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Summary: comprehensive H - H_2 - H^- - H_2^+ - H_3^+ He … databases

Roberto Celiberto, Detlev Reiter, Keiji Sawada, Dirk Wünderlich, Jung-Sik Yoon

3rd meeting of the CRP on Hydrogen and Helium, Mon-Wed 14-16 March 2016 at IAEA

Databases presented at CRP:

1.) K. Sawada (Nagano)
2.) D. Wünderlich (IPP)
3.) R.Janev/D.Reiter (FZJ)
4.) R. Celiberto (Bari)

Significant differences, but also:
Significant inter-dependencies,
not independent,
thanks to AMDS-unit community building

Additionally: IAEA, ORNL, ADAS (H_2 ?), NIFS,……,
plus: other communities

Customers in fusion:

Divertor (fusion) plasma dynamics
Fusion edge plasma spectroscopy
Ancillary (low T) technical plasmas

Data needs:
span 4-5 orders in key parameters:
plasma composition, density,
temperature, spatio-temporal scales

Categories of Processes

- e + H → H*, p, H^- + (electrons, photons)
- p + H → …..
- e/p/H + H^- → …..
- e + H_2(…) → …..
- p + H_2(…) → …..
- H,H_2,H^- + H_2 → …..
- Photonic processes in H_2
- e,H,H_2,H^- + H_2^+ → …..
- e,H,H_2,H^- + H_3+ →…..

If all processes are H(n,l,m), and H_2(N,v,J) resolved (and isotopes, isotopomeres, and He, He_2^+, HeH^+,…) →nearly endless list of data needs.

Consensus from all fusion user communities:

Identify

a) Most sensitive sub-models

b) discrepancies, inconsistencies, in existing databases, wrt. exp. data for single collision processes (e.g. evaluated data from NFRI: where are mismatches to existing databases?

and **prioritize data needs** from there:

1) Vibrational distribution in $H_2(X\ ^1\Sigma_g^+, v)$ (T=0.5 – 20 eV)

(such as e,p,H,H_2 collisions on H_2(X,v), v→v+1, v+2,…)

because of high v-sensitivity (in all presented databases) of processes involving H_2(X,v) and of the highest abundance of H_2(X,v)

Try to estimate from basic molecular physics: relaxation times of T_e (or eedf), T_{vib} or pdf(v), T_{rot} or pdf(v,J), compare to timescales of interest in particular application

T, E: 0.5 -- 20 eV, n_e, n_p, n_{H2}: 10^8 – 10^{15} cm^{-3}

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(Beam heating of fusion plasmas: 100 keV – MeV range,

no molecules, high energy asymptotics, mostly heavy particle collisions, is a separate matter..)

2) Excitation/Ionization cross sections of $H_2^*(\Lambda)$, $H_2^+(X)$, starting from $H_2(X,v)$. $H_2(\Lambda,v)$, $H_2(\Lambda,v,J)$ singlet, triplet states, start with N=2,N=3, and then proceed from there.

(Clarify mismatches with evaluated exp. data, if any

data evaluation: Miles, vs. Janev)

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$H_2(X) + e \rightarrow H_2^* + e$

R.K.Janev, D.Reiter, U.Samm,

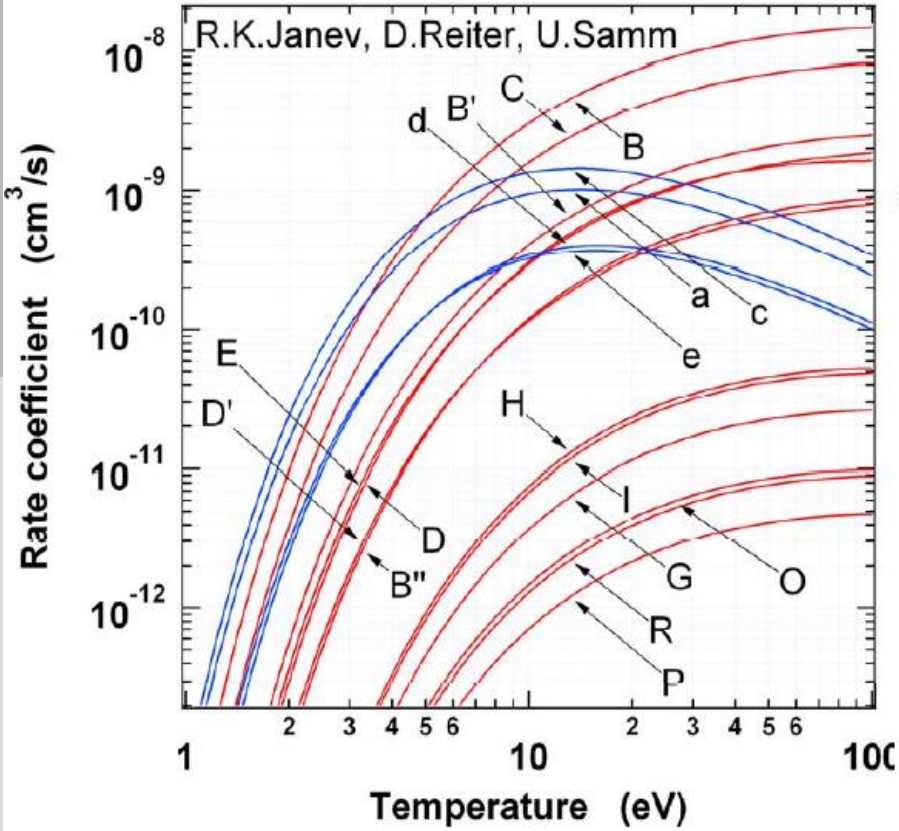
Collision Processes in Low-Temperature Hydrogen Plasmas,

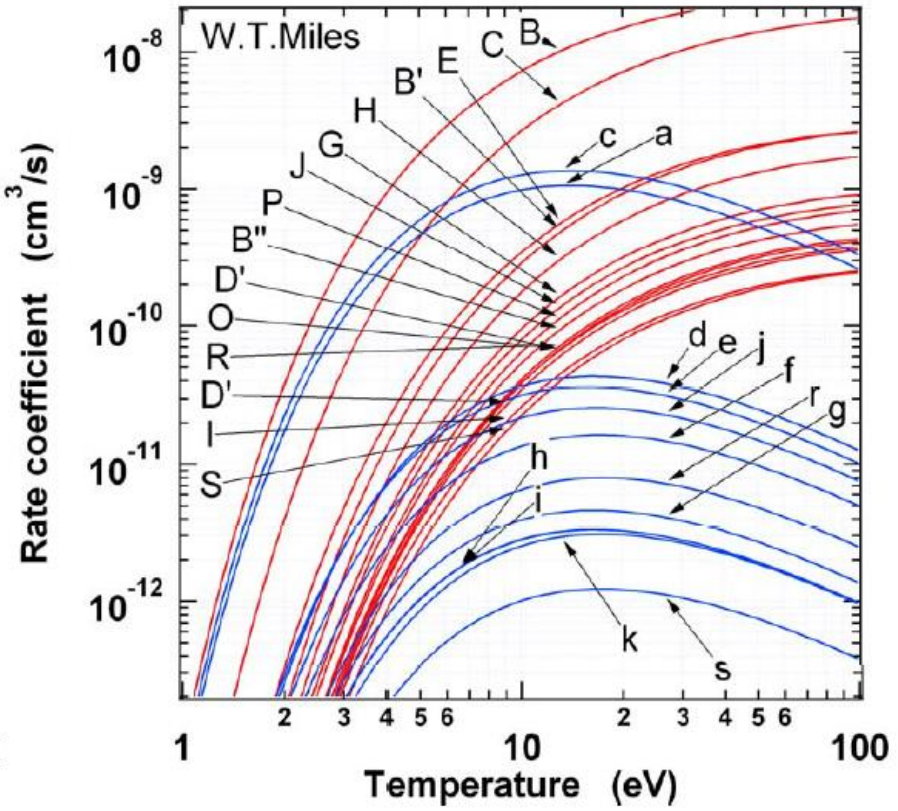
http://www.eirene.de/report_4105.pdf

W.T. Miles, R. Thompson, and A.E.S. Green, J. Appl. Phys. 43, 678 (1972).

Born-Bethe approximation modified at low energies by phenomenological techniques

All cross sections are given for n<=4.





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3) Isotopomeres: which reaction channels have an isotope effect, which can not be scaled, (Celiberto) if we use ro-vibrational energy rather than v,J states of H_2, D_2, T_2, HD, HT, DT, and their ions. (such as diss. electron attachment ??)

4.) Helium:

e,p,He^+,He^{++} + He:

e + He: full set of cross sections from R-Matrix, CCC calculations,
→ experimental evaluation, validation (see X.U. talk)

p, He^{++}, He^+, + He(GS,MS,…) CX involving (MS) excited states,
experimental evaluation, validation of CX rates

He_2^+, HHe^+ : formation (abundance of reaction partners, E, T) ? ,
lifetime in plasma, → relevant energy range

n.b.: DR paper on BeH^+ (I. Schneider, et al.) just rejected by editors of PPCF “out of scope of journal”, although BeH^+ clearly visible in JET, (ITER with Be walls): Energy, Temperature range !!

Special applications (with relation to Nucl. Fusion work, but not: fusion plasmas themselves)

- $e + H \rightarrow H^*, p, H^- + (electrons, photons)$
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For plasma sources, e.g. NBI sources

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For planetary atmospheres, re-entry

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For NBI-heating, (CX, CX recomb. on high Z)