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Quantum Mechanic Study of Electron Impact Ionization Cross Sections of Sodium-containing Molecules

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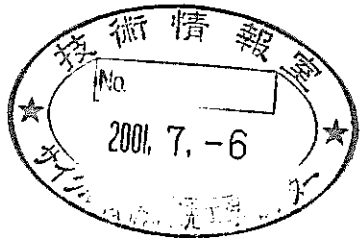

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Quantum Mechanic Study of Electron Impact Ionization Cross Sections of Sodium-containing Molecules

Jintao HUANG*

Abstract

Electron impact ionization is a common way used in high temperature mass spectrometry to obtain ion source for vaporization analysis. For most of the atomic vapor species, their electron impact ionization cross sections are experimentally measured and can be found in database. For various molecular vapor species, however, both theoretic estimation and experimentally measured data are very limited. The cross sections of sodium-containing molecules are the most important parameters to calculate their partial vapor pressures. Up to date, neither experiment data nor theoretic result can be found in literatures. So a theoretic estimation has to be made for further vapor pressure measurements.

In this study, the cross sections of sodium-containing molecules have been evaluated systematically in quantum mechanical level for the first time. The main possible sodium-containing vapor species in Fe-Na-O-H system, i.e. NaO(g), NaOH(g), Na_2O(g) and Na_2(g) are taken into account. It is found that the classic model such as additive rule as well as its modified version (MAR) are not suitable for calculation of ionization cross sections when electron impact energy is low. A recent Binary-Encounter-Bethe (BEB) model using molecular orbital parameters is employed to calculate the cross sections of sodium molecules. The results are demonstrated as a function of impact electron energy. Reliability of the data predicted by BEB model is investigated. These data are very valuable for future study on vaporization behaviors of sodium complex compounds by high temperature mass spectrometry.

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ナトリウムを含有する分子の電子衝撃イオン化断面積に対する量子力学的研究

黄　錦涛*

要　旨

高温質量分析では、蒸気圧解析に必要なイオン種を得るために電子衝撃イオン化断面積を必要とする。しかしながら、原子の蒸気種に対するイオン化断面積については、既に実験的に測定され、データベース化されているのに対して、分子の蒸気種のそれに対しては、理論的な評価および実験的データが非常に限定されているのが現状である。特に、ナトリウムを含有する分子のイオン化断面積は、現在のところ、実験データと理論的結果の両方とも報告されていない。

そこで、本研究では、ナトリウムを含有する分子のイオン化断面積を量子力学レベルで評価した。ここでは、Fe-Na-O-H系の中のナトリウムを含有する分子として、NaO(g)、NaOH(g)、Na_2O(g)およびNa_2(g)を評価対象とした。この結果、修正イオン化断面積相加法（MAR）のような古典的モデルでは、電子衝撃エネルギーが低い場合にイオン化断面積の計算に適さないことがわかった。一方、近年提案された分子パラメータを用いる Binary-Encounter-Bethe (BEB)モデルを用いてイオン化断面積を評価した結果、電子衝撃エネルギーの関数として示すことができた。さらに、この BEB モデルから得られた結果について信頼性評価を実施した。これらのデータは、高温質量分析によるナトリウム化合物の蒸発挙動評価の研究に反映できる。

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Quantum Mechanic Study of Electron Impact Ionization Cross Sections of Sodium-containing Molecules

1 Introduction

The principals of vapor pressure measurement by high temperature mass spectrometry have been reported in the previous report [1]. It is clear that the electron impact ionization cross section σ is one of the most important parameters to determine the partial vapor pressure as expressed in Eq.(1).

$$P(Pa) = K_s \times \frac{I \times T}{\alpha \times \beta \times \sigma} \quad \text{----------(1)}$$

where *Ks* is the proportional constant that should be determined by standard reference, *I* is the value of ion intensity measured by the Q-mass analyzer, *T* in Kelvin is the specimen temperature inside the K-cell, σ is the electron impact ionization cross section of the target ion in unit of 1E–16 cm^{-2}, α is the isotope abundance of the target ion, β is the electron magnification factor usually in unit of one.

As we can find in some literatures, there is another way to obtain the vapor pressure by measuring weight-loss of the sample. However, this method has some limitations as follows:

- It requires that testing sample does not absorb gases from its environment or the absorbed amount can be neglected compared to the evaporated mass of the testing materials. It is mainly due to the absorbed gas will be released at high temperatures that may significantly destroy the accuracy of this method.
- This method has to assume that the mass change of the sample after the whole test is equal to the lost amount of a dominant vapor species. So only the dominant vapor species in the testing system can be calculated. It is still difficult to determine other species with much lower partial vapor pressures.

As for the sodium compounds, almost all kinds of sodium compounds are strongly moisture absorptive. Multiple vapor species are often found over sodium compounds. For example, Na(g), NaO(g), Na_2O(g) and trance amounts of NaO_2(g) as well as Na_2O_2(g) were detected over Na_2O(s) [2]. Therefore, the weight-loss method is obviously not suitable for the present study.

In this situation, a systematic evaluation of molecular ionization cross section σ is very essential to measure vapor pressures for further attempts to evaluate thermodynamic properties of sodium compounds by means of high temperature mass spectrometry.

2 Electron Impact Ionization Cross Sections of Atoms

The electron impact ionization cross sections of most of the atoms in the Elementary Periodic Table are available now. One good database should be the AMDIS [3] developed by NIFS (日本核融合科学研究所), in which values of excitation and ionization cross sections by electron impact have been collected since 1961. A few examples like those of Ag, Na, O and H are given in the Appendix I because they are employed in this report to do further calculations.

Ionization potential of atom is another important value. It is equal to the energy required to remove one electron from the outmost orbital of a neutral atom. It means that a neutral atom can be ionized to its cation only if the impact electron possesses higher energy than the ionization potential. The ionization potentials are listed in Appendix II for all the elements. This can also be found in literatures or website of the National Institute of Standards and Technology (NIST) of USA.

3 Electron Impact Ionization Cross Sections of Molecules

3.1 The classic additive rule

By additive rule, ionization cross section of a molecule σ_M is assumed by Otvos and Stevenson to be sum of the corresponding atoms, i.e., $\sigma_M = \Sigma\sigma_A$ [4]. Since mass spectrometry was applied to thermal chemistry, this method had been used for a few decades as a rough estimation. As we can expect, it has some obstacles for practical applications. For example, an "Inverse problem"

occurred for some molecules such as silicon fluorides. Experiments show $\sigma(SiF_2)>\sigma(SiF_3)>\sigma(SiF_4)$ but the simple additive rule predicts molecule with more atoms has larger cross section.

3.2 The modified additive rule (MAR) method

Recently, a Modified Additive Rule (MAR) was built up by Deutsch et al [5]. It successfully overcomes the "Inverse problem" described in section 3.1. One important point is that it makes it possible to estimate polyatomic molecule like A_xB_y, $A_\alpha B_\beta C_\gamma$ and even $A_{n1}B_{n2}C_{n3}D_{n4}$ if nothing is known for a molecule. So, this method is firstly employed for a preliminary attempt to understand sodium compounds.

The formula is reproduced here.

$$\sigma(AxBy)=\left(\frac{r_A}{r_B}\right)^{2\alpha}\cdot\left[\frac{x\zeta_A}{x\xi_A+y\xi_B}\right]\cdot x\cdot\sigma(A)+\left(\frac{yr_B^2}{xr_A^2}\right)^{\beta}\cdot\left[\frac{y\xi_B}{x\xi_A+y\xi_B}\right]\cdot y\cdot\sigma(B) \quad \text{-------- (2)}$$

where r_A and r_B are the corresponding atomic radius; ξ_A and ξ_B are the effective electron numbers; the exponent α and β are determined by another function g_1 and g_2, respectively.

$$\alpha=g_1(\alpha^*) \text{ and } \beta=g_2(\beta^*) \quad \text{----------(3)}$$

$$\text{where } \alpha^*=\left(\frac{r_A}{r_B}\right)\cdot\left(\frac{\xi_A}{\xi_A+\xi_B}\right),\ \beta^*=\left(\frac{r_B}{r_A}\right)\cdot\left(\frac{\xi_B}{\xi_A+\xi_B}\right) \quad \text{----------(4)}$$

For easy usage, formula forms are given here by curve fitting according to the figure in Ref.[5].

When $\alpha^*<1$, $\log(g_1) = -0.2596 + 0.5040\log(\alpha^*)$ ----------(5)

When $\alpha^*>1$, $\log(g_1) = -0.2596 - 1.390\log(\alpha^*)$ ----------(6)

When $\beta^* < 0.6$, $\log(g_2) = -0.3170 + 0.3483 \log(\beta^*)$ ---------- (7)

When $\beta^* > 0.6$, $\log(g_2) = -2.404 - 3.737 \log(\beta^*)$ ---------- (8)

From http://www.webelements.com/webelements/, University of Sheffield, Royal Society of Chemistry, atomic data are obtained, i.e., r(Na) =180pm, ξ(Na)=1, r(O) =60pm, ξ(O)=6. From Eq. (3)-(8), we can obtain,

$\alpha^* = 3/7 < 1$, $\beta^* = 2/7 < 0.6$

$\alpha = g1(3/7) = 0.44$, $\beta = g2(2/7) = 0.28$

Then,

$$\sigma(NaO) = 0.37\,\sigma(Na) + 0.46\,\sigma(O) \quad \text{----------} (9)$$

Similarly, values of other sodium molecules are obtained as follows.

$$\sigma(Na_2O) = 0.80\,\sigma(Na) + 0.33\,\sigma(O) \quad \text{----------} (10)$$

$$\sigma(NaO_2) = 0.20\,\sigma(Na) + 1.25\,\sigma(O) \quad \text{----------} (11)$$

$$\sigma(NaOH) = 0.41\,\sigma(Na) + 0.01\,\sigma(O) + 0.01\,\sigma(H) \quad \text{----------} (12)$$

The calculation results by MAR are shown in Fig. 1. The ionization cross sections of sodium molecules of interests are plotted as a function of electron impact energy.

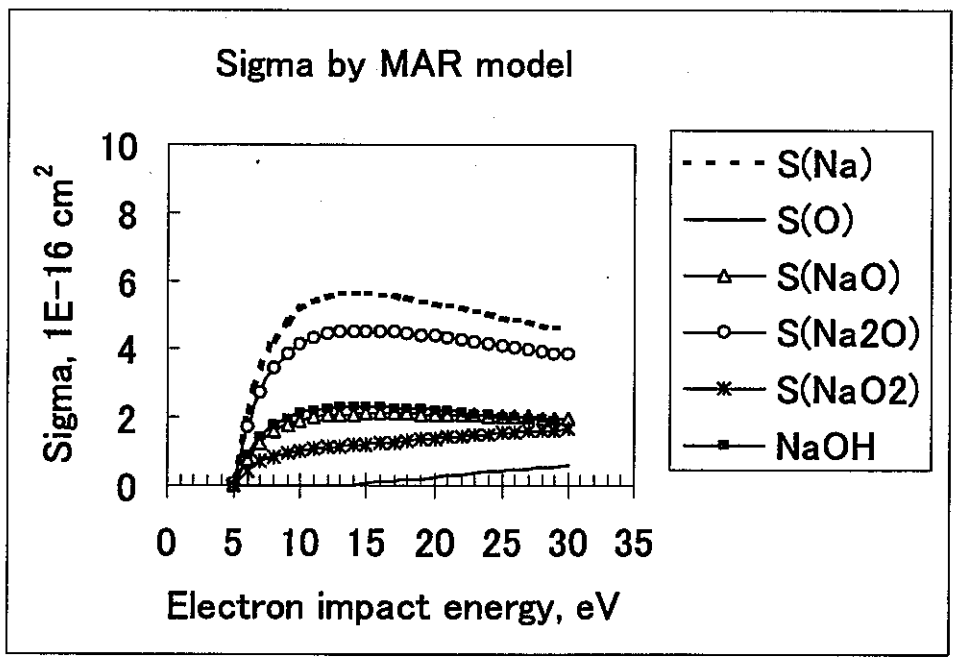

Fig. 1: Ionization cross sections of sodium molecules by MAR model

From Fig. 1, it is found that MAR gave the same ionization potential (about 5eV) to all these molecules. This is absolutely not correct. That means MAR model has difficulty to estimate ionization cross sections in low energy range.

It should be also noted MAR model seems not proper for treatment of dimmer vapor species. Here are two examples calculated by MAR,

$$\sigma(Na_2O_2) = 0.74\,\sigma(Na) + 0.92\,\sigma(O)$$
$$= 2\,\sigma(NaO) \quad (13)$$

$$\sigma(Na_2) = 0.5\,\sigma(Na) + 0.5\,\sigma(Na)$$
$$= \sigma(Na) \quad (14)$$

The result is not reasonable because experimental knowledge for dimmers should be about 1.5 to 2 times larger than that of monomers cross section.

For the above two reasons, we have to conclude that the classic models are not suitable for precise calculation of electron impact ionization cross sections, especially near the threshold energy. So new method in quantum mechanic level should be considered to satisfy high accuracy requirement for the present application.

3.3 Quantum mechanic BEB model

In the early 1990s, Dr. Yong-Ki Kim and his coworkers developed a rigorous method called Binary-Encounter-Bethe (BEB) model[6-18]. This model is based on quantum mechanic theory. The simplified formula employs only three orbital constants, i.e., the binding energy B, the orbital kinetic energy U, the electron occupation number N for each orbital. The early version of BEB model successfully calculated many simple molecules whose corresponding atoms are from the first two rows of the Elementary Periodic Table. To apply it for heavy atoms in the 3rd row or later, a modified version is developed recently. The total ionization cross section now is obtained by summing each orbital cross section as follows.

$$\sigma = \sum_i \sigma(i)$$

$$\sigma(i) = \frac{S(i)}{t(i) + \frac{u(i)+1}{n(i)}} \left[\frac{\ln(t(i))}{2} \left(1 - \frac{1}{t(i)^2} \right) + \left(1 - \frac{1}{t(i)} - \frac{\ln(t(i))}{t(i)+1} \right) \right] \quad \text{(15)}$$

where $\sigma(i)$ is the partial cross section from orbital i, $t(i) = T/B(i)$, $u(i) = U(i)/B(i)$, $S(i) = 4\pi\ a_0^2\ N(i)\ (R^2/B(i))^2$, $a_0 = 0.529\ 18$ Å, $R = 13.6057$ eV, and $N(i)$ is the number of occupied electrons in the I-th orbotal. T is the energy of impact electron. Parameters $B(i)$ and $U(i)$ can be calculated by using an ab initial method. Many computer codes have been developed for computation chemistry, for example, GAMESS [19] and Gaussian [20]. The constant $n(i)$ in Eq. (15) should be the principal quantum number of the atom if the Mulliken analysis shows more than 50% electron is from the large atoms like Na, otherwise $n(i) = 1$. It needs to be noted that $\sigma(i)=0$ when $T<B(i)$ because ionization occurs only if the impact energy is larger than the ionization potential.

According to Dr. Kim, the experimental value *I.P.* is recommended instead of using the lowest B but other orbital values are not very sensitive for the BEB cross section. If no experimental data is available, calculated *I.P.* by Gassian code is used for the lowest B in this study. Orbital constants obtained from the Hartree-Fock or similar wave functions are adequate. In many cases, the theory agrees with experiments in peak values within 10 %. Unlike most theories such as MAR, the BEB model is reliable near the threshold as well. This is very suitable for our mass spectrometric applications.

3.4 Ionization potentials of sodium-containing molecules

Ionization potential of a molecule is the energy required to remove one outmost electron from a neutral molecule. It is equal to the energy difference between the neutral molecule and its cation. For example, $IP(\mathrm{NaO.\ \ NaO^+}) = E(\mathrm{NaO^+}) - E(\mathrm{NaO})$. Some of ionization potentials of sodium compounds were measured by experiments. For those without experimental data, estimations was made by using the CBS-4M[21] model in Gaussian 98 and compared with mass spectrometric measurements. The results are listed in Table 1. All the data listed in the table are not corrected by the zero point energy E(ZPE) because neutral molecule and the cation have very close values of ZPE. For example, E(ZPE) of Na_2 is 0.000282 HF while E(ZPE) of Na_2^+ is 0.000264 HF. ΔE(ZPE) = 0.00002HF < 0.0005eV. It is unnecessary to consider it.

Table 1: Ionization potentials of sodium-containing molecules

Molecule	*E*(neutral) (Hartree)	*E*(cation) (Hartree)	Δ*E* (Hartree)	Δ*E* (eV)	Experimental *I.P.* (eV)
Na	-161.8505	-161.6643	0.1862	5.07	5.14 [22]
NaO(triplet)	-236.9332	-236.6561	0.2770	7.54	7.41 [23] 6.5±0.7 [5]
NaOH	-238.11015	-237.83801	0.2721	7.40	. 9 [24]
Na_2	-323.7268	-323.5504	0.1764	4.80	4.89 [25] 4.9 [26]
Na_2O	-398.8794	-398.6743	0.2051	5.58	5.5±0.5 [5]

From this table, we can see that calculated Δ*E* agrees well with experimental values. It indicates that the ab initio treatment correctly describe the molecular properties. Further calculation using the same theory will be reliable.

We also found that ionization potentials for some of the sodium-containing molecules are as low as about 5 eV. This result is very important for us to choose proper electron impact energies. No ions can be obtained if $E < I.P.$ On the other hand, possible fragmentations may occur if E is too large compared to *I.P.* So, the working range of electron impact energy should be a few eV higher than 5 eV.

3.5 Fragmentation

For sodium-containing molecules, there were long lasting arguments on the possible fragmentation of NaO_2. Early mass spectrometric study failed to identify the vapor species of NaO_2[5] but it was found stable in flame experiments [27]. Some ab initio calculations show that it may break into $Na+O_2$ as long as the impact energy is over 7.7eV[28-31]. However, mass spectrometric measurement repeated by Hildenbrand still could not find a consistent conclusion [32]. That means further study on mass spectrometry is in need to solve this unclear problem.

4 Molecular Orbitals and the Cross Sections of Sodium Molecules

In this section, the 3 main molecular parameters for BEB model, i.e., molecular

orbital energy, kinetic energy and the occupied number of electron will be determined by Gaussian computer code. To do this calculation, molecular structure is needed to make input files. As a basic rule, experimental data are preferentially used if they are available. In case of absence of experimental data, density function method "B3LYP"[33] is employed to find an equilibrium structure with minimum energy. Generally B3LYP method always does good work on this purpose. Bond lengths predicted by B3LYP with 6-31G Basis sets [34] or larger size are usually found to be very close to experimental value, for example, in accuracy of $\pm$0.01Å. That is good enough for further ab initio calculations.

4.1 Monosodium monoxide NaO(g)

The molecular structure of NaO is well known. The bond length between Na and oxygen is measured as 2.05155Å[35]. So, this value is used to calculate other molecular parameters as listed in Table 2. The input files for Gaussian calculation are given in Appendix III. As for the total number of electrons in a NaO molecule, simply counting the 11 electrons from sodium plus 8 electrons from oxygen. Since there is at least one unpaired electron, orbitals have to be divided into two kinds, alpha and beta orbitals in which electron with different spin direction occupy different orbital.

Table 2: NaO parameters calculated by Gaussian

MO No.	Occupied Electrons *N*	Binding Energy *B* (Hartree)	Kinetic Energy *U* (Hartree)	MO No.	Occupied Electrons *N*	Binding Energy *B* (Hartree)	Kinetic Energy *U* (Hartree)
A1	1	-38.48539	56.95875	B1	1	-38.48468	56.79473
A2	1	-19.00894	29.04489	B2	1	-18.98447	29.15411
A3	1	-2.24522	6.14600	B3	1	-2.24418	6.06662
A4	1	-1.18197	5.94376	B4	1	-1.18136	6.02428
A5	1	-1.18182	5.94376	B5	1	-1.18136	5.94371
A6	1	-1.18182	5.84158	B6	1	-1.17961	5.94371
A7	1	-0.78368	3.11636	B7	1	-0.70904	2.92286
A8	1	-0.26388	2.35202	B8	1	-0.15902	2.10245
A9	1	-0.18830	2.22336	B9	1	-0.15902	2.10245
A10	1	-0.18830	2.22336				

As discussed before, *I.P.* (7.41eV=0.2723H) of the NaO molecule will be used in BEB model for cross section calculation, although the lowest binding energy in Table 2 is 0.15902H=4.33eV (Beta 9 orbital)

Atomic occupiers analysis results are listed in Table 3 to determine the n(i) parameter in Eq.(15).

Table 3: Atomic occupiers in NaO molecular orbitals

Alpha Orbital	**Oxygen Contribution**	**Sodium Contribution**	***n(i)* Refer to Eq. (15)**
1	0.00000	1.00000	3
2	1.00000	0.00000	1
3	0.00549	0.99451>50%	3
4	0.00150	0.99850>50%	3
5	0.00150	0.99850>50%	3
6	0.00005	0.99995>50%	3
7	0.99909	0.00091	1
8	0.95298	0.04702	1
9	0.97548	0.02452	1
10	0.97548	0.02452	1
Beta Orbital	**Oxygen Contribution**	**Sodium Contribution**	***n(i)* Refer to Eq. (15)**
1	0.00000	1.00000	3
2	1.00000	0.00000	1
3	0.00738	0.99262>50%	3
4	0.00005	0.99995>50%	3
5	0.00150	0.99850>50%	3
6	0.00150	0.99850>50%	3
7	0.99375	0.00625	1
8	0.96181	0.03819	1
9	0.96181	0.01046	1

Based on the above calculation results, the electron impact ionization cross section of NaO can be obtained by Eq. (15). As shown in Fig. 2, σ(NaO) is a function of the electron impact energy.

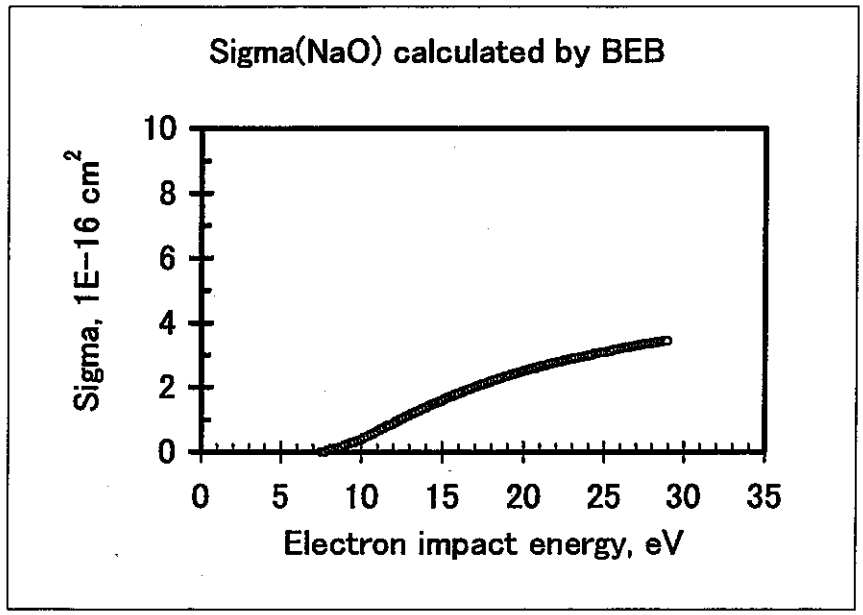

Fig. 2: Ionization cross section of NaO by BEB model

This relationship can also be expressed as a 4th degree polynomial equation,

$$\sigma(\mathrm{NaO}) = a + b\,x + c\,x^2 + d\,x^3 + e\,x^4 \quad (x<40\mathrm{eV}) \text{ ---------- } (16)$$

where the coefficient data:

a = –2.205
b = 0.261
c = 2.839E–3
d = –2.832E–4
e = 3.696E–6

4.2 Sodium hydroxide NaOH(g)

There are 20 electrons in a NaOH molecule. Molecular structure of NaOH(g) is also well known [36] . The location of atom Na, O and H can be expressed as follows.

Table 4: NaOH(g) molecule structure

Atom	*X*(Å)	*Y*(Å)	*Z*(Å)
O	0.0000	0.0000	0.0000
Na	0.0000	0.0000	1.9300
H	0.0000	0.0000	-0.9700

Therefore, a Gaussian calculation is made and the results are given in Table 5-6 and Fig. 3.

Table 5: NaOH parameters calculated by Gaussian

MO No.	Occupied Electrons *N*	Binding Energy *B* (Hartree)	Kinetic Energy *U* (Hartree)
A1	2	-40.45241	56.30356
A2	2	-20.36508	29.21951
A3	2	-2.76193	6.53747
A4	2	-1.49045	6.15891
A5	2	-1.49016	5.89145
A6	2	-1.49016	5.89145
A7	2	-1.10719	2.78316
A8	2	-0.47682	2.06244
A9	2	-0.32140	2.06244
A10	2	-0.32140	1.69921

Table 6: Atomic occupiers in NaOH molecular orbitals

Orbital	Oxygen	Sodium	Hydrogen	$n(i)$ Refer to Eq. (15)
1	0.00000	1.00000	0.00000	1
2	1.00000	0.00000	0.00000	1
3	0.00004	0.99996>50%	0.00000	3
4	0.00735	0.99244>50%	0.00021	3
5	0.00184	0.99816>50%	0.00000	3
6	0.00184	0.99816>50%	0.00000	3
7	0.98310	0.01472	0.00218	1
8	0.98261	0.01153	0.00587	1
9	0.98261	0.01153	0.00587	1
10	0.74182	0.01145	0.24673	1

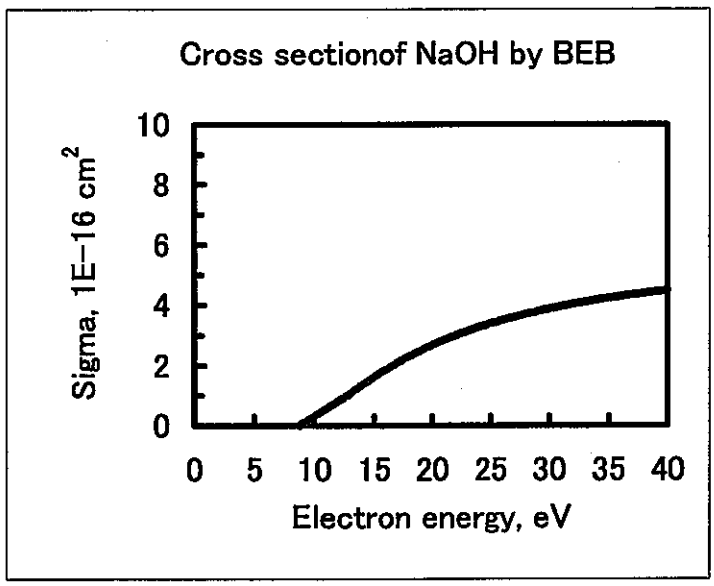

Fig. 3: Ionization cross section of NaOH by BEB model

The relationship is also expressed as a 4th degree polynomial equation.

$$\sigma(\mathrm{NaOH}) = a + b\,x + c\,x^2 + d\,x^3 + e\,x^4 \quad (x<40\mathrm{eV}) \text{ ---------- } (17)$$

where the coefficient data are:

a = –2.583
b = 0.324
c = 1.403E–3
d = –2.619E–4
e = 3.483E–6

4.3 Disodium oxide Na_2O(g)

As for Na_2O(g), it has 30 electrons. No structure data are given by experiments. So, a calculation by Gaussian is made by using B3LYP/6-311G(d) combination. It is found that the structure is almost linear not bent, i.e. bond length R(Na–O)=1.98Å and α(Na–O–Na). 179. The next step of Gaussian orbital calculation shows that molecular orbital parameters of disodium oxide are as follows.

Table 7: Na_2O parameters calculated by Gaussian

MO No.	Occupied Electrons N	Bindig Energy B (Hartree)	Kinetic Energy U (Hartree)
A1	2	–38.38723	56.85579
A2	2	–38.38723	56.85578
A3	2	–18.92030	29.14949
A4	2	–2.15004	6.18498
A5	2	–2.14984	6.18498
A6	2	–1.08727	5.92794
A7	2	–1.08727	5.92794
A8	2	–1.08724	5.92794
A9	2	–1.08724	5.92794
A10	2	–1.08461	5.90180
A11	2	–1.08335	5.90180
A12	2	–0.68300	2.90909
A13	2	–0.14125	1.92557
A14	2	–0.12009	1.89733
A15	2	–0.12009	1.89733

Table 8: Atomic occupiers in Na_2O molecular orbitals

Orbital	Oxygen	Sodium No.1	Sodium No.2	$n(i)$ refer to Eq. (15)
1	0.00000	0.00000	1.00000>50%	3
2	0.00000	1.00000>50%	0.00000	3
3	1.00000	0.00000	0.00000	1
4	0.00739	0.99238>50%	0.00022	3
5	0.00739	0.00022	0.99238>50%	3
6	0.00199	0.00000	0.99801>50%	3
7	0.00199	0.99801>50%	0.00000	3
8	0.00199	0.99801>50%	0.00000	3
9	0.00199	0.00000	0.99801>50%	3
10	0.00005	0.00001	0.99994>50%	3
11	0.00005	0.99994>50%	0.00001	3
12	0.98970	0.00515	0.00515	1
13	0.83802	0.08099	0.08099	1
14	0.94748	0.02626	0.02626	1
15	0.94748	0.02626	0.02626	1

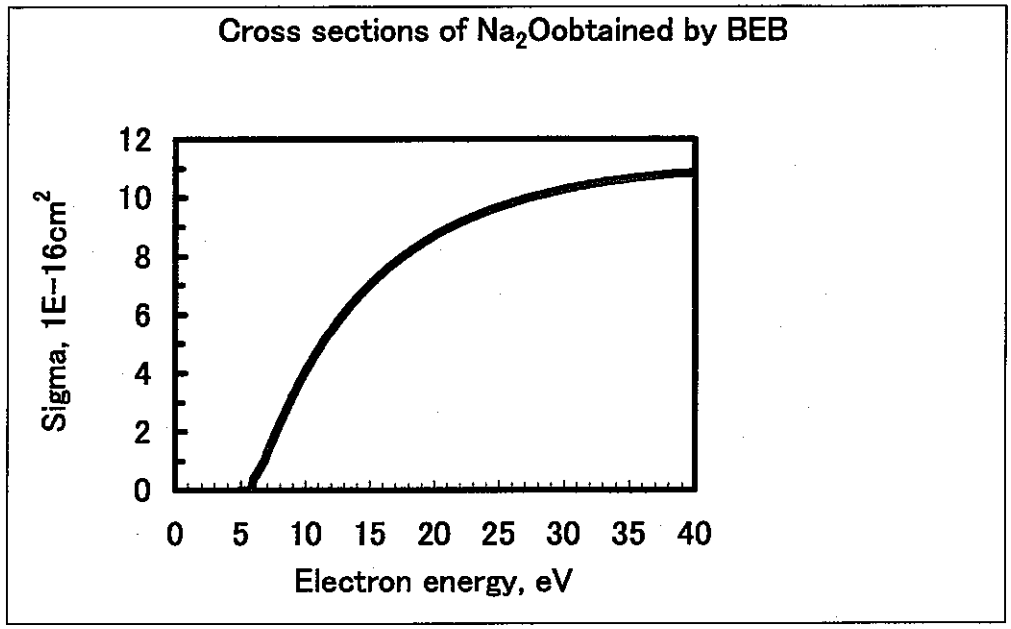

Fig. 4: Ionization cross section of Na_2O by BEB Model

The relationship is also expressed as a 4th degree polynomial equation.

$$\sigma(Na_2O) = a + b\,x + c\,x^2 + d\,x^3 + e\,x^4 \quad (x<40\text{eV}) \text{ ---------- } (18)$$

where the coefficient data are:

a = -9.015
b = 1.979
c = -8.278E-2
d = 1.671E-3
e = -1.322E-5

4.4 Disodium Na_2(g)

The bond length between the two sodium atoms is reported as 3.07887Å by Huber et al. [37]. It has 22 electrons. The calculation results are given in Table 9-10 and Fig. 5.

Table 9: Na_2 parameters calculated by Gaussian

MO No.	Occupied Electrons *N*	Binding Energy *B* (Hartree)	Kinetic Energy *U* (Hartree)
A1	2	-38.44251	57.20509
A2	2	-38.44251	56.27123
A3	2	-2.20030	6.64526
A4	2	-2.20025	5.95288
A5	2	-1.13815	5.95288
A6	2	-1.13691	5.93206
A7	2	-1.13691	5.93206
A8	2	-1.13665	5.93206
A9	2	-1.13665	5.93206
A10	2	-1.13610	5.71140
A11	2	-0.13026	0.36935

Table 10: Atomic occupiers in Na_2 molecular orbitals

Orbital	Sodium No.1	Sodium No.2	$n(i)$ Refer to Eq. (15)
1	1.00000	0.00000	3
2	0.00000	1.00000	3
3	0.00001	0.99999	3
4	0.00021	0.99979	3
5	0.99979	0.00021	3
6	0.00002	0.99998	3
7	0.99998	0.00002	3
8	0.00002	0.99998	3
9	0.99998	0.00002	3
10	0.99999	0.00001	3
11	0.50000	0.50000	3

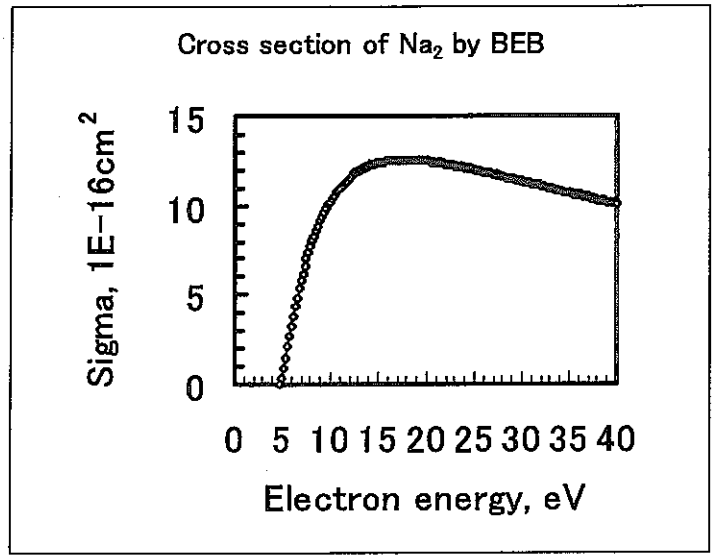

Fig. 5: Ionization cross section of Na_2 by BEB Model

The relationship can be expressed as a 5th degree polynomial equation.

$$\sigma(Na_2O) = a + b\,x + c\,x^2 + d\,x^3 + e\,x^4 + f\,x^5 \quad (x<40\text{eV}) \text{ ---------- } (19)$$

where the coefficient data are:

a = –25.619
b = 7.718
c = –0.6057
d = 2.322E–2
e = –4.3901E–4
f = 3.261E–6

4.5 Summary

The electron impact ionization cross sections of sodium-containing molecules were obtained in the previous sections. In Fig. 6, their cross sections are illustrated as a whole. It is quite clear that different molecules possess different values. For example, $\sigma(Na_2O)$ and $\sigma(NaO)$ are quite different compared to $\sigma(Na)$. It should be also noted that the dimmer sodium Na_2 has about double values of its monomer. Another particular point should be that NaO and NaOH show similar changing trends. The reasons will be discussed later in section 5.2.

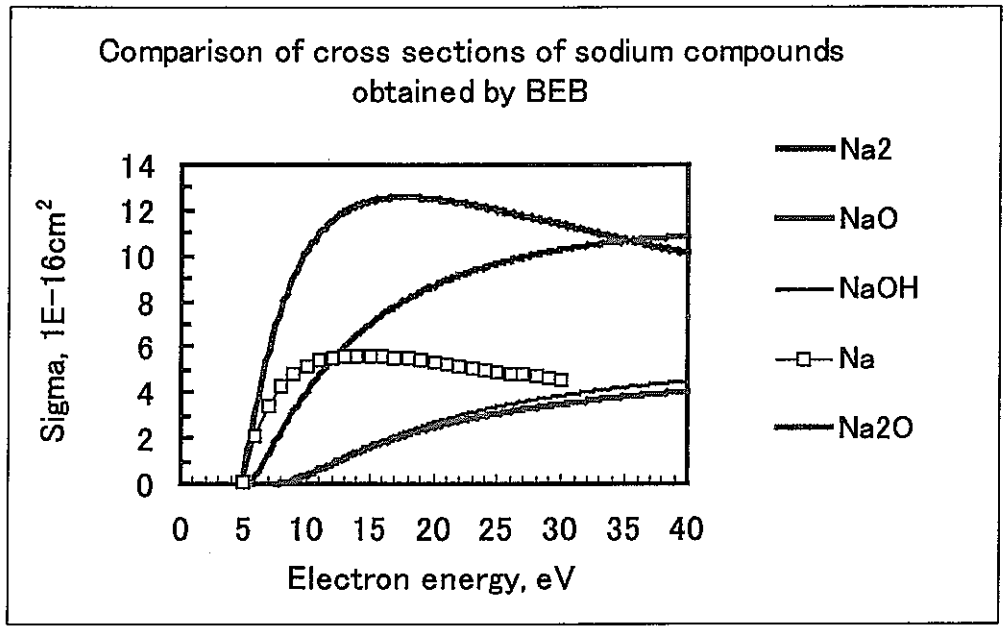

Fig. 6: Ionization cross sections by BEB model

The whole results are given in Table 11 to calculate partial vapor pressures for the application of high temperature mass spectrometry. The data of Na is taken from AMDIS database for comparison while the others are all the calculation results by BEB model as described above.

Table 11: The cross sections of some sodium molecules in unit of 10^{-16} cm^2

Impact Electron Energy *T*(eV)	σ(Na)	σ(NaO)	σ(NaOH)	σ(Na_2O)	σ(Na_2)
0-4	0.00	0.00	0.00	0.00	0.00
5	0.00	0.00	0.00	0.00	0.47
6	2.00	0.00	0.00	0.22	3.36
7	3.31	0.00	0.00	1.32	5.69
8	4.23	0.00	0.00	2.32	7.56
9	4.85	0.19	0.01	3.22	9.02
10	5.24	0.44	0.30	4.04	10.15
11	5.47	0.69	0.58	4.77	10.99
12	5.58	0.92	0.86	5.43	11.61
13	5.62	1.15	1.12	6.02	12.04
14	5.61	1.37	1.37	6.54	12.32
15	5.57	1.58	1.62	7.01	12.49
16	5.53	1.78	1.85	7.44	12.57
17	5.48	1.97	2.06	7.81	12.58
18	5.43	2.15	2.27	8.14	12.55
19	5.39	2.32	2.47	8.44	12.49
20	5.34	2.48	2.65	8.71	12.41
21	5.29	2.62	2.82	8.94	12.32
22	5.23	2.76	2.98	9.15	12.23
23	5.15	2.89	3.13	9.34	12.13
24	5.06	3.01	3.27	9.51	12.04
25	4.96	3.11	3.39	9.67	11.94
26	4.84	3.21	3.51	9.81	11.84
27	4.72	3.30	3.61	9.94	11.73
28	4.63	3.38	3.71	10.05	11.62
29	4.58	3.46	3.80	10.16	11.51
30	4.60	3.53	3.88	10.26	11.38

5 Discussions

5.1 Comparison with experimental data

In order to evaluate the calculated data of the sodium molecules, comparison with experimental data is needed. In the present situation, only sodium atom was experimental measured so it is used to check how well the BEB model would be.

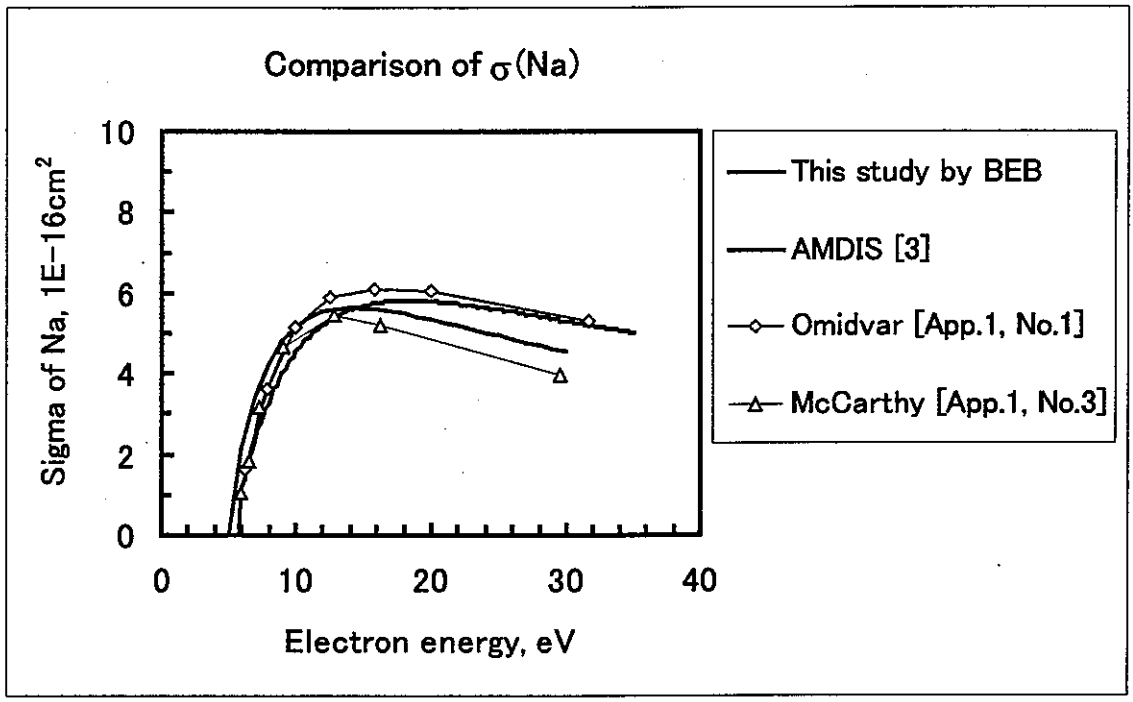

Fig. 7: Comparison of ionization cross section of Na atom

From this comparison, the BEB model agree well with other data. So, it is quite safe to conclude that the results calculated by BEB model for other sodium compounds should be reliable.

5.2 Similarity and dissimilarity of molecular properties

From the calculated results showed in the previous sections, it is noticed that the electron impact ionization cross section of NaO is very close to that of NaOH. A

theoretic explanation will be helpful to understand the reason for it.

The similarity could be attributed to the similar molecular parameters both in their energy level of corresponding molecular orbital and also the electron density distribution in space. The similarity in electron distribution is confirmed by drawing their electrostatic charge density surfaces as illustrated in Fig. 8.

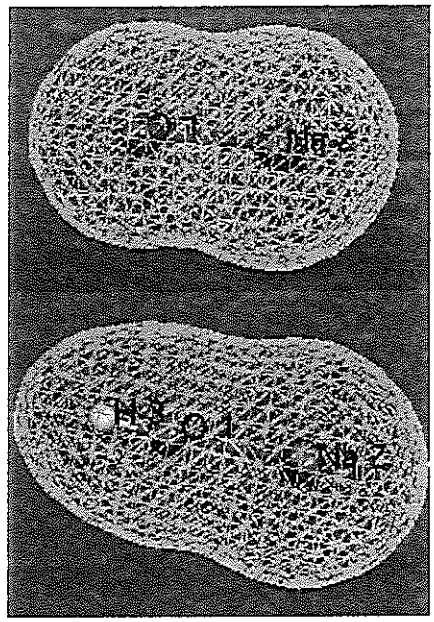

Fig. 8: Comparison of electron density surfaces of NaO and NaOH.

(Note: The number beside each atom only shows the location number in space. This picture is drawn by a freeware MOLEKEL, V.4.0 beta. 18.DEC.2000, OpenGL Version: 1.1.5. For inquiries please contact: Stefan Portmann, Centro Svizzero di Calcolo Scientifico (CSCS), Swiss Federal Institute of Technology, Via Cantonale, Galleria 2,CH-6928 Manno, Switzerland. Info: http://www.cscs.ch/molekel/)

The similarity in molecular orbitals is also found for NaO and NaOH. Fig. 9 shows their energy level and occupied number of electrons. Table 12 and 13 show that both NaO and NaOH possess similar orbital components. Influence from hydrogen on the molecular orbitals can be neglected so that NaO and NaOH produce similar ionization cross sections.

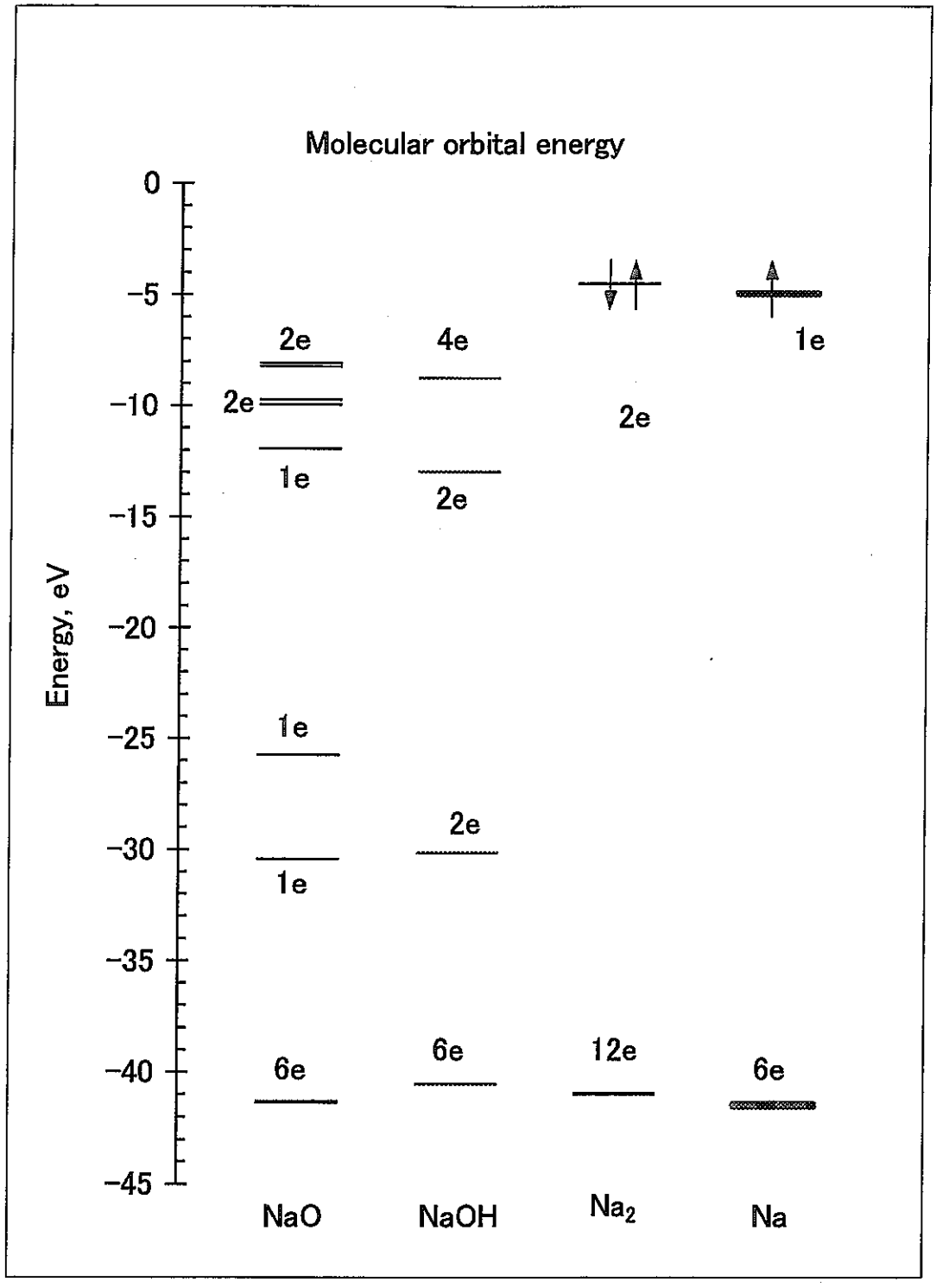

Fig. 9: Comparison of energy levels of molecular orbitals

Table 12: Atomic contributions for each atom in the molecule NaO

NaO	NaO
α1 (Na: 38%1s + 2s)	β1 (Na: 38%1s + 2s)
α2 (O: 55%1s + 2s)	β2 (O: 55%1s + 2s)
α3 (Na: 66%3s + 4s)	β3 (Na: 66%3s + 4s)
α4 (Na: 47%7Pz + 8Pz)	β4 (Na: 47%7Px + 8Px)
α5 (Na: 47%7Px + 8Px)	β5 (Na: 47%7Py + 8Py)
α6 (Na: 47%7Py + 8Py)	β6 (Na: 47%7Pz + 8Pz)
α7 (O: 60%3s + 4s)	β7 (O: 56%3s + 4s)
α8 (O: 29%2Pz + 45%3Pz + 4Pz)	β8 (O: 28%2Py + 40%3Py + 4Pz)
α9 (O: 29%2Px + 45%3Px + 4Px)	β9 (O: 28%2Px + 40%3Px + 4Px)
α10 (O: 29%2Pz + 45%3Pz + 4Pz)	

Table 13: Atomic contributions for each atom in molecule NaOH

NaOH
1 (Na: 38%1s + 2s)
2 (O: 55%1s + 2s)
3 (Na: 65%3s + 4s)
4 (Na: 47%7Px + 8Px)
5 (Na: 47%7Pz + 8Pz)
6 (Na: 47%7Py + 8Py)
7 (O: 54%3s + 4s) + (H: 12%1S+8%2s)
8 (O: 23%2Py + 34%3Py + 4Py) + (H: 17%1s+21%2s+3s)
9 (O: 29%2Px + 39%3Px + 4Px)
10 (O: 29%2Pz + 39%3Pz + 4Pz)

Similarity in molecular orbitals can also be found for Na and Na_2. But they differ in occupied number of electrons because electrons of dimmer Na_2 molecule are one time more than those of sodium atom as shown in Fig. 9. So it is reasonable to conclude that curves of dimmer sodium Na_2 and Na may have similar changing trend but the absolute values of the dimmer should be larger than that of sodium atom as shown in Fig. 6. The absolute magnitudes of their cross sections, however, are determined by the Eq. (15) so that they may not differ exactly in factor of 2.

5.3 Comparison of ab initio methods: GAMESS and Gaussian

Gamess can do ab initio calculations in Hartree Fock level and also Post Hartree Fock levels such as MP2 or MP4. It can provide kinetic energy of individual molecular orbital that is essential to calculate the ionization cross section by BEB theory. Another advantage is that it is a freeware and can be downloaded from its website. So GAMESS code is recommended by Dr. Kim, the BEB's developer. Up to now, it is the main tool employed to obtain the cross sections in BEB model. The disadvantage of it may lie in the following points:

- ✧ Unable to do density function calculation (DFT), one of the most successful geometry optimization method.

- ✧ It seems a little difficult to predict precisely ionization potentials of molecules. The electron-impact ionization cross section by BEB theory is very sensitive to this value.

Therefore, if there are no experimental data for the geometry of a target molecule, i.e. bond lengths and angles, and the ionization potentials, one have to try to look for other program like Gaussian to get satisfied data.

Gaussian code does not have above problems. The DFT methods included in Gaussian code, such as BLYP or B3LYP, are found very reliable to predict molecular geometry. The Complete Basis Set (CBS) method is good to compute ionization potential of molecules. So, Gaussian is a more powerful commercial code that can do much better job than GAMESS does. It can also give kinetic energy for each molecular orbital.

To compare Gaussian 98 and GAMESS, same ab initio method and Basis Set have to be exact the same. Some example outputs for NaO molecule are given in Table 14-17. They are all calculated in Hartree Fock level by using 6-311G Gaussian Basis Set.

Table 14: Molecular orbital of NaO by GAMESS using HF/6-311G

----- ALPHA SET -----
EIGENVECTORS

1	2	3	4	5
-40.4805	-20.4107	-2.7910	-1.5192	-1.5186
6	7	8	9	10
-1.5178	-1.1182	-0.4384	-0.3655	-0.3568

----- BETA SET -----
EIGENVECTORS

1	2	3	4
-40.4809	-20.3718	-2.7917	-1.5192
6	7	8	9
-1.5181	-0.9464	-0.3021	-0.2970

Table 15: Molecular orbitals of NaO by Gaussian 98 using HF/6-311G

Alpha Molecular Orbital Energies

	1	2	3	4	5
EIGENVALUES --	-40.50916	-20.40605	-2.81603	-1.54594	-1.54374
	6	7	8	9	10
EIGENVALUES --	-1.54374	-1.11163	-0.44315	-0.35244	-0.35244

Beta Molecular Orbital Energies:

	1	2	3	4	5
EIGENVALUES --	-40.50814	-20.36800	-2.81395	-1.54322	-1.54322
	6	7	8	9	
EIGENVALUES --	-1.54049	-0.94506	-0.29352	-0.29352	

Table 16: Kinetic energies of NaO orbitals by GAMESS using HF/6-311G

ALPHA ORBITALS

KINETIC ENERGY OF ORBITAL	1 IS	56.30753252
KINETIC ENERGY OF ORBITAL	2 IS	29.18155495
KINETIC ENERGY OF ORBITAL	3 IS	6.72925867
KINETIC ENERGY OF ORBITAL	4 IS	5.88477352
KINETIC ENERGY OF ORBITAL	5 IS	5.88801440
KINETIC ENERGY OF ORBITAL	6 IS	5.87385622
KINETIC ENERGY OF ORBITAL	7 IS	3.02776157
KINETIC ENERGY OF ORBITAL	8 IS	2.32939715
KINETIC ENERGY OF ORBITAL	9 IS	2.27560399
KINETIC ENERGY OF ORBITAL	10 IS	2.21974385

BETA ORBITALS

KINETIC ENERGY OF ORBITAL	1 IS	56.30798518
KINETIC ENERGY OF ORBITAL	2 IS	29.24669514
KINETIC ENERGY OF ORBITAL	3 IS	6.73185876
KINETIC ENERGY OF ORBITAL	4 IS	5.88859399
KINETIC ENERGY OF ORBITAL	5 IS	5.88344097
KINETIC ENERGY OF ORBITAL	6 IS	5.88497303
KINETIC ENERGY OF ORBITAL	7 IS	2.83808173
KINETIC ENERGY OF ORBITAL	8 IS	2.11132824
KINETIC ENERGY OF ORBITAL	9 IS	2.06383901

Table 17: Kinetic energies of NaO orbitals by Gaussian 98 using HF/6-311G

Alpha electrons:

Orb. numb.	Orbital occup.	Local. number	-Kinetic en. [au]
1	1.00000	1.00000	-56.30282
2	1.00000	1.00000	-29.17768
3	1.00000	1.00006	-6.58033
4	1.00000	1.00988	-6.11303
5	1.00000	1.00250	-5.90079
6	1.00000	1.00250	-5.90079
7	1.00000	1.00059	-2.96503
8	1.00000	1.06687	-2.33563
9	1.00000	1.02114	-2.20505
10	1.00000	1.02114	-2.20505

Beta electrons:

Orb. numb.	Orbital occup.	Local. number	-Kinetic en. [au]
1	1.00000	1.00000	-56.51015
2	1.00000	1.00000	-29.24083
3	1.00000	1.00006	-6.38258
4	1.00000	1.01238	-6.04984
5	1.00000	1.00247	-5.90154
6	1.00000	1.00247	-5.90154
7	1.00000	1.01075	-2.79489
8	1.00000	1.03860	-2.05086
9	1.00000	1.03860	-2.05086

So we can conclude that Gaussian and GAMESS may give close results as long as the same molecular structure, calculation method and the basis sets are inputted.

It is obviously that Gaussian code can do better job to look for equilibrium structure of molecules if their structures are completely unknown. In this case, probably Gaussian might be a wiser choice.

Conclusions

✧ A systematic study on electron impact ionization cross sections of sodium-containing molecules has been done in this report. The data evaluated are very essential to calculate partial vapor pressures in high temperature mass spectrometry.

✧ The classic model such as additive rule as well as its modified version are found not suitable for calculation of ionization cross sections near the threshold area where electron impact energy is low.

✧ The electron impact ionization cross sections of sodium-containing molecules have been calculated based on a quantum mechanic method BEB model for the first time. Their cross sections are given as a function of electron impact energy for most of the main vapor species in Fe-Na-O-H system, such as NaO, NaOH, Na_2 as well as Na_2O.

✧ Data predicted by BEB model are believed reliable and can be used for further study on vaporization behaviors of sodium complex compounds by high temperature mass spectrometry.

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The author would like to express his heartily thanks to Dr. Yong-Ki Kim, the developer of BEB model for his good suggestions in private communications. Without his help, this work could not have achieved fast improvements.

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Thanks should also go to Mr. Izumi Murakami, the manager of NIFS databases, Data and Planning Center, National Institute for Fusion Science, for the permission to make full use of their atomic cross section database, and Dr. Brett Bode, Interim GAMESS troubleshooter, Ames Laboratory Iowa State University, for providing the GAMESS freeware to do lots of valuable calculations in this report.

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Appendix Ⅰ:

Selected database for oxygen, hydrogen, sodium and silver

Note: The following data are taken from AMDIS database with permition of the manager in NIFS.

1. Oxygen atom O

1.1. Data Number 1

$O + e \rightarrow O^+ + 2e$
Zipf, E.C., Planet. & Space Sci. 33 (1985)1303

When the original data has no error bars for Y, 0 is displayed for the Y error (+, -) columns.

X = Electron energy (eV)	Y = Cross section (cm^2)	Y = Error Plus(cm^2)	Y = Error Minus(cm^2)
4.000000e+01	9.500000e-17	0.000000e+00	0.000000e+00
5.000000e+01	1.130000e-16	0.000000e+00	0.000000e+00
6.000000e+01	1.230000e-16	0.000000e+00	0.000000e+00
6.500000e+01	1.270000e-16	0.000000e+00	0.000000e+00
7.000000e+01	1.280000e-16	0.000000e+00	0.000000e+00
8.000000e+01	1.310000e-16	0.000000e+00	0.000000e+00
9.000000e+01	1.320000e-16	0.000000e+00	0.000000e+00
1.000000e+02	1.330000e-16	0.000000e+00	0.000000e+00
1.250000e+02	1.330000e-16	0.000000e+00	0.000000e+00
1.500000e+02	1.310000e-16	0.000000e+00	0.000000e+00
1.750000e+02	1.280000e-16	0.000000e+00	0.000000e+00
2.000000e+02	1.240000e-16	0.000000e+00	0.000000e+00
2.250000e+02	1.180000e-16	0.000000e+00	0.000000e+00
2.500000e+02	1.120000e-16	0.000000e+00	0.000000e+00
2.750000e+02	1.050000e-16	0.000000e+00	0.000000e+00
3.000000e+02	9.700000e-17	0.000000e+00	0.000000e+00

1.2. Data Number 2

$O + e \rightarrow O^+ + 2e$
Thompson, W.R. et al. J. Phys. B 28 (1995)1321

X = Electron energy (ev)	Y = Cross section (cm^2)	Y = Error Plus(cm^2)	Y = Error Minus(cm^2)
1.410000e+01	2.400000e-22	1.000000e-02	1.000000e-02
1.430000e+01	3.400000e-22	1.000000e-02	1.000000e-02
1.450000e+01	4.700000e-22	2.000000e-02	2.000000e-02
1.470000e+01	4.100000e-22	2.000000e-02	2.000000e-02
1.500000e+01	5.300000e-22	2.000000e-02	2.000000e-02
1.530000e+01	6.900000e-22	3.000000e-02	3.000000e-02
1.570000e+01	7.500000e-22	3.000000e-02	3.000000e-02
1.610000e+01	9.900000e-22	4.000000e-02	4.000000e-02
1.660000e+01	1.100000e-21	5.000000e-02	5.000000e-02
1.780000e+01	1.520000e-21	6.000000e-02	6.000000e-02
1.920000e+01	2.110000e-21	8.000000e-02	8.000000e-02
2.160000e+01	3.610000e-21	1.200000e-01	1.200000e-01
2.320000e+01	4.360000e-21	1.600000e-01	1.600000e-01
2.920000e+01	6.270000e-21	2.100000e-01	2.100000e-01
3.120000e+01	7.120000e-21	2.400000e-01	2.400000e-01
3.550000e+01	7.610000e-21	2.600000e-01	2.600000e-01
4.050000e+01	1.010000e-20	3.000000e-01	3.000000e-01
4.600000e+01	1.180000e-20	3.000000e-01	3.000000e-01
5.000000e+01	1.220000e-20	4.000000e-01	4.000000e-01
5.600000e+01	1.240000e-20	4.000000e-01	4.000000e-01
6.300000e+01	1.250000e-20	4.000000e-01	4.000000e-01
7.100000e+01	1.300000e-20	4.000000e-01	4.000000e-01
8.000000e+01	1.310000e-20	4.000000e-01	4.000000e-01
9.000000e+01	1.440000e-20	4.000000e-01	4.000000e-01
9.700000e+01	1.460000e-20	4.000000e-01	4.000000e-01
1.120000e+02	1.450000e-20	4.000000e-01	4.000000e-01
1.260000e+02	1.450000e-20	4.000000e-01	4.000000e-01
1.470000e+02	1.430000e-20	4.000000e-01	4.000000e-01
1.650000e+02	1.370000e-20	4.000000e-01	4.000000e-01
1.900000e+02	1.300000e-20	4.000000e-01	4.000000e-01
2.190000e+02	1.190000e-20	3.000000e-01	3.000000e-01
2.520000e+02	1.220000e-20	3.000000e-01	3.000000e-01
1.970000e+02	9.900000e-21	3.000000e-01	3.000000e-01
3.420000e+02	9.500000e-21	3.000000e-01	3.000000e-01
3.930000e+02	8.800000e-21	3.000000e-01	3.000000e-01
4.520000e+02	7.500000e-21	2.000000e-01	2.000000e-01
5.200000e+02	7.300000e-21	2.000000e-01	2.000000e-01
5.970000e+02	7.100000e-21	2.000000e-01	2.000000e-01
6.870000e+02	5.930000e-21	1.900000e-01	1.900000e-01
7.970000e+02	5.480000e-21	1.800000e-01	1.800000e-01
9.570000e+02	4.660000e-21	1.700000e-01	1.700000e-01
1.148000e+03	4.520000e-21	1.600000e-01	1.600000e-01

1.378000e+03	3.670000e-21	1.400000e-01	1.400000e-01
1.540000e+03	3.590000e-21	1.200000e-01	1.200000e-01
1.654000e+03	3.160000e-21	1.200000e-01	1.200000e-01
1.800000e+03	3.040000e-21	1.100000e-01	1.100000e-01
2.000000e+03	2.870000e-21	1.000000e-01	1.000000e-01

1.3. Data Number 3

$O + e \rightarrow O^+ + 2e$

Burnett, T.& Rountree, S.P. , Phys. Rev. A 20 (1979)1468

X = Electron energy (eV)	Y = Cross section (cm^2)	Y = Error Plus(cm^2)	Y = Error Minus(cm^2)
5.620000e+01	1.230000e-16	0.000000e+00	0.000000e+00
1.000000e+02	1.420000e-16	0.000000e+00	0.000000e+00
1.780000e+02	1.200000e-16	0.000000e+00	0.000000e+00
3.160000e+02	8.960000e-17	0.000000e+00	0.000000e+00
5.620000e+02	6.240000e-17	0.000000e+00	0.000000e+00
1.000000e+03	4.020000e-17	0.000000e+00	0.000000e+00
1.778000e+03	2.660000e-17	0.000000e+00	0.000000e+00
3.162000e+03	1.660000e-17	0.000000e+00	0.000000e+00

1.4. Data Number 4

$O + e \rightarrow O^+ + 2e$

Brook, E. et al., J. Phys. B 11 (1978)3115

X = Electron energy (eV)	Y = Cross section (cm^2)	Y = Error Plus(cm^2)	Y = Error Minus(cm^2)
1.290000e+01	4.700000e-18	2.200000e-01	2.200000e-01
1.390000e+01	5.700000e-18	2.400000e-01	2.400000e-01
1.490000e+01	9.300000e-18	3.900000e-01	3.900000e-01
1.590000e+01	1.700000e-17	3.200000e-01	3.200000e-01
1.690000e+01	2.310000e-17	3.400000e-01	3.400000e-01
1.790000e+01	2.460000e-17	3.800000e-01	3.800000e-01
1.890000e+01	2.410000e-17	2.000000e-01	2.000000e-01
2.090000e+01	3.530000e-17	2.200000e-01	2.200000e-01
2.190000e+01	4.270000e-17	2.900000e-01	2.900000e-01
2.290000e+01	4.390000e-17	1.300000e-01	1.300000e-01
2.490000e+01	5.760000e-17	2.700000e-01	2.700000e-01
2.690000e+01	5.960000e-17	4.100000e-01	4.100000e-01
3.190000e+01	7.350000e-17	3.400000e-01	3.400000e-01
3.690000e+01	8.790000e-17	2.600000e-01	2.600000e-01
4.700000e+01	1.067000e-16	1.200000e-01	1.200000e-01
4.700000e+01	1.137000e-16	3.700000e-01	3.700000e-01
5.700000e+01	1.223000e-16	2.200000e-01	2.200000e-01

7.200000e+01	1.303000e-16	9.000000e-02	9.000000e-02
9.700000e+01	1.356000e-16	5.000000e-02	5.000000e-02
9.700000e+01	1.301000e-16	1.100000e-01	1.100000e-01
1.220000e+02	1.334000e-16	3.000000e-02	3.000000e-02
1.470000e+02	1.281000e-16	4.000000e-02	4.000000e-02
1.470000e+02	1.324000e-16	2.300000e-01	2.300000e-01
1.970000e+02	1.239000e-16	7.000000e-02	7.000000e-02
2.470000e+02	1.093000e-16	6.000000e-02	6.000000e-02
2.970000e+02	9.940000e-17	4.000000e-02	4.000000e-02
2.970000e+02	1.050000e-16	7.000000e-02	7.000000e-02
3.970000e+02	8.630000e-17	4.000000e-02	4.000000e-02
3.970000e+02	8.160000e-17	7.000000e-02	7.000000e-02
4.970000e+02	7.840000e-17	4.000000e-02	4.000000e-02
5.970000e+02	6.860000e-17	1.200000e-01	1.200000e-01
7.970000e+02	5.710000e-17	6.000000e-02	6.000000e-02
9.970000e+02	4.820000e-17	7.000000e-02	7.000000e-02

1.5. Data Number 5

$O + e \rightarrow O^+ + 2e$

Fite, W.L.& Brackmann, R.T. „Phys. Rev. 113 (1959)815

X = Electron energy (eV)	Y = Cross section (cm^2)	Y = Error Plus(cm^2)	Y = Error Minus(cm^2)
3.400000e+01	1.190000e-16	0.000000e+00	0.000000e+00
4.800000e+01	1.280000e-16	0.000000e+00	0.000000e+00
5.710000e+01	1.450000e-16	0.000000e+00	0.000000e+00
6.750000e+01	1.420000e-16	0.000000e+00	0.000000e+00
7.460000e+01	1.500000e-16	0.000000e+00	0.000000e+00
8.800000e+01	1.460000e-16	0.000000e+00	0.000000e+00
8.800000e+01	1.510000e-16	0.000000e+00	0.000000e+00
1.000000e+02	1.480000e-16	0.000000e+00	0.000000e+00
1.200000e+02	1.420000e-16	0.000000e+00	0.000000e+00
1.350000e+02	1.430000e-16	0.000000e+00	0.000000e+00
1.400000e+02	1.360000e-16	0.000000e+00	0.000000e+00
1.500000e+02	1.410000e-16	0.000000e+00	0.000000e+00
2.000000e+02	1.250000e-16	0.000000e+00	0.000000e+00
2.500000e+02	1.060000e-16	0.000000e+00	0.000000e+00
3.000000e+02	1.040000e-16	0.000000e+00	0.000000e+00
3.500000e+02	9.330000e-17	0.000000e+00	0.000000e+00
4.000000e+02	8.710000e-17	0.000000e+00	0.000000e+00
4.500000e+02	8.270000e-17	0.000000e+00	0.000000e+00

1.6. Data Number 6

$O + e \rightarrow O^+ + 2e$

Ganas, P.S.& Green, A.E.S.

J. Quant. Spectrosc. & Radiat. Transfer 25 (1981)265

X = Electron energy (eV)	Y = Cross section (cm^2)	Y = Error Plus(cm^2)	Y = Error Minus(cm^2)
1.000000e+02	2.740000e-16	0.000000e+00	0.000000e+00
1.500000e+02	2.250000e-16	0.000000e+00	0.000000e+00
2.000000e+02	1.860000e-16	0.000000e+00	0.000000e+00
3.000000e+02	1.470000e-16	0.000000e+00	0.000000e+00
4.000000e+02	1.190000e-16	0.000000e+00	0.000000e+00
6.000000e+02	8.900000e-17	0.000000e+00	0.000000e+00
1.000000e+03	5.910000e-17	0.000000e+00	0.000000e+00
2.000000e+03	3.400000e-17	0.000000e+00	0.000000e+00
4.000000e+03	1.850000e-17	0.000000e+00	0.000000e+00

1.7. Data Number 7

$O + e \rightarrow O^+ + 2e$

McGuire, E.J., Phys. Rev. A 3 (1971)267

X = Electron energy (eV)	Y = Cross section (cm^2)	Y = Error Plus(cm^2)	Y = Error Minus(cm^2)
1.825000e+01	2.090000e-17	0.000000e+00	0.000000e+00
2.206000e+01	4.120000e-17	0.000000e+00	0.000000e+00
2.914000e+01	7.080000e-17	0.000000e+00	0.000000e+00
4.259000e+01	9.940000e-17	0.000000e+00	0.000000e+00
6.427000e+01	1.310000e-16	0.000000e+00	0.000000e+00
1.035000e+02	1.490000e-16	0.000000e+00	0.000000e+00
1.607000e+02	1.380000e-16	0.000000e+00	0.000000e+00
2.277000e+02	1.180000e-16	0.000000e+00	0.000000e+00
3.028000e+02	1.000000e-16	0.000000e+00	0.000000e+00
4.031000e+02	8.060000e-17	0.000000e+00	0.000000e+00
5.447000e+02	6.220000e-17	0.000000e+00	0.000000e+00

2. Oxygen molecule O_2

2.1. Data Number 1

$O_2 + e \rightarrow O_2^+ + 2e$

Mark, T.D. , J. Chem. Phys. 63 (1975)3731

X = Electron energy (eV)	Y = Cross section (cm^2)	Y = Error Plus(cm^2)	Y = Error Minus(cm^2)
1.300000e+01	4.900000e-19	5.000000e-04	5.000000e-04
1.350000e+01	8.700000e-19	9.000000e-04	9.000000e-04
1.500000e+01	2.900000e-18	2.900000e-03	2.900000e-03
1.750000e+01	7.300000e-18	7.000000e-03	7.000000e-03

1.900000e+01	1.140000e-17	1.100000e-02	1.100000e-02
2.250000e+01	2.300000e-17	2.300000e-02	2.300000e-02
2.800000e+01	3.930000e-17	3.900000e-02	3.900000e-02
3.150000e+01	4.960000e-17	5.000000e-02	5.000000e-02
3.700000e+01	6.400000e-17	6.000000e-02	6.000000e-02
4.400000e+01	8.300000e-17	8.000000e-02	8.000000e-02
4.800000e+01	9.100000e-17	9.000000e-02	9.000000e-02
5.150000e+01	9.900000e-17	1.000000e-01	1.000000e-01
5.500000e+01	1.080000e-16	1.100000e-01	1.100000e-01
5.850000e+01	1.160000e-16	1.200000e-01	1.200000e-01
6.200000e+01	1.250000e-16	1.300000e-01	1.300000e-01
6.600000e+01	1.320000e-16	1.300000e-01	1.300000e-01
7.000000e+01	1.390000e-16	1.400000e-01	1.400000e-01
7.300000e+01	1.480000e-16	1.500000e-01	1.500000e-01
8.000000e+01	1.570000e-16	1.600000e-01	1.600000e-01
9.450000e+01	1.660000e-16	1.700000e-01	1.700000e-01
1.000000e+02	1.700000e-16	1.700000e-01	1.700000e-01
1.090000e+02	1.750000e-16	1.800000e-01	1.800000e-01
1.150000e+02	1.730000e-16	1.700000e-01	1.700000e-01
1.260000e+02	1.700000e-16	1.700000e-01	1.700000e-01
1.390000e+02	1.660000e-16	1.700000e-01	1.700000e-01
1.470000e+02	1.630000e-16	1.600000e-01	1.600000e-01
1.560000e+02	1.580000e-16	1.600000e-01	1.600000e-01
1.670000e+02	1.460000e-16	1.500000e-01	1.500000e-01

2.2. Data Number 2

$O_2 + e \dashrightarrow O_2^+ + 2e$

Fite, W.L.& Brackmann, R.T. , Phys. Rev. 113 (1959)815

X = Electron energy (eV)	Y = Cross section (cm^2)	Y = Error Plus(cm^2)	Y = Error Minus(cm^2)
1.660000e+01	2.970000e-17	0.000000e+00	0.000000e+00
2.240000e+01	7.090000e-17	0.000000e+00	0.000000e+00
3.500000e+01	1.280000e-16	0.000000e+00	0.000000e+00
4.760000e+01	1.600000e-16	0.000000e+00	0.000000e+00
6.000000e+01	1.770000e-16	0.000000e+00	0.000000e+00
7.600000e+01	1.870000e-16	0.000000e+00	0.000000e+00
1.000000e+02	1.850000e-16	0.000000e+00	0.000000e+00
1.350000e+02	1.780000e-16	0.000000e+00	0.000000e+00
1.700000e+02	1.700000e-16	0.000000e+00	0.000000e+00
2.000000e+02	1.620000e-16	0.000000e+00	0.000000e+00
2.500000e+02	1.490000e-16	0.000000e+00	0.000000e+00
3.000000e+02	1.400000e-16	0.000000e+00	0.000000e+00
3.500000e+02	1.290000e-16	0.000000e+00	0.000000e+00
4.000000e+02	1.210000e-16	0.000000e+00	0.000000e+00

4.500000e+02	1.130000e-16	0.000000e+00	0.000000e+00
5.000000e+02	1.060000e-16	0.000000e+00	0.000000e+00

3. Hydrogen atom H

3.1. Data Number 1

$H + e \rightarrow H^+ + 2e$

Shah, M.B. et al. , J. Phys. B 20 (1987)3501

X = Electron energy (eV)	Y = Cross section (cm^2)	Y = Error Plus(cm^2)	Y = Error Minus(cm^2)
1.460000e+01	5.440000e-18	2.500000e-02	2.500000e-02
1.540000e+01	9.900000e-18	4.600000e-02	4.600000e-02
1.640000e+01	1.450000e-17	5.000000e-02	5.000000e-02
1.740000e+01	1.960000e-17	6.000000e-02	6.000000e-02
1.840000e+01	2.350000e-17	3.000000e-02	3.000000e-02
1.960000e+01	2.810000e-17	4.000000e-02	4.000000e-02
2.140000e+01	3.390000e-17	4.000000e-02	4.000000e-02
2.400000e+01	4.150000e-17	6.000000e-02	6.000000e-02
2.730000e+01	4.750000e-17	7.000000e-02	7.000000e-02
3.160000e+01	5.270000e-17	7.000000e-02	7.000000e-02
3.670000e+01	5.740000e-17	5.000000e-02	5.000000e-02
4.290000e+01	6.020000e-17	7.000000e-02	7.000000e-02
5.070000e+01	6.270000e-17	8.000000e-02	8.000000e-02
6.010000e+01	6.130000e-17	1.000000e-01	1.000000e-01
7.210000e+01	6.010000e-17	5.000000e-02	5.000000e-02
8.900000e+01	5.780000e-17	9.000000e-02	9.000000e-02
1.130000e+02	5.230000e-17	5.000000e-02	5.000000e-02
1.482000e+02	4.620000e-17	5.000000e-02	5.000000e-02
1.882000e+02	4.100000e-17	7.000000e-02	7.000000e-02
2.482000e+02	3.430000e-17	3.000000e-02	3.000000e-02
3.479000e+02	2.660000e-17	2.000000e-02	2.000000e-02
5.082000e+02	2.000000e-17	5.000000e-02	5.000000e-02
7.482000e+02	1.470000e-17	4.000000e-02	4.000000e-02
1.100000e+03	1.050000e-17	1.000000e-02	1.000000e-02
1.662700e+03	7.210000e-18	2.300000e-02	2.300000e-02
2.448100e+03	5.250000e-18	1.200000e-02	1.200000e-02
3.998100e+03	3.390000e-18	1.700000e-02	1.700000e-02

3.2. Data Number 2

$H + e \rightarrow H^+ + 2e$

Kao, H,C. et al., Phys. Rev. A 45 (1992)4646

X = Electron energy (eV)	Y = Cross section (cm^2)	Y = Error Plus(cm^2)	Y = Error Minus(cm^2)
1.538400e+01	4.354800e-17	0.000000e+00	0.000000e+00
1.727700e+01	4.638400e-17	0.000000e+00	0.000000e+00
1.957800e+01	5.556500e-17	0.000000e+00	0.000000e+00
2.270100e+01	6.746700e-17	0.000000e+00	0.000000e+00
2.492000e+01	7.630700e-17	0.000000e+00	0.000000e+00
2.878500e+01	8.639300e-17	0.000000e+00	0.000000e+00
3.191200e+01	9.171900e-17	0.000000e+00	0.000000e+00
3.462900e+01	9.341800e-17	0.000000e+00	0.000000e+00
3.784200e+01	9.341800e-17	0.000000e+00	0.000000e+00
4.591900e+01	8.979300e-17	0.000000e+00	0.000000e+00
5.317100e+01	8.639600e-17	0.000000e+00	0.000000e+00
6.108500e+01	8.141400e-17	0.000000e+00	0.000000e+00
6.842100e+01	7.699900e-17	0.000000e+00	0.000000e+00
7.666400e+01	7.258600e-17	0.000000e+00	0.000000e+00
8.424800e+01	6.874000e-17	0.000000e+00	0.000000e+00
9.372800e+01	6.444300e-17	0.000000e+00	0.000000e+00
1.026310e+02	6.048700e-17	0.000000e+00	0.000000e+00
1.131820e+02	5.653300e-17	0.000000e+00	0.000000e+00
1.238980e+02	5.280700e-17	0.000000e+00	0.000000e+00
1.360150e+02	4.897100e-17	0.000000e+00	0.000000e+00

3.3. Data Number 3

$H + e \rightarrow H^+ + 2e$

Younger, S.M., (1982)

When the original data has no error bars for Y, 0 is displayed for the Y error (+, -) columns.

X = Electron energy (eV)	Y = Cross section (cm^2)	Y = Error Plus(cm^2)	Y = Error Minus(cm^2)
1.700000e+01	3.100000e-17	0.000000e+00	0.000000e+00
2.040000e+01	4.440000e-17	0.000000e+00	0.000000e+00
3.060000e+01	6.730000e-17	0.000000e+00	0.000000e+00
4.760000e+01	7.640000e-17	0.000000e+00	0.000000e+00
5.440000e+01	7.540000e-17	0.000000e+00	0.000000e+00
6.800000e+01	7.160000e-17	0.000000e+00	0.000000e+00

3.4. Data Number 4

$H + e \rightarrow H^+ + 2e$

Dixon, A.J. et al. , Proc. R. Soc. London A 343 (1975)333

X = Electron energy (eV)	Y = Cross section (cm^2)	Y = Error Plus(cm^2)	Y = Error Minus(cm^2)

8.500000e+00	7.250000e-16	2.180000e+00	2.180000e+00
1.350000e+01	9.100000e-16	1.100000e+00	1.100000e+00
1.350000e+01	9.500000e-16	4.800000e+00	4.800000e+00
2.350000e+01	6.700000e-16	6.000000e-02	6.000000e-02
2.350000e+01	7.300000e-16	2.100000e+00	2.100000e+00
3.850000e+01	5.700000e-16	5.000000e-01	5.000000e-01
3.850000e+01	4.940000e-16	7.900000e-01	7.900000e-01
6.850000e+01	3.580000e-16	3.200000e-01	3.200000e-01
6.850000e+01	3.840000e-16	5.800000e-01	5.800000e-01
9.850000e+01	2.840000e-16	9.000000e-02	9.000000e-02
9.850000e+01	3.110000e-16	4.000000e-01	4.000000e-01
1.485000e+02	2.190000e-16	2.400000e-01	2.400000e-01
1.485000e+02	2.610000e-16	2.100000e-01	2.100000e-01
1.985000e+02	2.050000e-16	2.100000e-01	2.100000e-01
2.185000e+02	1.830000e-16	1.100000e-01	1.100000e-01
3.485000e+02	1.270000e-16	1.300000e-01	1.300000e-01
3.485000e+02	1.630000e-16	3.600000e-01	3.600000e-01
4.985000e+02	1.190000e-16	1.800000e-01	1.800000e-01

3.5. Data Number 5

$H + e \rightarrow H^+ + 2e$

Rothe, E.W. et al. , Phys. Rev. 125 (1962)582

X = Electron energy (eV)	Y = Cross section (cm^2)	Y = Error Plus(cm^2)	Y = Error Minus(cm^2)
1.000000e+02	4.860000e-17	0.000000e+00	0.000000e+00
1.200000e+02	4.800000e-17	0.000000e+00	0.000000e+00
1.500000e+02	4.160000e-17	0.000000e+00	0.000000e+00
2.000000e+02	3.680000e-17	0.000000e+00	0.000000e+00
2.500000e+02	3.170000e-17	0.000000e+00	0.000000e+00
3.000000e+02	2.670000e-17	0.000000e+00	0.000000e+00
3.300000e+02	2.820000e-17	0.000000e+00	0.000000e+00
4.000000e+02	2.370000e-17	0.000000e+00	0.000000e+00
4.500000e+02	2.110000e-17	0.000000e+00	0.000000e+00
5.000000e+02	2.050000e-17	0.000000e+00	0.000000e+00

3.6. Data Number 6

$H + e \rightarrow H^+ + 2e$

McGowan, J.W.& Clarke, E.M. , Phys. Rev. 167 (1968)43

X = Electron energy (eV)	Y = Cross section (cm^2)	Y = Error Plus(cm^2)	Y = Error Minus(cm^2)
1.350000e+01	1.760000e-19	0.000000e+00	0.000000e+00
1.390000e+01	2.380000e-18	0.000000e+00	0.000000e+00

1.440000e+01	5.280000e-18	0.000000e+00	0.000000e+00
1.480000e+01	7.920000e-18	0.000000e+00	0.000000e+00
1.540000e+01	1.080000e-17	0.000000e+00	0.000000e+00
1.580000e+01	1.340000e-17	0.000000e+00	0.000000e+00
1.640000e+01	1.620000e-17	0.000000e+00	0.000000e+00
1.680000e+01	1.810000e-17	0.000000e+00	0.000000e+00
1.730000e+01	2.070000e-17	0.000000e+00	0.000000e+00
1.780000e+01	2.250000e-17	0.000000e+00	0.000000e+00
1.820000e+01	2.430000e-17	0.000000e+00	0.000000e+00
1.870000e+01	2.590000e-17	0.000000e+00	0.000000e+00
1.920000e+01	2.740000e-17	0.000000e+00	0.000000e+00
1.970000e+01	2.860000e-17	0.000000e+00	0.000000e+00
2.010000e+01	2.950000e-17	0.000000e+00	0.000000e+00
2.060000e+01	3.100000e-17	0.000000e+00	0.000000e+00
2.110000e+01	3.200000e-17	0.000000e+00	0.000000e+00
2.160000e+01	3.320000e-17	0.000000e+00	0.000000e+00
2.220000e+01	3.420000e-17	0.000000e+00	0.000000e+00
2.250000e+01	3.470000e-17	0.000000e+00	0.000000e+00

3.7. Data Number 7

$H + e \rightarrow H^+ + 2e$

Fite, W.L.& Brackmann, R.T. , Phys. Rev. 112 (1958)1141

X = Electron energy (eV)	Y = Cross section (cm^2)	Y = Error Plus(cm^2)	Y = Error Minus(cm^2)
1.600000e+01	7.740000e-18	0.000000e+00	0.000000e+00
1.750000e+01	1.610000e-17	0.000000e+00	0.000000e+00
1.930000e+01	2.800000e-17	0.000000e+00	0.000000e+00
2.350000e+01	3.890000e-17	0.000000e+00	0.000000e+00
2.770000e+01	4.770000e-17	0.000000e+00	0.000000e+00
3.180000e+01	5.870000e-17	0.000000e+00	0.000000e+00
3.720000e+01	6.540000e-17	0.000000e+00	0.000000e+00
4.540000e+01	6.830000e-17	0.000000e+00	0.000000e+00
5.710000e+01	6.920000e-17	0.000000e+00	0.000000e+00
7.000000e+01	7.040000e-17	0.000000e+00	0.000000e+00
8.000000e+01	6.800000e-17	0.000000e+00	0.000000e+00
9.000000e+01	6.750000e-17	0.000000e+00	0.000000e+00
1.000000e+02	6.340000e-17	0.000000e+00	0.000000e+00
1.250000e+02	5.530000e-17	0.000000e+00	0.000000e+00
1.500000e+02	5.220000e-17	0.000000e+00	0.000000e+00
1.800000e+02	4.570000e-17	0.000000e+00	0.000000e+00
2.200000e+02	4.130000e-17	0.000000e+00	0.000000e+00
2.400000e+02	4.160000e-17	0.000000e+00	0.000000e+00
4.000000e+02	2.570000e-17	0.000000e+00	0.000000e+00
5.000000e+02	2.080000e-17	0.000000e+00	0.000000e+00

6.000000e+02	1.790000e-17	0.000000e+00	0.000000e+00
7.500000e+02	1.480000e-17	0.000000e+00	0.000000e+00
8.000000e+02	1.120000e-17	0.000000e+00	0.000000e+00

3.8. Data Number 8

$H + e \rightarrow H^+ + 2e$

Defrance, P. et al. , J. Phys. B 14 (1981)111

X = Electron energy (eV)	Y = Cross section (cm^2)	Y = Error Plus(cm^2)	Y = Error Minus(cm^2)
6.300000e+00	5.940000e-16	1.600000e+00	1.600000e+00
8.300000e+00	8.750000e-16	1.840000e+00	1.840000e+00
1.030000e+01	1.050000e-15	1.890000e+00	1.890000e+00
1.230000e+01	7.670000e-16	1.230000e+00	1.230000e+00
1.430000e+01	8.060000e-16	8.100000e-01	8.100000e-01
1.830000e+01	7.560000e-16	5.700000e-01	5.700000e-01
2.330000e+01	6.220000e-16	5.600000e-01	5.600000e-01
2.530000e+01	6.920000e-16	6.600000e-01	6.600000e-01
3.180000e+01	6.630000e-16	1.190000e+00	1.190000e+00
3.330000e+01	5.390000e-16	6.500000e-01	6.500000e-01
3.830000e+01	4.930000e-16	4.900000e-01	4.900000e-01
4.830000e+01	4.080000e-16	2.700000e-01	2.700000e-01
6.830000e+01	3.140000e-16	2.000000e-01	2.000000e-01
9.830000e+01	2.910000e-16	1.600000e-01	1.600000e-01
1.483000e+02	1.930000e-16	8.000000e-02	8.000000e-02
1.983000e+02	1.750000e-16	8.000000e-02	8.000000e-02
2.183000e+02	1.610000e-16	9.000000e-02	9.000000e-02
2.483000e+02	1.540000e-16	6.000000e-02	6.000000e-02
2.983000e+02	1.260000e-16	4.000000e-02	4.000000e-02
3.483000e+02	1.150000e-16	1.200000e-01	1.200000e-01
3.983000e+02	1.040000e-16	5.000000e-02	5.000000e-02
4.983000e+02	8.670000e-17	4.800000e-01	4.800000e-01
7.483000e+02	6.550000e-17	5.200000e-02	5.200000e-02
9.983000e+02	4.820000e-17	3.900000e-02	3.900000e-02

4. Hydrogen molecule H_2

4.1. Data Number 1

$H_2 + e \rightarrow H_2^+ + 2e$

Edwards,A.K. et al. , 37 (1988)3700

X = Electron energy (eV)	Y = Cross section (cm^2)	Y = Error Plus(cm^2)	Y = Error Minus(cm^2)

4.080000e+02	4.050000e-17	2.100000e-01	2.100000e-01
5.450000e+02	3.070000e-17	1.100000e-01	1.100000e-01
8.170000e+02	2.260000e-17	1.000000e-01	1.000000e-01
1.089000e+03	1.840000e-17	7.000000e-02	7.000000e-02
1.362000e+03	1.630000e-17	6.000000e-02	6.000000e-02
1.638000e+03	1.400000e-17	7.000000e-02	7.000000e-02
1.906000e+03	1.190000e-17	6.000000e-02	6.000000e-02

4.2. Data Number 2

$H_2 + e \rightarrow H_2^+ + 2e$

Adamczyk, B. et al. , J. Chem. Phys. 44 (1966)4640

X = Electron energy (eV)	Y = Cross section (cm^2)	Y = Error Plus(cm^2)	Y = Error Minus(cm^2)
2.000000e+01	2.400000e-17	0.000000e+00	0.000000e+00
3.000000e+01	5.800000e-17	0.000000e+00	0.000000e+00
5.000000e+01	8.100000e-17	0.000000e+00	0.000000e+00
7.000000e+01	8.600000e-17	0.000000e+00	0.000000e+00
1.000000e+02	8.000000e-17	0.000000e+00	0.000000e+00
1.500000e+02	7.100000e-17	0.000000e+00	0.000000e+00
2.000000e+02	6.200000e-17	0.000000e+00	0.000000e+00
3.000000e+02	4.800000e-17	0.000000e+00	0.000000e+00
4.000000e+02	4.100000e-17	0.000000e+00	0.000000e+00
5.000000e+02	3.300000e-17	0.000000e+00	0.000000e+00
6.000000e+02	2.900000e-17	0.000000e+00	0.000000e+00
7.000000e+02	2.600000e-17	0.000000e+00	0.000000e+00
8.000000e+02	2.400000e-17	0.000000e+00	0.000000e+00
9.000000e+02	2.300000e-17	0.000000e+00	0.000000e+00
1.000000e+03	2.100000e-17	0.000000e+00	0.000000e+00

4.3. Data Number 3

$H_2 + e \rightarrow H_2^+ + 2e$

McGowan, J.W. et al. , Phys. Rev. 167 (1968)52

X = Electron energy (eV)	Y = Cross section (cm^2)	Y = Error Plus(cm^2)	Y = Error Minus(cm^2)
1.527000e+01	1.000000e-22	0.000000e+00	0.000000e+00
1.530000e+01	1.800000e-22	0.000000e+00	0.000000e+00
1.533000e+01	4.600000e-22	0.000000e+00	0.000000e+00
1.536000e+01	1.070000e-21	0.000000e+00	0.000000e+00
1.539000e+01	2.340000e-21	0.000000e+00	0.000000e+00
1.542000e+01	4.720000e-21	0.000000e+00	0.000000e+00
1.545000e+01	9.070000e-21	0.000000e+00	0.000000e+00

1.548000e+01	1.540000e-20	0.000000e+00	0.000000e+00
1.551000e+01	2.560000e-20	0.000000e+00	0.000000e+00
1.554000e+01	3.750000e-20	0.000000e+00	0.000000e+00
1.557000e+01	5.280000e-20	0.000000e+00	0.000000e+00
1.560000e+01	6.980000e-20	0.000000e+00	0.000000e+00
1.563000e+01	8.640000e-20	0.000000e+00	0.000000e+00
1.566000e+01	1.043000e-19	0.000000e+00	0.000000e+00
1.569000e+01	1.210000e-19	0.000000e+00	0.000000e+00
1.572000e+01	1.382000e-19	0.000000e+00	0.000000e+00
1.575000e+01	1.555000e-19	0.000000e+00	0.000000e+00
1.578000e+01	1.755000e-19	0.000000e+00	0.000000e+00
1.581000e+01	1.964000e-19	0.000000e+00	0.000000e+00
1.584000e+01	2.199000e-19	0.000000e+00	0.000000e+00
1.587000e+01	2.424000e-19	0.000000e+00	0.000000e+00
1.590000e+01	2.611000e-19	0.000000e+00	0.000000e+00
1.593000e+01	2.807000e-19	0.000000e+00	0.000000e+00
1.596000e+01	2.990000e-19	0.000000e+00	0.000000e+00
1.599000e+01	3.165000e-19	0.000000e+00	0.000000e+00
1.602000e+01	3.344000e-19	0.000000e+00	0.000000e+00
1.605000e+01	3.546000e-19	0.000000e+00	0.000000e+00
1.608000e+01	3.798000e-19	0.000000e+00	0.000000e+00
1.611000e+01	3.997000e-19	0.000000e+00	0.000000e+00
1.614000e+01	4.188000e-19	0.000000e+00	0.000000e+00
1.617000e+01	4.357000e-19	0.000000e+00	0.000000e+00
1.620000e+01	4.526000e-19	0.000000e+00	0.000000e+00
1.623000e+01	4.751000e-19	0.000000e+00	0.000000e+00
1.625000e+01	4.920000e-19	0.000000e+00	0.000000e+00

4.4. Data Number 4

$H_2 + e \rightarrow H_2^+ + 2e$
Crowe, A.& McConkey, J.W. , J. Phys. B 6 (1973)2088

X = Electron energy (eV)	Y = Cross section (cm^2)	Y = Error Plus(cm^2)	Y = Error Minus(cm^2)
1.480000e+01	7.900000e-20	0.000000e+00	0.000000e+00
1.520000e+01	2.510000e-19	0.000000e+00	0.000000e+00
1.540000e+01	5.280000e-19	0.000000e+00	0.000000e+00
1.570000e+01	1.380000e-18	0.000000e+00	0.000000e+00
1.600000e+01	2.600000e-18	0.000000e+00	0.000000e+00
1.630000e+01	3.730000e-18	0.000000e+00	0.000000e+00
1.660000e+01	5.170000e-18	0.000000e+00	0.000000e+00
1.700000e+01	7.530000e-18	0.000000e+00	0.000000e+00
1.770000e+01	1.070000e-17	0.000000e+00	0.000000e+00
1.810000e+01	1.330000e-17	0.000000e+00	0.000000e+00

5. Sodium atom Na

5.1. Data Number 1

Na + e --> Na^+ + 2e

Omidvar, K. et al. , Phys. Rev. A 5 (1972)1174

X = Electron energy (eV)	Y = Cross section (cm^2)	Y = Error Plus(cm^2)	Y = Error Minus(cm^2)
6.310000e+00	1.610000e-16	0.000000e+00	0.000000e+00
7.940000e+00	3.630000e-16	0.000000e+00	0.000000e+00
1.000000e+01	5.150000e-16	0.000000e+00	0.000000e+00
1.260000e+01	5.890000e-16	0.000000e+00	0.000000e+00
1.580000e+01	6.110000e-16	0.000000e+00	0.000000e+00
2.000000e+01	6.040000e-16	0.000000e+00	0.000000e+00
3.160000e+01	5.290000e-16	0.000000e+00	0.000000e+00
5.010000e+01	4.420000e-16	0.000000e+00	0.000000e+00
1.000000e+02	3.120000e-16	0.000000e+00	0.000000e+00
1.585000e+02	2.470000e-16	0.000000e+00	0.000000e+00
3.162000e+02	1.680000e-16	0.000000e+00	0.000000e+00
1.000000e+03	8.040000e-17	0.000000e+00	0.000000e+00

5.2. Data Number 2

Na + e --> Na^+ + 2e

Tate, J.T.& Smith, P.T. , Phys. Rev. 46 (1934)773

X = Electron energy (eV)	Y = Cross section (cm^2)	Y = Error Plus(cm^2)	Y = Error Minus(cm^2)
5.000000e+00	2.360000e-16	0.000000e+00	0.000000e+00
7.000000e+00	9.520000e-16	0.000000e+00	0.000000e+00
1.000000e+01	1.040000e-15	0.000000e+00	0.000000e+00
1.700000e+01	9.880000e-16	0.000000e+00	0.000000e+00
2.000000e+01	9.150000e-16	0.000000e+00	0.000000e+00
2.500000e+01	8.510000e-16	0.000000e+00	0.000000e+00
3.000000e+01	7.940000e-16	0.000000e+00	0.000000e+00
3.500000e+01	7.560000e-16	0.000000e+00	0.000000e+00
4.000000e+01	6.860000e-16	0.000000e+00	0.000000e+00
4.500000e+01	6.510000e-16	0.000000e+00	0.000000e+00
5.000000e+01	6.030000e-16	0.000000e+00	0.000000e+00
5.500000e+01	5.690000e-16	0.000000e+00	0.000000e+00
7.000000e+01	5.260000e-16	0.000000e+00	0.000000e+00
7.500000e+01	4.920000e-16	0.000000e+00	0.000000e+00
8.800000e+01	4.610000e-16	0.000000e+00	0.000000e+00
1.000000e+02	4.380000e-16	0.000000e+00	0.000000e+00

1.230000e+02	3.850000e-16	0.000000e+00	0.000000e+00
1.500000e+02	3.340000e-16	0.000000e+00	0.000000e+00
1.700000e+02	3.040000e-16	0.000000e+00	0.000000e+00
2.000000e+02	2.750000e-16	0.000000e+00	0.000000e+00
2.500000e+02	2.420000e-16	0.000000e+00	0.000000e+00
3.000000e+02	2.220000e-16	0.000000e+00	0.000000e+00
3.500000e+02	2.040000e-16	0.000000e+00	0.000000e+00
4.000000e+02	1.760000e-16	0.000000e+00	0.000000e+00
4.500000e+02	1.630000e-16	0.000000e+00	0.000000e+00
5.000000e+02	1.480000e-16	0.000000e+00	0.000000e+00
5.500000e+02	1.250000e-16	0.000000e+00	0.000000e+00
6.000000e+02	1.200000e-16	0.000000e+00	0.000000e+00
6.500000e+02	1.120000e-16	0.000000e+00	0.000000e+00
7.000000e+02	1.050000e-16	0.000000e+00	0.000000e+00

5.3. Data Number 3

$Na + e \rightarrow Na^+ + 2e$

McCarthy, I.E.& Stelbovics, A.T. , Phys. Rev. A 28 (1983)1322

X = Electron energy (eV)	Y = Cross section (cm^2)	Y = Error Plus(cm^2)	Y = Error Minus(cm^2)
5.900000e+00	1.020000e-16	0.000000e+00	0.000000e+00
6.500000e+00	1.840000e-16	0.000000e+00	0.000000e+00
7.300000e+00	3.170000e-16	0.000000e+00	0.000000e+00
9.100000e+00	4.650000e-16	0.000000e+00	0.000000e+00
1.290000e+01	5.450000e-16	0.000000e+00	0.000000e+00
1.620000e+01	5.180000e-16	0.000000e+00	0.000000e+00
2.960000e+01	3.950000e-16	0.000000e+00	0.000000e+00
5.140000e+01	2.900000e-16	0.000000e+00	0.000000e+00
9.790000e+01	1.920000e-16	0.000000e+00	0.000000e+00
1.625000e+02	1.310000e-16	0.000000e+00	0.000000e+00
3.096000e+02	8.800000e-17	0.000000e+00	0.000000e+00
5.138000e+02	6.510000e-17	0.000000e+00	0.000000e+00
1.025200e+03	4.050000e-17	0.000000e+00	0.000000e+00

6. Silver atom Ag

6.1. Data Number 1

$Ag + e \rightarrow Ag^+ + 2e$

Freund, R.S. et al., Phys. Rev. A 41 (1990)3575

X = Electron energy (eV)	Y = Cross section (cm^2)	Y = Error Plus(cm^2)	Y = Error Minus(cm^2)
5.000000e+00	0.000000e+00	0.000000e+00	0.000000e+00

6.000000e+00	5.000000e-18	0.000000e+00	0.000000e+00
7.000000e+00	2.600000e-17	0.000000e+00	0.000000e+00
8.000000e+00	8.300000e-17	0.000000e+00	0.000000e+00
9.000000e+00	1.590000e-16	0.000000e+00	0.000000e+00
1.000000e+01	2.140000e-16	0.000000e+00	0.000000e+00
1.100000e+01	2.570000e-16	0.000000e+00	0.000000e+00
1.200000e+01	2.920000e-16	0.000000e+00	0.000000e+00
1.400000e+01	3.470000e-16	0.000000e+00	0.000000e+00
1.500000e+01	3.700000e-16	0.000000e+00	0.000000e+00
1.600000e+01	3.970000e-16	0.000000e+00	0.000000e+00
1.700000e+01	4.180000e-16	0.000000e+00	0.000000e+00
1.800000e+01	4.280000e-16	0.000000e+00	0.000000e+00
2.000000e+01	4.500000e-16	0.000000e+00	0.000000e+00
2.200000e+01	4.700000e-16	0.000000e+00	0.000000e+00
2.400000e+01	4.880000e-16	0.000000e+00	0.000000e+00
2.500000e+01	5.000000e-16	0.000000e+00	0.000000e+00
2.600000e+01	5.080000e-16	0.000000e+00	0.000000e+00
2.700000e+01	5.100000e-16	0.000000e+00	0.000000e+00
2.800000e+01	5.030000e-16	0.000000e+00	0.000000e+00
2.900000e+01	5.050000e-16	0.000000e+00	0.000000e+00
3.000000e+01	5.160000e-16	0.000000e+00	0.000000e+00
3.200000e+01	5.270000e-16	0.000000e+00	0.000000e+00
3.400000e+01	5.260000e-16	0.000000e+00	0.000000e+00
3.600000e+01	5.330000e-16	0.000000e+00	0.000000e+00
4.000000e+01	5.430000e-16	0.000000e+00	0.000000e+00
4.500000e+01	5.470000e-16	0.000000e+00	0.000000e+00
5.500000e+01	5.370000e-16	0.000000e+00	0.000000e+00
6.000000e+01	5.350000e-16	0.000000e+00	0.000000e+00
6.500000e+01	5.260000e-16	0.000000e+00	0.000000e+00
7.500000e+01	5.140000e-16	0.000000e+00	0.000000e+00
8.500000e+01	4.950000e-16	0.000000e+00	0.000000e+00
9.000000e+01	4.880000e-16	0.000000e+00	0.000000e+00
1.050000e+02	4.600000e-16	0.000000e+00	0.000000e+00
1.200000e+02	4.430000e-16	0.000000e+00	0.000000e+00
1.250000e+02	4.320000e-16	0.000000e+00	0.000000e+00
1.300000e+02	4.280000e-16	0.000000e+00	0.000000e+00
1.350000e+02	4.190000e-16	0.000000e+00	0.000000e+00
1.400000e+02	4.150000e-16	0.000000e+00	0.000000e+00
1.450000e+02	4.080000e-16	0.000000e+00	0.000000e+00
1.500000e+02	4.040000e-16	0.000000e+00	0.000000e+00
1.600000e+02	3.920000e-16	0.000000e+00	0.000000e+00
1.650000e+02	3.830000e-16	0.000000e+00	0.000000e+00
1.750000e+02	3.750000e-16	0.000000e+00	0.000000e+00
1.800000e+02	3.630000e-16	0.000000e+00	0.000000e+00
1.850000e+02	3.600000e-16	0.000000e+00	0.000000e+00
1.900000e+02	3.510000e-16	0.000000e+00	0.000000e+00

1.950000e+02	3.450000e-16	0.000000e+00	0.000000e+00
2.000000e+02	3.320000e-16	0.000000e+00	0.000000e+00

6.2. Data Number 2

$Ag + e \rightarrow Ag^{+} + 2e$

Franzreb, K. et al. , Z. Phys. D 19 (1991)77

X = Electron energy (eV)	Y = Cross section (cm^2)	Y = Error Plus(cm^2)	Y = Error Minus(cm^2)
8.100000e+00	2.700000e-17	0.000000e+00	0.000000e+00
8.800000e+00	7.900000e-17	0.000000e+00	0.000000e+00
1.010000e+01	1.330000e-16	0.000000e+00	0.000000e+00
1.110000e+01	1.810000e-16	0.000000e+00	0.000000e+00
1.270000e+01	2.340000e-16	0.000000e+00	0.000000e+00
1.400000e+01	2.810000e-16	0.000000e+00	0.000000e+00
1.530000e+01	3.260000e-16	0.000000e+00	0.000000e+00
1.710000e+01	3.710000e-16	0.000000e+00	0.000000e+00
1.930000e+01	4.170000e-16	0.000000e+00	0.000000e+00
2.230000e+01	4.510000e-16	0.000000e+00	0.000000e+00
2.540000e+01	4.810000e-16	0.000000e+00	0.000000e+00
2.890000e+01	4.880000e-16	0.000000e+00	0.000000e+00
3.090000e+01	5.150000e-16	0.000000e+00	0.000000e+00
3.320000e+01	5.150000e-16	0.000000e+00	0.000000e+00
3.620000e+01	5.340000e-16	0.000000e+00	0.000000e+00
4.090000e+01	5.400000e-16	0.000000e+00	0.000000e+00
4.640000e+01	5.490000e-16	0.000000e+00	0.000000e+00
5.080000e+01	5.650000e-16	0.000000e+00	0.000000e+00
5.600000e+01	5.740000e-16	0.000000e+00	0.000000e+00
6.090000e+01	5.720000e-16	0.000000e+00	0.000000e+00
6.540000e+01	5.630000e-16	0.000000e+00	0.000000e+00
7.090000e+01	5.590000e-16	0.000000e+00	0.000000e+00
7.550000e+01	5.540000e-16	0.000000e+00	0.000000e+00
8.080000e+01	5.410000e-16	0.000000e+00	0.000000e+00
8.520000e+01	5.380000e-16	0.000000e+00	0.000000e+00
9.030000e+01	5.350000e-16	0.000000e+00	0.000000e+00
9.540000e+01	5.260000e-16	0.000000e+00	0.000000e+00
1.000000e+02	5.130000e-16	0.000000e+00	0.000000e+00
1.054000e+02	5.010000e-16	0.000000e+00	0.000000e+00
1.104000e+02	4.900000e-16	0.000000e+00	0.000000e+00
1.150000e+02	4.830000e-16	0.000000e+00	0.000000e+00
1.199000e+02	4.750000e-16	0.000000e+00	0.000000e+00

6.3. Data Number 3

$Ag + e \rightarrow Ag^{+} + 2e$

Crawford, C.K. Wang, K.I. , J. Chem. Phys. 47 (1967)4667

X = Electron energy (eV)	Y = Cross section (cm^2)	Y = Error Plus(cm^2)	Y = Error Minus(cm^2)
2.090000e+01	3.600000e-16	0.000000e+00	0.000000e+00
4.190000e+01	4.190000e-16	0.000000e+00	0.000000e+00
4.640000e+01	4.390000e-16	0.000000e+00	0.000000e+00
5.620000e+01	4.660000e-16	0.000000e+00	0.000000e+00
6.740000e+01	4.800000e-16	0.000000e+00	0.000000e+00
8.080000e+01	4.710000e-16	0.000000e+00	0.000000e+00
8.570000e+01	4.570000e-16	0.000000e+00	0.000000e+00
1.030000e+02	4.080000e-16	0.000000e+00	0.000000e+00
1.210000e+02	3.310000e-16	0.000000e+00	0.000000e+00
1.410000e+02	2.620000e-16	0.000000e+00	0.000000e+00
1.600000e+02	2.230000e-16	0.000000e+00	0.000000e+00
2.000000e+02	1.880000e-16	0.000000e+00	0.000000e+00
2.500000e+02	1.570000e-16	0.000000e+00	0.000000e+00
3.000000e+02	1.330000e-16	0.000000e+00	0.000000e+00
3.500000e+02	1.090000e-16	0.000000e+00	0.000000e+00
4.000000e+02	9.400000e-17	0.000000e+00	0.000000e+00
4.550000e+02	7.900000e-17	0.000000e+00	0.000000e+00
5.000000e+02	7.000000e-17	0.000000e+00	0.000000e+00
6.000000e+02	5.600000e-17	0.000000e+00	0.000000e+00
7.000000e+02	4.500000e-17	0.000000e+00	0.000000e+00
7.800000e+02	3.700000e-17	0.000000e+00	0.000000e+00
8.000000e+02	3.200000e-17	0.000000e+00	0.000000e+00

Appendix II:

Ionization Energies of Neutral Atoms

Table 18: Ionization energies for the neutral atoms

Z		Element	Ground-state configuration	Ground level	Ionization energy (eV)
1	H	Hydrogen	$1s$	$^2S_{1/2}$	13.5984
2	He	Helium	$1s^2$	$^1S_0$	24.5874
3	Li	Lithium	$1s^2\ 2s$	$^2S_{1/2}$	5.3917
4	Be	Beryllium	$1s^2\ 2s^2$	$^1S_0$	9.3227
5	B	Boron	$1s^2\ 2s^2\ 2p$	$^2P^o_{1/2}$	8.2980
6	C	Carbon	$1s^2\ 2s^2\ 2p^2$	$^3P_0$	11.2603
7	N	Nitrogen	$1s^2\ 2s^2\ 2p^3$	$^4S^o_{3/2}$	14.5341
8	O	Oxygen	$1s^2\ 2s^2\ 2p^4$	$^3P_2$	13.6181
9	F	Fluorine	$1s^2\ 2s^2\ 2p^5$	$^2P^o_{3/2}$	17.4228
10	Ne	Neon	$1s^2\ 2s^2\ 2p^6$	$^1S_0$	21.5646
11	Na	Sodium	[Ne] $3s$	$^2S_{1/2}$	5.1391
12	Mg	Magnesium	[Ne] $3s^2$	$^1S_0$	7.6462
13	Al	Aluminum	[Ne] $3s^2\ 3p$	$^2P^o_{1/2}$	5.9858
14	Si	Silicon	[Ne] $3s^2\ 3p^2$	$^3P_0$	8.1517
15	P	Phosphorus	[Ne] $3s^2\ 3p^3$	$^4S^o_{3/2}$	10.4867
16	S	Sulfur	[Ne] $3s^2\ 3p^4$	$^3P_2$	10.3600
17	Cl	Chlorine	[Ne] $3s^2\ 3p^5$	$^2P^o_{3/2}$	12.9676
18	Ar	Argon	[Ne] $3s^2\ 3p^6$	$^1S_0$	15.7596
19	K	Potassium	[Ar] $4s$	$^2S_{1/2}$	4.3407
20	Ca	Calcium	[Ar] $4s^2$	$^1S_0$	6.1132
21	Sc	Scandium	[Ar] $3d\ 4s^2$	$^2D_{3/2}$	6.5615
22	Ti	Titanium	[Ar] $3d^2\ 4s^2$	$^3F_2$	6.8281
23	V	Vanadium	[Ar] $3d^3\ 4s^2$	$^4F_{3/2}$	6.7462

24	Cr	Chromium	[Ar] $3d^5\ 4s$	$^7S_3$	6.7665
25	Mn	Manganese	[Ar] $3d^5\ 4s^2$	$^6S_{5/2}$	7.4340
26	Fe	Iron	[Ar] $3d^6\ 4s^2$	$^5D_4$	7.9024
27	Co	Cobalt	[Ar] $3d^7\ 4s^2$	$^4F_{9/2}$	7.8810
28	Ni	Nickel	[Ar] $3d^8\ 4s^2$	$^3F_4$	7.6398
29	Cu	Copper	[Ar] $3d^{10}\ 4s$	$^2S_{1/2}$	7.7264
30	Zn	Zinc	[Ar] $3d^{10}\ 4s^2$	$^1S_0$	9.3942
31	Ga	Gallium	[Ar] $3d^{10}\ 4s^2\ 4p$	$^2P^o_{1/2}$	5.9993
32	Ge	Germanium	[Ar] $3d^{10}\ 4s^2\ 4p^2$	$^3P_0$	7.8994
33	As	Arsenic	[Ar] $3d^{10}\ 4s^2\ 4p^3$	$^4S^o_{3/2}$	9.7886
34	Se	Selenium	[Ar] $3d^{10}\ 4s^2\ 4p^4$	$^3P_2$	9.7524
35	Br	Bromine	[Ar] $3d^{10}\ 4s^2\ 4p^5$	$^2P^o_{3/2}$	11.8138
36	Kr	Krypton	[Ar] $3d^{10}\ 4s^2\ 4p^6$	$^1S_0$	13.9996
37	Rb	Rubidium	[Kr] $5s$	$^2S_{1/2}$	4.1771
38	Sr	Strontium	[Kr] $5s^2$	$^1S_0$	5.6949
39	Y	Yttrium	[Kr] $4d\ 5s^2$	$^2D_{3/2}$	6.2171
40	Zr	Zirconium	[Kr] $4d^2\ 5s^2$	$^3F_2$	6.6339
41	Nb	Niobium	[Kr] $4d^4\ 5s$	$^6D_{1/2}$	6.7589
42	Mo	Molybdenum	[Kr] $4d^5\ 5s$	$^7S_3$	7.0924
43	Tc	Technetium	[Kr] $4d^5\ 5s^2$	$^6S_{5/2}$	7.28
44	Ru	Ruthenium	[Kr] $4d^7\ 5s$	$^5F_5$	7.3605
45	Rh	Rhodium	[Kr] $4d^8\ 5s$	$^4F_{9/2}$	7.4589
46	Pd	Palladium	[Kr] $4d^{10}$	$^1S_0$	8.3369
47	Ag	Silver	[Kr] $4d^{10}\ 5s$	$^2S_{1/2}$	7.5762
48	Cd	Cadmium	[Kr] $4d^{10}\ 5s^2$	$^1S_0$	8.9938
49	In	Indium	[Kr] $4d^{10}\ 5s^2\ 5p$	$^2P^o_{1/2}$	5.7864
50	Sn	Tin	[Kr] $4d^{10}\ 5s^2\ 5p^2$	$^3P_0$	7.3439
51	Sb	Antimony	[Kr] $4d^{10}\ 5s^2\ 5p^3$	$^4S^o_{3/2}$	8.6084
52	Te	Tellurium	[Kr] $4d^{10}\ 5s^2\ 5p^4$	$^3P_2$	9.0096
53	I	Iodine	[Kr] $4d^{10}\ 5s^2\ 5p^5$	$^2P^o_{3/2}$	10.4513
54	Xe	Xenon	[Kr] $4d^{10}\ 5s^2\ 5p^6$	$^1S_0$	12.1298
55	Cs	Cesium	[Xe] $6s$	$^2S_{1/2}$	3.8939
56	Ba	Barium	[Xe] $6s^2$	$^1S_0$	5.2117

57	La	Lanthanum	[Xe] $5d\,6s^2$	$^2D_{3/2}$	5.5769
58	Ce	Cerium	[Xe] $4f\ 5d\,6s^2$	$^1G^o_4$	5.5387
59	Pr	Praseodymium	[Xe] $4f^3\ 6s^2$	$^4I^o_{9/2}$	5.473
60	Nd	Neodymium	[Xe] $4f^4\ 6s^2$	$^5I_4$	5.5250
61	Pm	Promethium	[Xe] $4f^5\ 6s^2$	$^6H^o_{5/2}$	5.582
62	Sm	Samarium	[Xe] $4f^6\ 6s^2$	$^7F_0$	5.6436
63	Eu	Europium	[Xe] $4f^7\ 6s^2$	$^8S^o_{7/2}$	5.6704
64	Gd	Gadolinium	[Xe] $4f^7\ 5d\ 6s^2$	$^9D^o_2$	6.1501
65	Tb	Terbium	[Xe] $4f^9\ 6s^2$	$^6H^o_{15/2}$	5.8638
66	Dy	Dysprosium	[Xe] $4f^{10}\ 6s^2$	$^5I_8$	5.9389
67	Ho	Holmium	[Xe] $4f^{11}\ 6s^2$	$^4I^o_{15/2}$	6.0215
68	Er	Erbium	[Xe] $4f^{12}\ 6s^2$	$^3H_6$	6.1077
69	Tm	Thulium	[Xe] $4f^{13}\ 6s^2$	$^2F^o_{7/2}$	6.1843
70	Yb	Ytterbium	[Xe] $4f^{14}\ 6s^2$	$^1S_0$	6.2542
71	Lu	Lutetium	[Xe] $4f^{14}\ 5d\ 6s^2$	$^2D_{3/2}$	5.4259
72	Hf	Hafnium	[Xe] $4f^{14}\ 5d^2\ 6s^2$	$^3F_2$	6.8251
73	Ta	Tantalum	[Xe] $4f^{14}\ 5d^3\ 6s^2$	$^4F_{3/2}$	7.5496
74	W	Tungsten	[Xe] $4f^{14}\ 5d^4\ 6s^2$	$^5D_0$	7.8640
75	Re	Rhenium	[Xe] $4f^{14}\ 5d^5\ 6s^2$	$^6S_{5/2}$	7.8335
76	Os	Osmium	[Xe] $4f^{14}\ 5d^6\ 6s^2$	$^5D_4$	8.4382
77	Ir	Iridium	[Xe] $4f^{14}\ 5d^7\ 6s^2$	$^4F_{9/2}$	8.9670
78	Pt	Platinum	[Xe] $4f^{14}\ 5d^9\ 6s$	$^3D_3$	8.9587
79	Au	Gold	[Xe] $4f^{14}\ 5d^{10}\ 6s$	$^2S_{1/2}$	9.2255
80	Hg	Mercury	[Xe] $4f^{14}\ 5d^{10}\ 6s^2$	$^1S_0$	10.4375
81	Tl	Thallium	[Xe] $4f^{14}\ 5d^{10}\ 6s^2\ 6p$	$^2P^o_{1/2}$	6.1082
82	Pb	Lead	[Xe] $4f^{14}\ 5d^{10}\ 6s^2\ 6p^2$	$^3P_0$	7.4167
83	Bi	Bismuth	[Xe] $4f^{14}\ 5d^{10}\ 6s^2\ 6p^3$	$^4S^o_{3/2}$	7.2856
84	Po	Polonium	[Xe] $4f^{14}\ 5d^{10}\ 6s^2\ 6p^4$	$^3P_2$	8.417 ?
85	At	Astatine	[Xe] $4f^{14}\ 5d^{10}\ 6s^2\ 6p^5$	$^2P^o_{3/2}$	
86	Rn	Radon	[Xe] $4f^{14}\ 5d^{10}\ 6s^2\ 6p^6$	$^1S_0$	10.7485
87	Fr	Francium	[Rn] $7s$	$^2S_{1/2}$	4.0727
88	Ra	Radium	[Rn] $7s^2$	$^1S_0$	5.2784
89	Ac	Actinium	[Rn] $6d\ 7s^2$	$^2D_{3/2}$	5.17

90	Th	Thorium	[Rn] $6d^2\ 7s^2$	$^3F_2$	6.3067
91	Pa	Protactinium	[Rn] $5f^2(^3H_4)\ 6d\ 7s^2$	$(4,^3/_2)_{11/2}$	5.89
92	U	Uranium	[Rn] $5f^3(^4I^o_{9/2})\ 6d\ 7s^2$	$(^9/_2,^3/_2)^o_6$	6.1941
93	Np	Neptunium	[Rn] $5f^4(^5I_4)\ 6d\ 7s^2$	$(4,^3/_2)_{11/2}$	6.2657
94	Pu	Plutonium	[Rn] $5f^6\ 7s^2$	$^7F_0$	6.0262
95	Am	Americium	[Rn] $5f^7\ 7s^2$	$^8S^o_{7/2}$	5.9738
96	Cm	Curium	[Rn] $5f^7\ 6d\ 7s^2$	$^9D^o_2$	5.9915
97	Bk	Berkelium	[Rn] $5f^9\ 7s^2$	$^6H^o_{15/2}$	6.1979
98	Cf	Californium	[Rn] $5f^{10}\ 7s^2$	$^5I_8$	6.2817
99	Es	Einsteinium	[Rn] $5f^{11}\ 7s^2$	$^4I^o_{15/2}$	6.42
100	Fm	Fermium	[Rn] $5f^{12}\ 7s^2$	$^3H_6$	6.50
101	Md	Mendelevium	[Rn] $5f^{13}\ 7s^2$	$^2F^o_{7/2}$	6.58
102	No	Nobelium	[Rn] $5f^{14}\ 7s^2$	$^1S_0$	6.65
103	Lr	Lawrencium	[Rn] $5f^{14}\ 7s^2\ 7p$?	$^2P^o_{1/2}$?	4.9 ?
104	Rf	Rutherfordium	[Rn] $5f^{14}\ 6d^2\ 7s^2$?	$^3F_2$?	6.0 ?

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References for Ionization Energies of the neutral atoms in Table 18 .

1 H

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Appendix Ⅲ:

Gaussian Input Files

1. Monosodium monoxide NaO

1.1. No.1:

Purpose: Determination of geometry structure of NaO and check the vibration frequencies:

```
# OPT Freq B3LYP/6-311G(d) SCF=tight

Geometry
0,2
O
Na,1,R
        Variables:
R=3.0
```

1.2. No.2:

Purpose: Determination of geometry structure of cation NaO^+, compare singlet and triplet state and check the vibration frequencies:

```
# OPT Freq B3LYP/6-311G(d) SCF=tight

Geometry

1,1
O
Na,1,R
      Variables:
R=3.0

--Link1--
# OPT Freq B3LYP/6-311G(d) SCF=tight

Geometry

1,3
O
Na,1,R
      Variables:
R=3.0
```

1.3. No. 3:

Purpose: Calculate orbital parameters by using experiment bond length

```
# B3LYP/6-311G SCF=tight AIM=ALL POP=FULL

Geometry

0,2
O
Na,1,2.05155
```

1.4. No. 4:

Purpose: Calculate I.P. of NaO by CBS-4 method, using structure data of cation obtained in No. 2.

```
# CBS-4M/6-311G(d) SCF=tight

I.P. NaO + e >> NaO+ + 2e

0,2
O
Na,1, 2.05155

--Link1--

# CBS-4M/6-311G(d), SCF=tight

I.P. NaO + e >> NaO+ + 2e

1,1
O
Na,1, 2.4942

--Link1--
# CBS-4M/6-311G(d) SCF=tight

I.P. NaO + e >> NaO+ + 2e

1,3
O
Na,1, 2.5118
```

2. Sodium hydroxide NaOH

For NaOH, there exists a theoretic problem when using B3LYP/6-31G(d). It failed to give correct geometry but could only find a false bent structure, i.e. α (Na-O-H) =126° instead of 180°. That is quite unusual because diffuse functions must be considered when electrons are far from the nucleus. So B3LYP/6-31+G(d) or MP2/6-31G(d) combinations are employed in this case. Both of them can give much close answer to the experiment values.

2.1. No. 1:

Purpose: Calculating geometry, check frequencies and then orbital parameters

```
#MP2/6-311G(d) OPT=z-matrix AIM=all POP=Full

NaOH

0, 1
O
Na 1 1.9300
H 1 0.9700 2 180.0
```

Or

```
# B3LYP/6-31+G(d) OPT=z-matrix FREQ SCF=tight AIM=ALL POP=FULL

NaOH

0, 1
O
X 1 1.0
Na 1 rna 2 90.0
H 1 rh 2 ah 3 beta
 variables:
rna 1.9782
rh 0.9666
ah 36.374
beta=180.0
```

2.2. No. 2:

Purpose: Calculating orbital parameters by using experimental data of geometry structure.

```
#MP2FU/6-311G(d) OPT=z-matrix FREQ AIM=all POP=Full

NaOH

0, 1
O
Na 1 r1
H 1 r2 2 alpha
      variables:
r1=2.0
r2=1.0
alpha=178.0
```

2.3. No. 3:

Purpose: Looking for geometry of cation NaOH

```
#B3LYP/6-31G* OPT=z-matrix FREQ

NaOH


1, 2
O
X 1 1.0
Na 1 rna 2 90.0
H 1 rh 2 ah 3 180.0

rna 2.5
rh 1.5
ah 36.374
```

3. Disodium monoxide Na_2O

3.1. No. 1:

Purpose: Searching geometry structure of $Na_2O(g)$ and check vibration frequencies.

```
# Opt Freq B3LYP/6-311G(d) SCF=tight POP=FULL

Na2O Geometry Optimization

 0 1
 O
 NA,1,R
 NA,1,R,2,A
       Variables:
 R=1.5
 A=180.00000
```

3.2. No. 2:

Purpose: Calculating orbital parameters by using structure data obtained in No. 1

```
# B3LYP/6-311G(d) SCF=tight aim=all Pop=Full

K.E.

 0 1
 O
 NA,1,1.98
 NA,1,1.98,2,180.0
```

3.3. No. 3:

Purpose: Searching structure of cation Na_2O^+

```
# OPT B3LYP/6-311G(d) SCF=tight

Optimize Na2O+

1 2
 O
 NA,1,R
 NA,1,R,2,A
  variables:
 R=2.5
 A=180.0
```

3.4. No. 4:

Purpose: Calculating I.P. of Na2O by CBS-4 with structure data obtained in No. 1 and No. 3.

```
# CBS-4M/6-311G(d) SCF=tight

I.P. of Na2O + e >> Na2O+ + 2e

 0 1
 O
 NA,1,1.98
 NA,1,1.98,2,180.0

--Link1--

# CBS-4M/6-311G(d), SCF=tight

Na2O Geometry Optimization

1 2
O
NA,1,2.05626191
NA,1,2.05626191,2,180.0
```

4. Disodium Na_2

4.1. No. 1

Purpose: Check structure, vibration frequency of Na_2 and searching the structure of cation Na_2^+

```
#OPT Freq BLYP/6-311G(d) SCF=tight

Geometry

0,1
Na
Na,1,R
        Variables:
R=3.0

--Link1--
#Opt Freq BLYP/6-311G(d) SCF=tight

Geometry

1,2
Na
Na,1,R
      Variables:
R=3.0
```

4.2. No. 2:

Purpose: Obtaining orbital parameters of Na^2 by using experimental bond length

```
# B3LYP/6-311G SCF=tight AIM=ALL POP=FULL

test K.E.

0,1
Na
Na,1,3.07887
```

4.3. No. 3:

Purpose: Calculating I.P of Na2 with results obtained in No. 1.

```
# CBS-4M/6-311G(d) SCF=tight

I.P. Na2 + 2 >> Na2+ + 2e

0,1
Na
Na,1,3.07887

--Link1--

# CBS-4M/6-311G(d) SCF=tight

I.P. Na2 + 2 >> Na2+ + 2e

1,2
Na
Na,1,3.6485
```

Appendix Ⅳ:

GAMESS Input and Selected Parts of Output Files

Note:

- ✧ All the calculation by GAMESS are in Hartree Hock level with 6-311G Basis Sets.
- ✧ In the output file, only the orbital energy, kinetic energy and Mulliken analysis results are printed here to save the size of the report.

1. Monosodium monoxide NaO

1.1. Input file:

```
$contrl scftyp=UHF MULT=2 $end
$system memory=300000 $end
$SCF VTSCAL=.TRUE. $end
$basis   gbasis=N311 ngauss=6 $end
$guess   guess=huckel $end
$data
NaO
Cnv 1

O, 8.0, 0.0, 0.0, 0.0
Na, 11.0, 0.0, 0.0, 2.05155
$end
```

1.2. Selected output data:

----- ALPHA SET -----

EIGENVECTORS

1	2	3	4	5
-40.4805	-20.4107	-2.7910	-1.5192	-1.5186
6	7	8	9	10
-1.5178	-1.1182	-0.4384	-0.3655	-0.3568
11	12	13	14	15
-0.0120	0.0301	0.0321	0.0572	0.1198
16	17	18	19	20
0.1216	0.1242	0.2001	0.5505	0.5541

----- BETA SET -----

EIGENVECTORS

1	2	3	4	5
-40.4809	-20.3718	-2.7917	-1.5192	-1.5190
6	7	8	9	10
-1.5181	-0.9464	-0.3021	-0.2970	-0.0119
11	12	13	14	15
0.0276	0.0326	0.0572	0.1093	0.1225
16	17	18	19	20
0.1246	0.2052	0.3025	0.5520	0.5523

MULLIKEN AND LOWDIN POPULATION ANALYSES

MULLIKEN ATOMIC POPULATION IN EACH MOLECULAR ORBITAL
ALPHA ORBITALS

	1	2	3	4	5
	1.000000	1.000000	1.000000	1.000000	1.000000
1	0.000000	0.999983	0.000314	-0.000001	-0.000010
2	1.000000	0.000017	0.999686	1.000001	1.000010
	6	7	8	9	10
	1.000000	1.000000	1.000000	1.000000	1.000000
1	0.004089	0.991475	0.987356	0.953775	0.977211
2	0.995911	0.008525	0.012644	0.046225	0.022789

MULLIKEN ATOMIC POPULATION IN EACH MOLECULAR ORBITAL
BETA ORBITALS

	1	2	3	4	5
	1.000000	1.000000	1.000000	1.000000	1.000000
1	0.000000	0.999992	0.000298	-0.000010	-0.000033
2	1.000000	0.000008	0.999702	1.000010	1.000033
	6	7	8	9	
	1.000000	1.000000	1.000000	1.000000	
1	0.001998	0.982730	0.920007	0.957993	
2	0.998002	0.017270	0.079993	0.042007	

VIRIAL ANALYSIS

ALPHA ORBITALS

KINETIC ENERGY OF ORBITAL	1 IS	56.30753252
KINETIC ENERGY OF ORBITAL	2 IS	29.18155495
KINETIC ENERGY OF ORBITAL	3 IS	6.72925867
KINETIC ENERGY OF ORBITAL	4 IS	5.88477352
KINETIC ENERGY OF ORBITAL	5 IS	5.88801440
KINETIC ENERGY OF ORBITAL	6 IS	5.87385622
KINETIC ENERGY OF ORBITAL	7 IS	3.02776157
KINETIC ENERGY OF ORBITAL	8 IS	2.32939715
KINETIC ENERGY OF ORBITAL	9 IS	2.27560399
KINETIC ENERGY OF ORBITAL	10 IS	2.21974385

BETA ORBITALS

KINETIC ENERGY OF ORBITAL	1 IS	56.30798518
KINETIC ENERGY OF ORBITAL	2 IS	29.24669514
KINETIC ENERGY OF ORBITAL	3 IS	6.73185876
KINETIC ENERGY OF ORBITAL	4 IS	5.88859399
KINETIC ENERGY OF ORBITAL	5 IS	5.88344097
KINETIC ENERGY OF ORBITAL	6 IS	5.88497303
KINETIC ENERGY OF ORBITAL	7 IS	2.83808173
KINETIC ENERGY OF ORBITAL	8 IS	2.11132824
KINETIC ENERGY OF ORBITAL	9 IS	2.06383901

2. Sodium hydroxide NaOH

2.1. Input file

```
 $contrl scftyp=RHF MULT=1 COORD=ZMT $end
 $system memory=300000 $end
 $SCF VTSCAL=.TRUE. $end
 $basis   gbasis=N31 ngauss=6 $end
 $guess   guess=huckel $end
 $data
NaOH
Cnh 1

O
X 1 1.
Na 1 rna 2 90.
H 1 rh 2 ah 3 180. 0.0

rna=1.9300
rh=0.9700
ah=36.374
 $end
```

2.2. Output file (Selected parts in short)

```
------------
EIGENVECTORS
------------
          1         2         3         4         5
   -40.4482  -20.3795   -2.7736   -1.4958   -1.4954
          6         7         8         9        10
    -1.4951   -1.1130   -0.4602   -0.3229   -0.3192
         11        12        13        14        15
    -0.0013    0.0509    0.0564    0.0942    0.1554
         16        17        18        19        20
     0.2264    0.2319    0.3197    0.3890    1.2941
         21        22        23        24
     1.3528    1.3822    1.5442    1.7803
```

```
---------------------------------------
 MULLIKEN AND LOWDIN POPULATION ANALYSES
---------------------------------------
MULLIKEN ATOMIC POPULATION IN EACH MOLECULAR ORBITAL

          1         2         3         4         5
      2.000000  2.000000  2.000000  2.000000  2.000000
1    -0.000014  1.999530 -0.000179  0.002842  0.000039
2     2.000014  0.000143  2.000209  1.997221  1.999961
3     0.000000  0.000327 -0.000030 -0.000063  0.000000
          6         7         8         9        10
      2.000000  2.000000  2.000000  2.000000  2.000000
1     0.010308  1.786585  1.448141  1.900560  1.927148
2     1.989944  0.026179  0.056833  0.098382  0.072852
3    -0.000252  0.187236  0.495027  0.001058  0.000000
```

```
---------------
VIRIAL ANALYSIS
---------------

      ALPHA ORBITALS
KINETIC ENERGY OF ORBITAL    1 IS   56.27897824
KINETIC ENERGY OF ORBITAL    2 IS   29.20792448
KINETIC ENERGY OF ORBITAL    3 IS    6.84858074
KINETIC ENERGY OF ORBITAL    4 IS    5.85645218
KINETIC ENERGY OF ORBITAL    5 IS    5.86735575
KINETIC ENERGY OF ORBITAL    6 IS    5.83005808
KINETIC ENERGY OF ORBITAL    7 IS    2.69001710
KINETIC ENERGY OF ORBITAL    8 IS    1.87153204
KINETIC ENERGY OF ORBITAL    9 IS    2.12198403
KINETIC ENERGY OF ORBITAL   10 IS    2.06083744
```

3. Disodium monoxide Na_2O

3.1. Input file

```
$contrl RUNTYP=OPTIMIZE MAXIT=100 scftyp=UHF MULT=1 $end
$system memory=300000 $end
$SCF VTSCAL=.TRUE. $end
$basis   gbasis=N311 ngauss=6 $end
$guess   guess=huckel $end
$data
Na2O
Cnv 1
CARD>
O, 8.0, 0.0, 0.0, 0.0
Na, 11.0, 0.0, 0.0, 2.0
CARD> Na, 11.0, 0.0, 0.0, -2.0
$end
```

3.2. Selected output results

MULLIKEN ATOMIC POPULATION IN EACH MOLECULAR ORBITAL
ALPHA ORBITALS

	1	2	3	4	5
	1.000000	1.000000	1.000000	1.000000	1.000000
1	0.000004	0.000000	0.999966	0.001265	0.000049
2	0.500014	0.499984	0.000017	0.499368	0.499976
3	0.499982	0.500016	0.000017	0.499367	0.499976
	6	7	8	9	10
	1.000000	1.000000	1.000000	1.000000	1.000000
1	-0.000082	-0.000082	0.000000	0.000000	0.006951
2	0.500042	0.500042	0.499999	0.499999	0.496524
3	0.500041	0.500041	0.500001	0.500001	0.496524
	11	12	13	14	15
	1.000000	1.000000	1.000000	1.000000	1.000000
1	-0.000535	0.965829	0.867977	0.885389	0.885389
2	0.500267	0.017086	0.066012	0.057305	0.057305
3	0.500267	0.017086	0.066012	0.057305	0.057305

MULLIKEN ATOMIC POPULATION IN EACH MOLECULAR ORBITAL
BETA ORBITALS

	1	2	3	4	5
	1.000000	1.000000	1.000000	1.000000	1.000000
1	0.000004	0.000000	0.999966	0.001265	0.000049
2	0.500014	0.499984	0.000017	0.499368	0.499976
3	0.499982	0.500016	0.000017	0.499367	0.499976
	6	7	8	9	10
	1.000000	1.000000	1.000000	1.000000	1.000000
1	-0.000082	-0.000082	0.000000	0.000000	0.006951
2	0.500042	0.500042	0.499999	0.499999	0.496524
3	0.500041	0.500041	0.500001	0.500001	0.496524
	11	12	13	14	15
	1.000000	1.000000	1.000000	1.000000	1.000000
1	-0.000535	0.965829	0.867977	0.885389	0.885389
2	0.500267	0.017086	0.066012	0.057305	0.057305
3	0.500267	0.017086	0.066012	0.057305	0.057305

VIRIAL ANALYSIS

ALPHA ORBITALS

KINETIC ENERGY OF ORBITAL	1 IS	56.31553829
KINETIC ENERGY OF ORBITAL	2 IS	56.31580313
KINETIC ENERGY OF ORBITAL	3 IS	29.22249293
KINETIC ENERGY OF ORBITAL	4 IS	6.73264152
KINETIC ENERGY OF ORBITAL	5 IS	6.73287125
KINETIC ENERGY OF ORBITAL	6 IS	5.87904727
KINETIC ENERGY OF ORBITAL	7 IS	5.87904727
KINETIC ENERGY OF ORBITAL	8 IS	5.88056738
KINETIC ENERGY OF ORBITAL	9 IS	5.88056738
KINETIC ENERGY OF ORBITAL	10 IS	5.84757775
KINETIC ENERGY OF ORBITAL	11 IS	5.88095456
KINETIC ENERGY OF ORBITAL	12 IS	2.90460716
KINETIC ENERGY OF ORBITAL	13 IS	2.10757604
KINETIC ENERGY OF ORBITAL	14 IS	1.83755557
KINETIC ENERGY OF ORBITAL	15 IS	1.83755557

BETA ORBITALS

KINETIC ENERGY OF ORBITAL	1 IS	56.31553829
KINETIC ENERGY OF ORBITAL	2 IS	56.31580313
KINETIC ENERGY OF ORBITAL	3 IS	29.22249293
KINETIC ENERGY OF ORBITAL	4 IS	6.73264152
KINETIC ENERGY OF ORBITAL	5 IS	6.73287125
KINETIC ENERGY OF ORBITAL	6 IS	5.87904727
KINETIC ENERGY OF ORBITAL	7 IS	5.87904727
KINETIC ENERGY OF ORBITAL	8 IS	5.88056738
KINETIC ENERGY OF ORBITAL	9 IS	5.88056738
KINETIC ENERGY OF ORBITAL	10 IS	5.84757775
KINETIC ENERGY OF ORBITAL	11 IS	5.88095456
KINETIC ENERGY OF ORBITAL	12 IS	2.90460716
KINETIC ENERGY OF ORBITAL	13 IS	2.10757604
KINETIC ENERGY OF ORBITAL	14 IS	1.83755557
KINETIC ENERGY OF ORBITAL	15 IS	1.83755557

4. Disodium Na_2

4.1. Input file

```
$contrl scftyp=RHF MULT=1 $end
 $system memory=300000 $end
 $SCF VTSCAL=.TRUE. $end
 $basis   gbasis=N311 ngauss=6 $end
 $guess   guess=huckel $end
 $data
 Na2
 Cnv 1

 Na, 11.0, 0.0, 0.0, 0.0
 Na, 11.0, 0.0, 0.0, 3.07887
 $end
```

4.2. Selected output data

```
            ------------
            EIGENVECTORS
            ------------

     1         2         3         4         5
-40.4681  -40.4681   -2.7805   -2.7804   -1.5069
     6         7         8         9        10
 -1.5055   -1.5055   -1.5052   -1.5052   -1.5050
    11        12        13        14        15
 -0.1660    0.0025    0.0242    0.0242    0.0347
```

VIRIAL ANALYSIS

ALPHA ORBITALS

KINETIC ENERGY OF ORBITAL	1 IS	56.33478474
KINETIC ENERGY OF ORBITAL	2 IS	56.33499332
KINETIC ENERGY OF ORBITAL	3 IS	6.75909723
KINETIC ENERGY OF ORBITAL	4 IS	6.76129574
KINETIC ENERGY OF ORBITAL	5 IS	5.88029404
KINETIC ENERGY OF ORBITAL	6 IS	5.89458938
KINETIC ENERGY OF ORBITAL	7 IS	5.89458938
KINETIC ENERGY OF ORBITAL	8 IS	5.89895442
KINETIC ENERGY OF ORBITAL	9 IS	5.89895442
KINETIC ENERGY OF ORBITAL	10 IS	5.90805823
KINETIC ENERGY OF ORBITAL	11 IS	0.28714748

MULLIKEN ATOMIC POPULATION IN EACH MOLECULAR ORBITAL

	1	2	3	4	5
	2.000000	2.000000	2.000000	2.000000	2.000000
1	1.000000	1.000000	1.000000	1.000000	1.000000
2	1.000000	1.000000	1.000000	1.000000	1.000000
	6	7	8	9	10
	2.000000	2.000000	2.000000	2.000000	2.000000
1	1.000000	1.000000	1.000000	1.000000	1.000000
2	1.000000	1.000000	1.000000	1.000000	1.000000
	11				
	2.000000				
1	1.000000				
2	1.000000				