

# Élaboration d'une base de données nécessaire à la modélisation des plasmas thermiques

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Le rapport contient

# Logiciels de calcul de la composition chimique

Les codes permettant le calcul de la composition	
<b>ESM Software</b> TAPP HSC Factsage/sage Chemsheet Chemapp	<a href="http://www.esmsoftware.com/tapp/">http://www.esmsoftware.com/tapp/</a> <a href="http://www.esm-software.com/hsc/">http://www.esm-software.com/hsc/</a> <a href="http://www.esmsoftware.com/factsage/">http://www.esmsoftware.com/factsage/</a> <a href="http://www.esmsoftware.com/chemsheet/">http://www.esmsoftware.com/chemsheet/</a> <a href="http://www.esm-software.com/chemapp">http://www.esm-software.com/chemapp</a>
<b>Thermodata</b> Coach Gemini 1 et 2 Gemplot	<a href="http://thermodata.online.fr/index.html">http://thermodata.online.fr/index.html</a>
<b>SGTE</b> Pure, SSUB, SSOL	<a href="http://www.sgte.org/">http://www.sgte.org/</a>
<b>CODATA</b>	<a href="http://www.codata.org/index.html">http://www.codata.org/index.html</a>
<b>MELTS</b>	<a href="http://www1.gly.bris.ac.uk/cetsei/melts/Melts.htm">http://www1.gly.bris.ac.uk/cetsei/melts/Melts.htm</a>
<b>THERMO-CALC</b>	<a href="http://www.thermocalc.com/">http://www.thermocalc.com/</a> <a href="http://www.thermocalc.com/Filer/Pdf/Manuals/TCCQ_UsersGuide.pdf">http://www.thermocalc.com/Filer/Pdf/Manuals/TCCQ_UsersGuide.pdf</a>
<b>MT-DATA</b>	<a href="http://www.npl.co.uk/mtdata/winmt.htm">http://www.npl.co.uk/mtdata/winmt.htm</a>
<b>TTWINNER</b>	<a href="http://ttwinner.free.fr/">http://ttwinner.free.fr/</a>
Les codes permettant le calcul du rayonnement	
<b>LIFBASE</b>	<a href="http://www.sri.com/psd/lifbase/">http://www.sri.com/psd/lifbase/</a>
<b>DIATOMIC</b>	<a href="http://www.sri.com/psd/diatomic/">http://www.sri.com/psd/diatomic/</a>

# Sources de données spectroscopiques

	Données numériques	Ref biblio	Calcul en ligne
Harvard-Smithsonian Cfa (USA) - kelly, Krurucz	EL-WL-TP		
IAEA (Autriche) - AMDIS - ALLADIN - AAEXCITE - RATES	CR-RC	MSC	CS KP
IAPCM (chine) - CAMBD	MSC	MSC	
ISAN (russie) - BIBL		MSC	
KAERI (Corée) - AMODS	MSC		EL-WL-TP
LANL ( USA) - LAPC			MSC
NASA ( USA) - TIPTOP	EL-WL-TP- CR-RC		
NIFS (Japon) - PLAM	CR-RC	MSC	
NIST (USA) - ASD - Chandra - ATP - ASL	EL-WL-TP EL-WL-TP	EL-WL-TP TP TP LB	SP
ORNL (USA) - Bibliography - MIRF	CS	MSC	
Vanderbilt University (USA) - MCHF/MCDHF	EL-WL-TP		WF
VNIITF-VNIIFTR - SPECTR-W <sup>3</sup>	MSC	MSC	

CS section efficace

EL niveaux d'énergie

KP paramètres  
cinétiques

LB élargissement ra

TP probabilité de  
transition

WL longueur d'onde

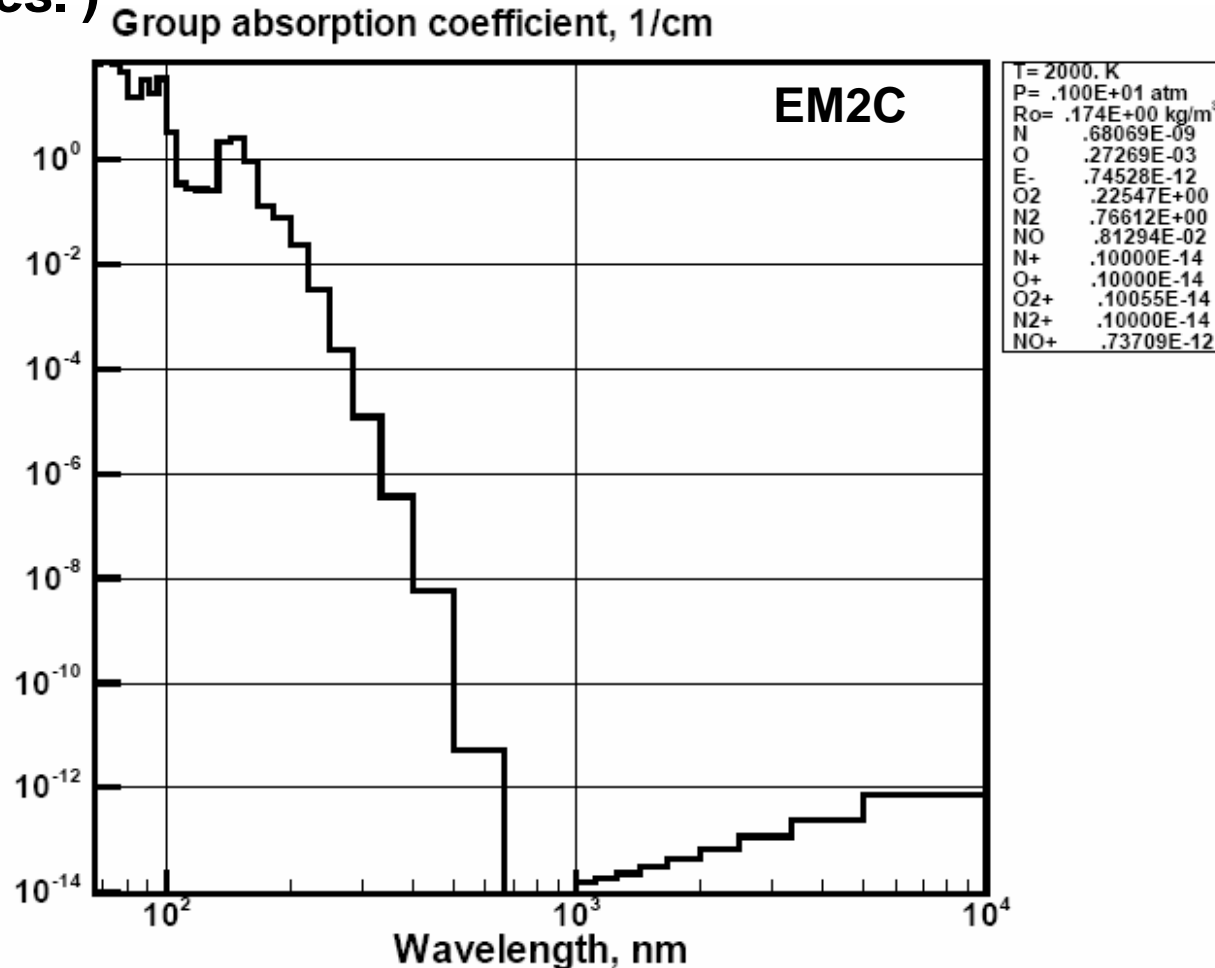
# Quelques propriétés de transport

**Ar, He, Cu, SF<sub>6</sub>, O<sub>2</sub>, N<sub>2</sub>, CO, CO<sub>2</sub>, Fe, CO, air, POM, PE, PMMA, PA66, PC, SF<sub>6</sub>-Cu, SF<sub>6</sub>, N<sub>2</sub>, ... + certains de leur mélange. )**

Propriétés T Temperature	H Enthalpie	ROEL Masse vol. volumique	CPEL Chaleur massique	SIGEL Conductivité électrique	VISEL Viscosité dynamique	XLABEL Conductivité thermique	XKABEL Coefficient d'absorption
K	J/kg	kg/m <sup>3</sup>	J/(kg K)	ohm/m	kg/(m s)	w/(m K)	-
300.00	14000.	1.6225	520.33	0.13214E-03	0.34224E-04	0.26712E-01	0.10000E-09
400.00	65800.	1.2169	520.33	0.13214E-03	0.34224E-04	0.26712E-01	0.10000E-09
500.00	0.11699E+06	0.97353	520.33	0.13214E-03	0.34224E-04	0.26712E-01	0.10000E-09
600.00	0.16905E+06	0.81121	520.63	0.13214E-03	0.39245E-04	0.30631E-01	0.10000E-09
700.00	0.22110E+06	0.69530	520.53	0.13214E-03	0.44858E-04	0.35011E-01	0.10000E-09
800.00	0.27215E+06	0.60839	520.48	0.13214E-03	0.49742E-04	0.38823E-01	0.10000E-09
900.00	0.31319E+06	0.54079	520.44	0.13214E-03	0.53921E-04	0.42085E-01	0.10000E-09
1000.0	0.36524E+06	0.48672	520.41	0.13214E-03	0.57633E-04	0.44982E-01	0.10484E-08
1100.0	0.41727E+06	0.44248	520.39	0.13214E-03	0.61076E-04	0.47669E-01	0.25818E-07
1200.0	0.46931E+06	0.40561	520.38	0.13214E-03	0.64374E-04	0.50243E-01	0.37184E-06
1300.0	0.52135E+06	0.37441	520.37	0.13214E-03	0.67598E-04	0.52760E-01	0.35842E-05
1400.0	0.57339E+06	0.34767	520.36	0.13214E-03	0.70787E-04	0.55249E-01	0.25194E-04
1500.0	0.62542E+06	0.32450	520.36	0.13214E-03	0.73960E-04	0.57725E-01	0.13753E-03
1600.0	0.67746E+06	0.30422	520.35	0.13214E-03	0.77125E-04	0.60195E-01	0.61060E-03
1700.0	0.72949E+06	0.28633	520.35	0.13214E-03	0.80284E-04	0.62661E-01	0.22896E-02
1800.0	0.78152E+06	0.27042	520.34	0.13214E-03	0.83437E-04	0.65122E-01	0.74442E-02
1900.0	0.83356E+06	0.25619	520.34	0.13214E-03	0.86582E-04	0.67576E-01	0.21465E-01
2000.0	0.88559E+06	0.24338	520.34	0.13214E-03	0.89715E-04	0.70022E-01	0.55868E-01
2100.0	0.93763E+06	0.23179	520.34	0.13214E-03	0.92834E-04	0.72456E-01	0.13314E+00
2200.0	0.98966E+06	0.22126	520.34	0.13214E-03	0.95935E-04	0.74877E-01	0.29398E+00
2300.0	0.10417E+07	0.21164	520.33	0.13214E-03	0.99017E-04	0.77282E-01	0.60630E+00
2400.0	0.10937E+07	0.20282	520.33	0.13214E-03	0.10208E-03	0.79669E-01	0.11774E+01
2500.0	0.11458E+07	0.19471	520.33	0.13214E-03	0.10511E-03	0.82038E-01	0.21652E+01
2600.0	0.11978E+07	0.18722	520.33	0.13214E-03	0.10812E-03	0.84387E-01	0.37889E+01
2700.0	0.12498E+07	0.18029	520.33	0.13214E-03	0.11110E-03	0.86714E-01	0.63317E+01
2800.0	0.13019E+07	0.17385	520.33	0.13214E-03	0.11405E-03	0.89019E-01	0.10133E+02
2900.0	0.13539E+07	0.16786	520.33	0.13214E-03	0.11698E-03	0.91301E-01	0.15563E+02
3000.0	0.14059E+07	0.16226	520.33	0.13214E-03	0.11987E-03	0.93561E-01	0.22960E+02

# Quelques propriétés radiatives

( Ar, He, Cu, SF<sub>6</sub>, O<sub>2</sub>, N<sub>2</sub>, CO, CO<sub>2</sub>, H<sub>2</sub>O, CH<sub>4</sub>, Fe, CO, air, SF<sub>6</sub>-Cu, SF<sub>6</sub>, N<sub>2</sub>, mélanges. )



Group absorption coefficients of high temperature air at  $p = 1$  atm and  $T = 2000$  F

## Propriétés de transports et radiatives



• Composition + intégrales de collision

		sigma (Å)	Eps (K/particle)
C	C	3	100
CH <sub>4</sub>	CH <sub>4</sub>	3.8	144
CH <sub>4</sub> O	CH <sub>4</sub> O	3.585	507
CO	CO	3.60	100
CO <sub>2</sub>	CO <sub>2</sub>	4	200
C <sub>2</sub> H	C <sub>2</sub> H	4	235
C <sub>2</sub> H <sub>2</sub>	C <sub>2</sub> H <sub>2</sub>	4.221	184
C <sub>2</sub> H <sub>4</sub>	C <sub>2</sub> H <sub>4</sub>	4.232	205
C <sub>2</sub> H <sub>6</sub>	C <sub>2</sub> H <sub>6</sub>	4.418	230
C <sub>3</sub> H <sub>4</sub>	C <sub>3</sub> H <sub>4</sub>	4.602	274.5
C <sub>3</sub> H <sub>6</sub>	C <sub>3</sub> H <sub>6</sub>	4.592	276.34
C <sub>3</sub> H <sub>8</sub>	C <sub>3</sub> H <sub>8</sub>	5.061	254
C <sub>4</sub> H <sub>6</sub>	C <sub>4</sub> H <sub>6</sub>	5.086	309
C <sub>4</sub> H <sub>8</sub>	C <sub>4</sub> H <sub>8</sub>	5.228	306.9
C <sub>2</sub> H <sub>4</sub> O	C <sub>2</sub> H <sub>4</sub> O	4.373	325.45
C <sub>2</sub> H <sub>4</sub> O <sub>2</sub>	C <sub>2</sub> H <sub>4</sub> O <sub>2</sub>	4.672	449.65
C <sub>2</sub> H <sub>6</sub> O	C <sub>2</sub> H <sub>6</sub> O	4.455	391.0
C <sub>3</sub> H <sub>6</sub> O	C <sub>3</sub> H <sub>6</sub> O	4.994	378.35
C <sub>3</sub> H <sub>8</sub> O	C <sub>3</sub> H <sub>8</sub> O	5.069	425.5
C <sub>4</sub> H <sub>8</sub> O	C <sub>4</sub> H <sub>8</sub> O	5.42	404.80
H	H	2.6	40
H <sub>2</sub>	H <sub>2</sub>	2.968	37.30
H	H	2.8	40
O	O	2.8	117
O <sub>2</sub>	O <sub>2</sub>	3.499	100
O	O	3.011	107.3
O <sub>2</sub>	NO	3.479	111.65
O	NO	3.150	120.5
O <sub>3</sub>	O <sub>3</sub>	3.756	100
N	N	2.98	119
N <sub>2</sub>	N <sub>2</sub>	3.68	91.5
N	N	3.33	104.5
N <sub>2</sub>	O <sub>2</sub>	3.557	101.85
N <sub>2</sub>	NO	3.6	109.14
NO	NO	3.53	105
NO <sub>2</sub>	NO <sub>2</sub>	4.06	97
N <sub>2</sub> O	N <sub>2</sub> O	3.85	219

Chemical species	$\alpha$ ( $10^{-30} \text{m}^3$ )	References
H	0.666793	[25]
C	1.76	[25]
N	1.10	[25]
O	0.802	[25]
CO	1.95	[25]
H <sub>2</sub>	0.8059	[25]
N <sub>2</sub>	1.7403	[25]
NO	1.70	[25]
O <sub>2</sub>	1.5812	[25]
OH	1.470	[13]
CH	2.270	[13]
C <sub>2</sub>	3.200	[13]
CO <sub>2</sub>	2.911	[25]
H <sub>2</sub> O	1.45	[25]
HCN	2.525	[25]
C <sub>2</sub> H	3.870	[13]
N <sub>2</sub> O	3.03	[25]
NO <sub>2</sub>	3.02	[25]
CH <sub>2</sub>	2.940	[13]
CH <sub>3</sub>	2.76	approximation
C <sub>2</sub> H <sub>2</sub>	3.63	[25]
O <sub>3</sub>	3.21	[25]
C <sub>3</sub>	4.9	approximation
CH <sub>2</sub> O	3.740	[13]
CH <sub>4</sub>	2.593	[25]

Table 4. Parameter A and B that characterized resonant charge exchange.

		A	B	References
C	C <sup>+</sup>	20.1	0.864	Evaluate from [42][43]
H	H <sup>+</sup>	28.69	1.3	[30][34]
N	N <sup>+</sup>	26.61	1.27	[37]
N <sub>2</sub>	N <sub>2</sub> <sup>+</sup>	24.5	1.032	[37]
NO	NO <sup>+</sup>	23.61	1.095	[37]
O	O <sup>+</sup>	19.5	0.832	[37]
O <sub>2</sub>	O <sub>2</sub> <sup>+</sup>	24.05	1.132	[37]

# Quelques données spectroscopiques



## Nécessaires pour calcul composition chimique

### Atomique + moléculaire (N, N<sub>2</sub>, O<sub>2</sub>, O<sub>2</sub><sup>+</sup>, N<sub>2</sub><sup>+</sup>,.....)

-----  
 ATOM = N Z = 1. ATOMW = 14.

NTSMAX = 228 NIMAX = 90 NPterm = 2

Comments: #S=2S+1, #S''=2S''+1.

n	E(n,l)	J	n	l	q	#S	L	$\pi$	#S''	L''	$\pi''$	sh
---	--------	---	---	---	---	----	---	-------	------	-----	---------	----

1	0.	1.5	2	1	3	4	0	0	0	0	0	0
2	19223.	2.5	2	1	3	2	2	0	0	0	0	0
2	19231.	1.5	2	1	3	2	2	0	0	0	0	0
3	28840.	1.5	2	1	3	2	1	0	0	0	0	0
3	28840.	0.5	2	1	3	2	1	0	0	0	0	0
4	83285.5	0.5	3	0	1	4	1	1	3	1	1	0
4	83319.3	1.5	3	0	1	4	1	1	3	1	1	0
4	83366.0	2.5	3	0	1	4	1	1	3	1	1	0
5	86131.4	0.5	3	0	1	2	1	1	3	1	1	0
5	86223.2	1.5	3	0	1	2	1	1	3	1	1	0
6	88109.5	2.5	2	1	4	4	1	1	0	0	0	0
6	88153.4	1.5	2	1	4	4	1	1	0	0	0	0
6	88173.0	0.5	2	1	4	4	1	1	0	0	0	0
7	93582.3	0.5	3	1	1	3	1	0	3	1	1	0
8	94772.2	0.5	3	1	1	4	2	0	3	1	1	0
8	94794.8	1.5	3	1	1	4	2	0	3	1	1	0
8	94832.1	2.5	3	1	1	4	2	0	3	1	1	0
8	94883.1	3.5	3	1	1	4	2	0	3	1	1	0
9	95476.5	0.5	3	1	1	4	1	0	3	1	1	0
9	95494.9	1.5	3	1	1	4	1	0	3	1	1	0
9	95533.2	2.5	3	1	1	4	1	0	3	1	1	0
10	96751.7	1.5	3	1	1	4	0	0	3	1	1	0
11	96788.2	1.5	3	1	1	2	2	0	3	1	1	0
26	109813.5	0.5	5	0	1	4	1	1	3	1	1	0
26	109857.8	1.5	5	0	1	4	1	1	3	1	1	0
26	109927.9	2.5	5	0	1	4	1	1	3	1	1	0
27	110029.2	0.5	5	0	1	2	1	1	3	1	1	0
27	110108.5	1.5	5	0	1	2	1	1	3	1	1	0
28	110196.	1.5	4	2	1	4	3	1	3	1	1	0
28	110214.	2.5	4	2	1	4	3	1	3	1	1	0
28	110248.	3.5	4	2	1	4	3	1	3	1	1	0
28	110304.	4.5	4	2	1	4	3	1	3	1	1	0
29	110221.	0.5	4	2	1	4	2	1	3	1	1	0
29	110275.	1.5	4	2	1	4	2	1	3	1	1	0
29	110288.	2.5	4	2	1	4	2	1	3	1	1	0
29	110339.	3.5	4	2	1	4	2	1	3	1	1	0
30	110221.7	1.5	4	2	1	2	1	1	3	1	1	0
30	110244.6	0.5	4	2	1	2	1	1	3	1	1	0
31	110311.0	2.5	4	2	1	2	3	1	3	1	1	0
31	110373.	3.5	4	2	1	2	3	1	3	1	1	0
32	110325.	0.5	4	2	1	4	1	1	3	1	1	0
32	110351.	1.5	4	2	1	4	1	1	3	1	1	0
32	110403.	2.5	4	2	1	4	1	1	3	1	1	0
33	110448.3	1.5	4	2	1	2	2	1	3	1	1	0
33	110470.5	2.5	4	2	1	2	2	1	3	1	1	0
34	110521.9	1.5	3	1	1	2	2	0	1	2	1	0

# Quelques donnees spectroscopiques

→ Nécessaires pour calcul du transfert radiatif

Force d'oscillateur, coef. D'Einstein, .....

## Atomique

Atom: N

Nlines = 1706

.....E.....:OMEGA::::g...:f:::::C4.....

0.0	83285.5	4.00	0.011401	0.05576	19223.0	67000.2	6.00	0.036349	0.05652
0.0	83319.3	4.00	0.022802	0.06000	19231.0	66900.4	4.00	0.030291	0.05576
0.0	83366.0	4.00	0.034203	0.03219	19231.0	66992.2	4.00	0.006058	0.06000
0.0	103618.1	4.00	0.001318	0.23133	19223.0	85004.4	6.00	0.005050	0.25069
0.0	103668.1	4.00	0.002635	0.25417	19231.0	84911.2	4.00	0.004208	0.23133
0.0	103736.8	4.00	0.003953	0.20102	19231.0	84996.4	4.00	0.000842	0.25417
0.0	109813.5	4.00	0.000427	0.00463	19223.0	90885.5	6.00	0.001690	0.00115
0.0	109857.8	4.00	0.000854	0.00463	19231.0	90798.2	4.00	0.001408	0.00463
0.0	109927.9	4.00	0.001281	0.00463	19231.0	90877.5	4.00	0.000282	0.00463
0.0	112565.9	4.00	0.000205	0.00463	19223.0	93600.0	6.00	0.000657	0.00115
0.0	112610.6	4.00	0.000410	0.00463	19231.0	93504.0	4.00	0.000548	0.00463
0.0	112682.6	4.00	0.000615	0.00463	19231.0	93592.0	4.00	0.000110	0.00463
0.0	114015.0	4.00	0.000142	0.00463	19223.0	94940.0	6.00	0.000425	0.00115
0.0	114072.0	4.00	0.000283	0.00463	19231.0	94899.0	4.00	0.000354	0.00463
0.0	114146.0	4.00	0.000425	0.00463	19231.0	94932.0	4.00	0.000071	0.00463
0.0	114809.0	4.00	0.000142	0.00463	19223.0	95727.0	6.00	0.000425	0.00115
0.0	114890.0	4.00	0.000283	0.00463	19231.0	95719.0	4.00	0.000354	0.00463
0.0	114942.0	4.00	0.000425	0.00463	19231.0	95719.0	4.00	0.000071	0.00463
0.0	115483.0	4.00	0.000142	0.00463	19223.0	96257.0	6.00	0.000425	0.00115
0.0	115483.0	4.00	0.000283	0.00463	19231.0	96249.0	4.00	0.000354	0.00463
0.0	115483.0	4.00	0.000425	0.00463	19231.0	96249.0	4.00	0.000071	0.00463
0.0	115855.0	4.00	0.000142	0.00463	19223.0	96619.0	6.00	0.000425	0.00115
0.0	115855.0	4.00	0.000283	0.00463	19231.0	96611.0	4.00	0.000354	0.00463

# Conclusion

Ce qu'il serait bon de faire !!

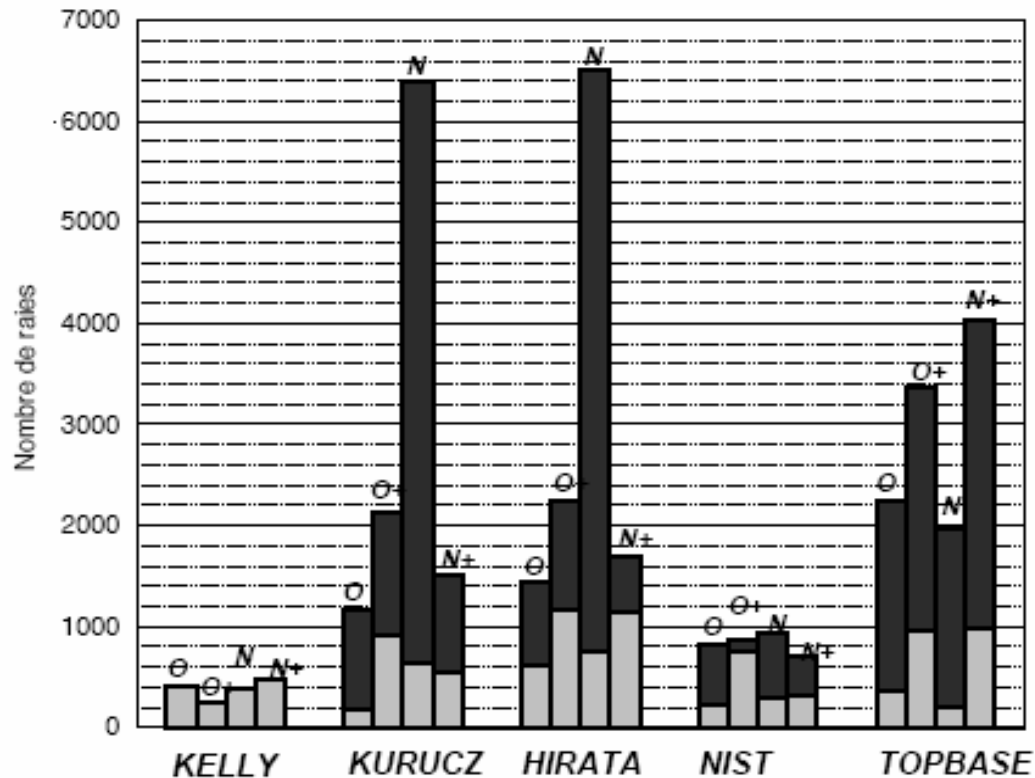
Pour aboutir à une base de données  
utilisable

- 1- Analyse critique et descriptive de l'ensemble des données déjà recensées et tabulées

# Rayonnement

→ Selon les bases de données utilisées

Thèse Chauveau, EM2C, 2001



Nombre de raies contenues dans chacune des bases. Le nombre de raies ayant des nombres d'onde supérieurs à  $28500 \text{ cm}^{-1}$  est indiqué en "gris clair", le nombre des autres raies est indiqué en "gris foncé".

# Rayonnement

→ Selon les bases de données utilisées

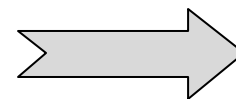
Thèse Chauveau, EM2C, 2001 ( N, N<sup>+</sup>, O, O<sup>+</sup>)

Nom	Nature de données	types de transitions <sup>1</sup>	structure fine type de couplage	Contenu
KELLY	expérimentales et/ou théoriques	E1,E2,M1	oui L-S, intermédiaire	$E_u, E_l, g_u, g_l$
KURUCZ	expérimentales et/ou théoriques	E1,E2,M1	oui L-S, intermédiaire	$E_u, E_l, g_u, g_l$ $A_{ul}, f_{lu}$
TOPBASE	théoriques	E1	non	$E_u, E_l, g_u, g_l$ $A_{ul}, f_{lu}$
HIRATA	expérimentales et/ou théoriques	E1,E2,M1	oui L-S, intermédiaire	$E_u, E_l, g_u, g_l$ $f_{lu}$
NIST	expérimentales et/ou théoriques	E1,E2,M1	oui L-S, intermédiaire	$E_u, E_l, g_u, g_l$ $A_{ul}, f_{lu}, S_{lu}$

<sup>1</sup> E1: dipolaire électrique, E2: quadrupolaire électrique, M1: dipolaire magnétique.

→ Adaptées au calcul de la composition T>2000K

HIRATA, TOPBASE et NIST

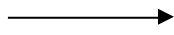


rayonnement

# Rayonnement

⇒ Selon la technique utilisée (CEN, CAM, CP, R/R)

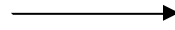
**Coefficient d'émission nette**  
(*rayon plasma, facteur de fuite*)



Adéquat au haute températures (10 000K)  
Mais pas absorption du rayonnement

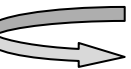
**Méthode raie par raie**  
(*nombre de raies*)

**Coefficient d'absorption moyen**  
(nombre de bandes, traitement  
raies auto absorbées)



Permet de modéliser absorption du  
rayonnement dans les zones périphérique  
de l'arc

⇒ Selon la prise en compte ou non des molécules à basse température (IR)  
(*Aussi bien dans le calcul de la composition que dans celui du rayonnement IR*)



Si non prise en compte, données a ne pas utiliser pour les flammes

Différences fondamentales sur le domaine d'application  
des données

# Propriétés de transport

⇒ Selon les hypothèses sous lesquelles elles ont été calculées

→ Type de potentiel utilisé: LJ, sphères rigides,.....

→ Extrapolation aux faibles énergie < 1eV interaction neutre- électro

Interaction	States	Type	Parameter values
O-O	$b^1\Sigma_g^+$	HH	$D_e = 3.5772 \text{ eV}, r_e = 1.2269 \text{ \AA}$ $a = 3.75996, \beta = 4.21172, \gamma = 0.932099$
	$2^1\Sigma_g^+$	E	$V_0 = 948.13 \text{ eV}, B = 3.2421 \text{ \AA}^{-1}$
	$A'^3\Sigma_u^+$	HH	$D_e = 0.83049 \text{ eV}, r_e = 1.52106 \text{ \AA}$ $a = 5.58325, \beta = 52.0591, \gamma = 2.47077$
	$2^3\Sigma_u^+$	E	$V_0 = 978.88 \text{ eV}, B = 3.2519 \text{ \AA}^{-1}$
	$1^3\Sigma_g^+$	E	$V_0 = 2010.2 \text{ eV}, B = 3.8993 \text{ \AA}^{-1}$
	$2^3\Sigma_g^+$	E	$V_0 = 1689.7 \text{ eV}, B = 3.453 \text{ \AA}^{-1}$
	$c^1\Sigma_u^-$	HH	$D_e = 1.1121 \text{ eV}, r_e = 1.5184 \text{ \AA}$ $a = 4.44766, \beta = 14.2768, \gamma = 1.97906$
	$X^3\Sigma_g^-$	HH	$D_e = 5.2141 \text{ eV}, r_e = 1.2075 \text{ \AA}$ $a = 3.39788, \beta = 4.23436, \gamma = 3.07850$
	$5^1\Sigma_u^-$	HH	$D_e = 7.401 \text{ meV}, r_e = 3.035 \text{ \AA}$ $a = 6.7048, \beta = 9.2833, \gamma = 1.2181$
	$1^1\Pi_g$	HH	$D_e = 17.08 \text{ meV}, r_e = 3.2226 \text{ \AA}$ $a = 5.39018, \beta = 8.83439, \gamma = 2.07834$
	$1^1\Pi_u$	HH	$D_e = 2.585 \text{ meV}, r_e = 3.639 \text{ \AA}$ $a = 6.4861, \beta = 8.0082, \gamma = 1.0946$
	$3^1\Pi_u$	HH	$D_e = 27.73 \text{ meV}, r_e = 2.91 \text{ \AA}$ $a = 4.80766, \beta = 19.9624, \gamma = 1.6192$
	$3^1\Pi_g$	E	$V_0 = 733.3 \text{ eV}, B = 3.5882 \text{ \AA}^{-1}$
	$5^1\Pi_g$	HH	$D_e = 0.16 \text{ eV}, r_e = 2.1167 \text{ \AA}$ $a = 5.50248, \beta = 14.2535, \gamma = 1.93411$
	$5^1\Pi_u$	HH	$D_e = 4.35 \text{ meV}, r_e = 3.264 \text{ \AA}$ $a = 7.4819, \beta = 11.283, \gamma = 1.2576$
$a^1\Delta_g$	HH	$D_e = 4.2315 \text{ eV}, r_e = 1.2156 \text{ \AA}$ $a = 3.51336, \beta = 1.46520, \gamma = 3.24691$	
$A'^3\Delta_u$	HH	$D_e = 0.9059 \text{ eV}, r_e = 1.5135 \text{ \AA}$ $a = 5.34885, \beta = 44.3777, \gamma = 2.43003$	
$5^1\Delta_g$	E	$V_0 = 2190.0 \text{ eV}, B = 3.264 \text{ \AA}^{-1}$	

Interaction	States	Type	Parameter values
N-O	$X^2\Pi$	HH	$D_e = 6.6144 \text{ eV}, r_e = 1.15077 \text{ \AA}$ $a = 3.16513, \beta = 2.12662, \gamma = 4.05347$
	$a^4\Pi$	HH	$D_e = 1.8485 \text{ eV}, r_e = 1.417 \text{ \AA}$ $a = 3.91864, \beta = 9.92562, \gamma = 5.06010$
	$6^1\Pi$	E	$V_0 = 1109.6 \text{ eV}, B = 3.5581 \text{ \AA}^{-1}$
	$2^2\Sigma$	E	$V_0 = 65.02 \text{ eV}, B = 2.4178 \text{ \AA}^{-1}$
	$4^2\Sigma$	E	$V_0 = 802.9 \text{ eV}, B = 3.4679 \text{ \AA}^{-1}$
	$6^2\Sigma$	E	$V_0 = 983.4 \text{ eV}, B = 3.5096 \text{ \AA}^{-1}$
Interaction	States	Type	Parameter values
N-N	$X^1\Sigma_g^+$	HH	$D_e = 9.90517 \text{ eV}, r_e = 1.09769 \text{ \AA}$ $a = 2.95154, \beta = 2.14862, \gamma = 3.00407$
	$A^3\Sigma_u^+$	HH	$D_e = 3.68066 \text{ eV}, r_e = 1.28660 \text{ \AA}$ $a = 3.51450, \beta = 5.47820, \gamma = 3.02859$
	$A'^5\Sigma_g^+$	HH	$D_e = 0.42291 \text{ eV}, r_e = 1.61823 \text{ \AA}$ $a = 6.95367, \beta = 1.64708, \gamma = 4.158871$
	$7^1\Sigma_u^+$	HH	$D_e = 5.265 \text{ meV}, r_e = 3.71483 \text{ \AA}$ $a = 5.86380, \beta = -4.85121, \gamma = 0.898288$

## Aubreton SPCTS

Recenser l'ensemble des potentiels d'interaction ou des intégrales de collisions pour une collision donnée

# Et surtout

2- Continuer à recenser les données existantes ( Ni, Na, Ag, Hg,.....) et les fournir sous format numérique

# Proprietes de transport

## Fournir les données sous format numérique

Proprietes T Temperature	H Enthalpie	ROEL Masse vol. volumique kg/m3	CPHEL Chaleur massique J/(kg K)	SIGEL Conductivite electrique ohm/m	VISEL viscosite dynamique kg/(m s)	XLABEL Conductivite thermique w/(m K)
K	J/kg					
500	4.14490E+06	9.7557E-02	5.1931E+03	2.9209E-24	2.8964E-05	2.2562E-01
600	4.6642E+06	8.1297E-02	5.1931E+03	2.6384E-24	3.3144E-05	2.5818E-01
700	5.1835E+06	6.9683E-02	5.1931E+03	2.4200E-24	3.7170E-05	2.8954E-01
800	5.7028E+06	6.0973E-02	5.1931E+03	2.2446E-24	4.1075E-05	3.1996E-01
900	6.2221E+06	5.4198E-02	5.1931E+03	2.0997E-24	4.4883E-05	3.4962E-01
1000	6.7415E+06	4.8778E-02	5.1931E+03	1.9776E-24	4.8608E-05	3.7864E-01
1100	7.2608E+06	4.4344E-02	5.1931E+03	1.8728E-24	5.2263E-05	4.0711E-01
1200	7.7801E+06	4.0649E-02	5.1931E+03	1.7818E-24	5.5856E-05	4.3510E-01
1300	8.2994E+06	3.7522E-02	5.1931E+03	1.7018E-24	5.9394E-05	4.6266E-01
1400	8.8187E+06	3.4842E-02	5.1931E+03	1.6308E-24	6.2883E-05	4.8984E-01
1500	9.3380E+06	3.2519E-02	5.1931E+03	1.5674E-24	6.6327E-05	5.1667E-01
1600	9.8573E+06	3.0486E-02	5.1931E+03	1.5102E-24	6.9731E-05	5.4318E-01
1700	1.0377E+07	2.8693E-02	5.1931E+03	1.4584E-24	7.3099E-05	5.6942E-01
1800	1.0896E+07	2.7099E-02	5.1931E+03	1.4112E-24	7.6432E-05	5.9538E-01
1900	1.1415E+07	2.5673E-02	5.1931E+03	1.3679E-24	7.9735E-05	6.2111E-01
2000	1.1937E+07	2.4389E-02	5.1931E+03	3.2311E-24	8.3008E-05	6.4661E-01
2100	1.2454E+07	2.3228E-02	5.1931E+03	9.7793E-23	8.6255E-05	6.7190E-01
2200	1.2973E+07	2.2172E-02	5.1931E+03	2.1741E-21	8.9477E-05	6.9700E-01
2300	1.3493E+07	2.1208E-02	5.1931E+03	3.6959E-20	9.2676E-05	7.2192E-01
2400	1.4012E+07	2.0324E-02	5.1931E+03	4.9677E-19	9.5854E-05	7.4667E-01
2500	1.4531E+07	1.9511E-02	5.1931E+03	5.4303E-18	9.9011E-05	7.7126E-01
2600	1.5050E+07	1.8761E-02	5.1931E+03	4.9438E-17	1.0215E-04	7.9571E-01
2700	1.5570E+07	1.8066E-02	5.1931E+03	3.8253E-16	1.0527E-04	8.2001E-01
2800	1.6089E+07	1.7421E-02	5.1931E+03	2.5598E-15	1.0837E-04	8.4418E-01
2900	1.6608E+07	1.6820E-02	5.1931E+03	1.5038E-14	1.1146E-04	8.6823E-01
3000	1.7128E+07	1.6259E-02	5.1931E+03	7.8572E-14	1.1453E-04	8.9216E-01
3100	1.7647E+07	1.5735E-02	5.1931E+03	3.6927E-13	1.1759E-04	9.1598E-01
3200	1.8166E+07	1.5243E-02	5.1931E+03	1.5766E-12	1.2063E-04	9.3970E-01
3300	1.8686E+07	1.4781E-02	5.1931E+03	6.1688E-12	1.2366E-04	9.6331E-01
3400	1.9205E+07	1.4347E-02	5.1931E+03	2.2289E-11	1.2668E-04	9.8683E-01
3500	1.9724E+07	1.3937E-02	5.1931E+03	7.4881E-11	1.2969E-04	1.0103E+00
3600	2.0244E+07	1.3550E-02	5.1931E+03	2.3532E-10	1.3269E-04	1.0336E+00
3700	2.0763E+07	1.3183E-02	5.1931E+03	6.9552E-10	1.3567E-04	1.0569E+00
3800	2.1282E+07	1.2836E-02	5.1931E+03	1.9427E-09	1.3865E-04	1.0800E+00
3900	2.1802E+07	1.2507E-02	5.1931E+03	5.1504E-09	1.4162E-04	1.1031E+00
4000	2.2321E+07	1.2195E-02	5.1931E+03	1.3011E-08	1.4457E-04	1.1262E+00
4100	2.2840E+07	1.1897E-02	5.1931E+03	3.1429E-08	1.4752E-04	1.1492E+00
4200	2.3359E+07	1.1614E-02	5.1931E+03	7.2830E-08	1.5046E-04	1.1721E+00
4300	2.3879E+07	1.1344E-02	5.1931E+03	1.6236E-07	1.5339E-04	1.1949E+00
4400	2.4398E+07	1.1086E-02	5.1931E+03	3.4914E-07	1.5632E-04	1.2677E+00
4500	2.4917E+07	1.0840E-02	5.1931E+03	7.2595E-07	1.5924E-04	1.2404E+00

Ex: Hélium (Bateyron, SPCTS)

# Fournir les données sous format numérique

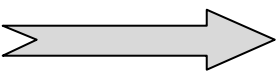
Propriétés T Temperature	H Enthalpie	ROEL Masse vol. volumique	CPEL Chaleur massique	SIGEL Conductivite electrique	VISEL Viscosite dynamique	XLABEL Conductivite thermique	XKABEL Coefficient d'absorption
K	J/kg	kg/m <sup>3</sup>	J/(kg K)	ohm/m	kg/(m s)	w/(m K)	-
300.00	14000.	1.6225	520.33	0.13214E-03	0.34224E-04	0.26712E-01	0.10000E-09
400.00	65800.	1.2169	520.33	0.13214E-03	0.34224E-04	0.26712E-01	0.10000E-09
500.00	0.11699E+06	0.97353	520.33	0.13214E-03	0.34224E-04	0.26712E-01	0.10000E-09
600.00	0.16905E+06	0.81121	520.63	0.13214E-03	0.39245E-04	0.30631E-01	0.10000E-09
700.00	0.22110E+06	0.69530	520.53	0.13214E-03	0.44858E-04	0.35011E-01	0.10000E-09
800.00	0.27215E+06	0.60839	520.48	0.13214E-03	0.49742E-04	0.38823E-01	0.10000E-09
900.00	0.31319E+06	0.54079	520.44	0.13214E-03	0.53921E-04	0.42085E-01	0.10000E-09
1000.0	0.36524E+06	0.48672	520.41	0.13214E-03	0.57633E-04	0.44982E-01	0.10484E-08
1100.0	0.41727E+06	0.44248	520.39	0.13214E-03	0.61076E-04	0.47669E-01	0.25818E-07
1200.0	0.46931E+06	0.40561	520.38	0.13214E-03	0.64374E-04	0.50243E-01	0.37184E-06
1300.0	0.52135E+06	0.37441	520.37	0.13214E-03	0.67598E-04	0.52760E-01	0.35842E-05
1400.0	0.57339E+06	0.34767	520.36	0.13214E-03	0.70787E-04	0.55249E-01	0.25194E-04
1500.0	0.62542E+06	0.32450	520.36	0.13214E-03	0.73960E-04	0.57725E-01	0.13753E-03
1600.0	0.67746E+06	0.30422	520.35	0.13214E-03	0.77125E-04	0.60195E-01	0.61060E-03
1700.0	0.72949E+06	0.28633	520.35	0.13214E-03	0.80284E-04	0.62661E-01	0.22896E-02
1800.0	0.78152E+06	0.27042	520.34	0.13214E-03	0.83437E-04	0.65122E-01	0.74442E-02
1900.0	0.83356E+06	0.25619	520.34	0.13214E-03	0.86582E-04	0.67576E-01	0.21465E-01
2000.0	0.88559E+06	0.24338	520.34	0.13214E-03	0.89715E-04	0.70022E-01	0.55868E-01
2100.0	0.93763E+06	0.23179	520.34	0.13214E-03	0.92834E-04	0.72456E-01	0.13314E+00
2200.0	0.98966E+06	0.22126	520.34	0.13214E-03	0.95935E-04	0.74877E-01	0.29398E+00
2300.0	0.10417E+07	0.21164	520.33	0.13214E-03	0.99017E-04	0.77282E-01	0.60630E+00
2400.0	0.10937E+07	0.20282	520.33	0.13214E-03	0.10208E-03	0.79669E-01	0.11774E+01
2500.0	0.11458E+07	0.19471	520.33	0.13214E-03	0.10511E-03	0.82038E-01	0.21652E+01
2600.0	0.11978E+07	0.18722	520.33	0.13214E-03	0.10812E-03	0.84387E-01	0.37889E+01
2700.0	0.12498E+07	0.18029	520.33	0.13214E-03	0.11110E-03	0.86714E-01	0.63317E+01
2800.0	0.13019E+07	0.17385	520.33	0.13214E-03	0.11405E-03	0.89019E-01	0.10133E+02
2900.0	0.13539E+07	0.16786	520.33	0.13214E-03	0.11698E-03	0.91301E-01	0.15563E+02
3000.0	0.14059E+07	0.16226	520.33	0.13214E-03	0.11987E-03	0.93561E-01	0.22960E+02
3100.0	0.14580E+07	0.15703	520.33	0.13214E-03	0.12274E-03	0.95798E-01	0.32571E+02
3200.0	0.15100E+07	0.15212	520.33	0.30489E-03	0.12557E-03	0.98014E-01	0.44430E+02
3300.0	0.15620E+07	0.14751	520.33	0.67299E-03	0.12837E-03	0.10021	0.58284E+02
3400.0	0.16141E+07	0.14200	520.33	0.14257E-02	0.13114E-03	0.10240	0.73558E+02
3500.0	0.16661E+07	0.13700	520.33	0.29073E-02	0.13389E-03	0.10458	0.89358E+02
3600.0	0.17181E+07	0.13522	520.33	0.57210E-02	0.13660E-03	0.10679	0.10490E+03
3700.0	0.17702E+07	0.13157	520.33	0.10891E-01	0.13928E-03	0.10904	0.11969E+03

Ex: Argon (Bateyron SPCTS)

# Fournir les donnees sous format numerique

Proprietes T Temperature	H Enthalpie	ROEL Masse vol. volumique kg/m3	CEPL Chaleur massique J/(kg K)	SIGEL Conductivite electrique 1/(ohm m)	VISEL viscosite dynamique kg/(m s)	XLABEL Conductivite thermique w/(m K)	XKABEL Coefficient d'absorption -
300	0.12400E+04	0.12400E+01	751.	0.10600E-07	0.21600E-04	0.31800E-01	0.10000E-09
400	0.76400E+05	0.92800E+00	752.	0.10600E-07	0.27100E-04	0.39400E-01	0.10000E-09
500	0.15200E+06	0.74300E+00	752.	0.10600E-07	0.32000E-04	0.46300E-01	0.10000E-09
600	0.22700E+06	0.61900E+00	753.	0.10600E-07	0.36500E-04	0.52600E-01	0.10000E-09
700	0.30200E+06	0.53000E+00	753.	0.10600E-07	0.40600E-04	0.58500E-01	0.10000E-09
800	0.37800E+06	0.46400E+00	755.	0.10600E-07	0.44600E-04	0.64100E-01	0.10000E-09
900	0.45300E+06	0.41300E+00	757.	0.10600E-07	0.48300E-04	0.69400E-01	0.10000E-09
1000	0.52900E+06	0.37100E+00	760.	0.10600E-07	0.51900E-04	0.74600E-01	0.10484E-08
1100	0.60500E+06	0.33800E+00	763.	0.10600E-07	0.55300E-04	0.79600E-01	0.25818E-07
1200	0.68200E+06	0.30900E+00	767.	0.10600E-07	0.58700E-04	0.84400E-01	0.37184E-06
1300	0.75800E+06	0.28600E+00	770.	0.10600E-07	0.61900E-04	0.89200E-01	0.35842E-05
1400	0.83600E+06	0.26500E+00	774.	0.10600E-07	0.65000E-04	0.93900E-01	0.25194E-04
1500	0.91300E+06	0.24800E+00	779.	0.10600E-07	0.68100E-04	0.98800E-01	0.13753E-03
1600	0.99100E+06	0.23200E+00	784.	0.10600E-07	0.71100E-04	0.10400E+00	0.61060E-03
1700	0.10700E+07	0.21800E+00	790.	0.10600E-07	0.74000E-04	0.11100E+00	0.22896E-02
1800	0.11500E+07	0.20600E+00	800.	0.10600E-07	0.76900E-04	0.11900E+00	0.74442E-02
1900	0.12300E+07	0.19500E+00	814.	0.10600E-07	0.79700E-04	0.13200E+00	0.21465E-01
2000	0.13100E+07	0.18600E+00	836.	0.10600E-07	0.82500E-04	0.15100E+00	0.55868E-01
2100	0.14000E+07	0.17700E+00	870.	0.10600E-07	0.85200E-04	0.18000E+00	0.13314E+00
2200	0.14900E+07	0.16900E+00	919.	0.47500E-07	0.87900E-04	0.22400E+00	0.29398E+00
2300	0.15800E+07	0.16100E+00	990.	0.18500E-06	0.90500E-04	0.28800E+00	0.60630E+00
2400	0.16900E+07	0.15400E+00	1090.	0.64100E-06	0.93100E-04	0.37900E+00	0.11774E+01
2500	0.18000E+07	0.14800E+00	1210.	0.19800E-05	0.95800E-04	0.50300E+00	0.21652E+01
2600	0.19300E+07	0.14100E+00	1380.	0.55500E-05	0.98400E-04	0.66400E+00	0.37889E+01
2700	0.20800E+07	0.13600E+00	1580.	0.14200E-04	0.10100E-03	0.86800E+00	0.63317E+01
2800	0.22500E+07	0.13000E+00	1830.	0.33300E-04	0.10400E-03	0.11100E+01	0.10133E+02
2900	0.24400E+07	0.12500E+00	2110.	0.72700E-04	0.10600E-03	0.13900E+01	0.15563E+02
3000	0.26700E+07	0.11900E+00	2420.	0.14800E-03	0.10900E-03	0.17000E+01	0.22960E+02
3100	0.29300E+07	0.11400E+00	2740.	0.28500E-03	0.11200E-03	0.20100E+01	0.32571E+02
3200	0.32200E+07	0.10900E+00	3060.	0.52100E-03	0.11400E-03	0.22900E+01	0.44430E+02
3300	0.35400E+07	0.10400E+00	3340.	0.91200E-03	0.11700E-03	0.25200E+01	0.58284E+02
3400	0.38800E+07	0.99700E-01	3560.	0.15400E-02	0.12000E-03	0.26700E+01	0.73558E+02
3500	0.42500E+07	0.95300E-01	3680.	0.25300E-02	0.12300E-03	0.27200E+01	0.89358E+02
3600	0.46200E+07	0.91100E-01	3690.	0.40700E-02	0.12500E-03	0.26600E+01	0.10490E+03
3700	0.49800E+07	0.87200E-01	3570.	0.64400E-02	0.12800E-03	0.25000E+01	0.11969E+03

**Ex: Argon - hydrogène (Aubreton, SPCTS)**



# Pour aboutir à une base de données utilisable

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