|
| C01 | Hydrogen,Deuterium,Tritium | 62% | 130 | 12 |
| C02 | H + Noble Gases (He,Ne,Ar,Kr,Xe,Rn) + .. | 72% | 130 | 12 |
| C03 | H + Mono-,bi- and trivalent elements + .. | 60% | 130 | 12 |
| C04 | H + Carbon/Titanium Groups + .. | 48% | 410 | 30 |
| ... | see List in the Web | ... | ... | ... |
| C17 | Surfaces/Clusters | 52% | 130 | 12 |
| Thematic Volumes | | | | |
| T00 | Cross Sections/Reaction Rates (Numerical values) | 100% | 110 | 10 |
| ... | see List in the Web | ... | ... | ... |
| T30 | Electronic Collisions (Section 3) | 62% | 210 | 18 |
| T50 | Macro.Prop. of Gases (Section 5: Transport coefficients,..) | 58% | 210 | 15 |
| | | Σ | 4640 | 321 |

Table 3: Handbook Volumes

8 Appendix 1

Section 1. Structure

EN **Energy levels , wave functions**
EA Unstable energy levels
EI Energy of isomerization
VR Potentiel curves, structure of molecules
DP Dipolar moments
PE Electric (or magnetic) polarizability
TR **Radiative transition (probability,...)**
IN Autoionization
DT Autodetachment

Section 2. Photonic collisions

SN **Effective absorption, total diffusion**
AN True absorption
SC Angular diffusion (scattering)
EL Elastic diffusion (Thomson, Rayleigh)
DO Depolarization, Change of polarization
EX **Photoexcitation**
ER Emission of line
DX Photodeexcitation (stimulated emission)
FF Free-free absorption(inv. bremsstrahlung)
IN **Photoionization**
IM Creation of an ion pair (positive-negative)
DT Photodetachment
DS Photodissociation
EE Photoemission of electrons (ions) by solids

Section 3. Electronic Collisions

SN **Total cross sections**
SM Transport cross sections (momentum, ...)
EL Elastic collision
DO Depolarization, Change of polarization
EX **Excitation**
DX Deexcitation
BS Bremsstrahlung
IN **Ionization**
IM Creation of an ion pair (positive-negative)
DT Detachment
AT Attachment
RR Radiative recombination
RD Dielectronic recombination
RE e-e-i recombination
RO e-i-o recombination
RS Dissociative recombination
DS Dissociation
DG **Desorption**
EE Emission of electrons by a solid
PU Emission of neutrals or ions by solids (sputtering)

Section 4. Atom./mol. Coll. (and Reactions)

EN **Energy or enthalpy of reaction**
KE Constant of chemical equilibrium
SN **Total cross sections**

SM Transport cross sections (momentum, ...)
SC Angular diffusion (scattering)
SP Stopping power
EL Elastic collision
DO Depolarization, change of polarization
EX **Excitation**
DX Deexcitation (quenching)
TE Excitation transfer
IN **Ionization**
IM Creation of an ion pair (positive-negative)
DT Detachment
TI Ionizing charge transfer
RI Recombination ion-ion
CX Charge transfer
XD Dissociative charge transfer
CA Capture of electrons
SR Loss of electrons (stripping)
DS **Dissociation**
IR Interchange reaction (of one or several atoms)
IA Associative interchange reaction
ID Dissociative interchange reaction
AS Association
DG **Desorption**
AD Adsorption
EE Emission of electrons by a solid
PU Emission of neutrals or ions by solids (sputtering)

Section 5. Macroscopic properties

ST **Statistics of levels**
FT Thermodynamic functions
PV Compressibility, equation of state
PE Dielectric and magnetic constants
DN **Diffusion**
VI Viscosity
CT Thermal conductivity
LW **Line broadening and shift (collisional effects)**
PI **First coefficient of Townsend**
DT Detachment
AT Attachment
FE Distribution function of electrons
ME Mobility of electrons
CE Electrical conductivity
DE Diffusion of electrons
MD Characteristic temperature of electrons (D/μ)
PC Power delivered by electron-neutral collisions
FI **Distribution function of ions**
MI Mobility of ions
DI Diffusion of ions
DA Ambipolar diffusion

Remark This list is slightly simplified (see the Web)