

2011年12月13-14日
原子分子データ応用フォーラムセミナー

核融合研の原子分子データ ベースと世界の原子分子データ ベースについて

核融合科学研究所
村上 泉

原子分子データベースの発展

1981
AMDIS

1985
CHART
SPUTY
BACKS

ALADDIN

1997
WWW

1998
AMDIS
Rec.

2001
AMOL
CMOL

2001
GENIE

1990代～ サテライトデータベース

1977-1989
IPPJ-AM (64 reports)

1990-
NIFS-DATA (111 reports)

1978-1989
名古屋大学プラズマ研究所

1989-2004
核融合研 研究・企画情報センター

2004-2009
核融合研
連携研究センター
原子分子
データ研究室

2010-
核融合研
核融合システム研究系
原子分子過程研究部門

1977-
IAEA 核融合のための原子データ諮問委員会、データセンターネットワーク

1973-1977
名古屋大学プラズマ研
原子過程作業グループ
データ収集
IPPJ-DT-48 ('75), 50('76)

30年以上に及ぶデータ収集と蓄積
(Data Bank)

核融合プラズマ→より広いプラズマ分野へ

1. NIFS 原子分子数値データベース

<http://dbshino.nifs.ac.jp/>

NIFS DATABASE
<National Institute for Fusion Science>

Atomic & Molecular Numerical Databases

Cross Sections and Rate Coefficients for Ionization, Excitation, and Recombination by Electron Impact, Charge Transfer by Heavy Particle Collision, and Collision Processes of Molecules, Sputtering Yields of Solids, and Back Scattering Coefficients from Solids

Bibliographic Databases

Fusion and Plasma Sciences, Atomic and Molecular Physics, and Atomic Collision Processes

Made by [A&M and PWI data research section](#)

More detailed information is [here](#). Samples on Numerical Data are [here](#).
We welcome your [data submission](#). Details are [here](#).
We welcome your [comments and suggestions](#). Please send email to dbadmin@dbshino.nifs.ac.jp.

Please Logon Free

[Logon Free](#)

Information on Database Service

<No Service Stop is scheduled.>

Free Access Databases on Atomic and Molecular Data provided by NIFS:

- [ALADDIN](#) (Ionization Cross Sections and Excitation Rate Coefficients by Electron Impact)
- [Data for Autoionizing States](#) (Energy Levels of Autoionizing States and Satellite Lines by Dielectronic Recombination)
- [Differential Cross Sections for Molecules by Electron Impact](#)
- [Differential Cross Sections of Ionization for Atomic Hydrogen by Proton Impact](#)
- [Sputtering yield, Reflection coefficient and Range value of solid surfaces](#) (Calculated by Dr. W. Eckstein)
- [Electron Dissociative Attachment to Molecular Hydrogen](#)
- [ION FRACTION](#) (Ion Abundance Tables in Ionization Equilibrium)
- [Recommended data set of electron collision cross sections of atoms and molecules](#) (compiled by The Institute of Electrical Engineers of Japan)

[Links to Atomic and Molecular Databases in the World](#)

By [A&M and PWI data research section](#), [Coordination Research Center in NIFS](#)

入り口

各データベースの略称をクリックしてアクセス

各データベースの簡単な紹介

衛星データベース

Welcome to NIFS DATABASE

Please select the database. Atomic and Molecular Research Center, NIFS is making the Atomic and Molecular Numerical databases for various collisional processes and the Bibliographic Databases. You can access the databases only which you applied for at the registration. Information on each database will be found from [here](#).

Atomic and Molecular Numerical Databases

AMDIS	EXC	ION	REC	DIO
CHART	AMOL	CMOL		
BACKS	SPUTY	CURVE		

Bibliographic Database

ORNL

Atomic and Molecular Numerical Databases

Atomic and Molecular Research Center, NIFS is making the Atomic and Molecular Numerical databases for various collisional processes. When you use the data from our databases in your papers, you are requested to refer to our databases and let us know it by sending the email. We are interested in your atomic data needs for the activities relating to atomic data in our center. Your requests to add data to our databases are appreciated as well. Please send your data needs and requests to dbadmin@dbshino.nifs.ac.jp.

- AMDIS**
Cross sections and rate coefficients for ionization, excitation, and recombination by electron impact (since 1961). Please use AMOL for molecule targets.
 - ION**: Ionization cross sections and rate coefficients by electron impact.
 - EXC**: Excitation cross sections and rate coefficients by electron impact.
 - REC**: Recombination cross sections and rate coefficients by electron impact.
 - DIO**: Dissociation cross sections of molecules. (until 2000. Please use AMOL.)

[Tables for number of data records in AMDIS ION and EXC.](#)

- CHART**
Cross sections for charge transfer and ionization by heavy particle collision. Please use CMOL for molecule targets.

AM and PWI 数值Database (<http://dbshino.nifs.ac.jp>)

データベース名	内容	Period	データ件数 (2011年8月)
AMDIS	EXC	1961-2011	463,592 (408,164 (Aug. 2009))
	ION		
	DIO		
	REC		
CHART	原子-イオン衝突の荷電交換・電離過程	1957-2010	7,054 (5,305)
AMDIS MOL (AMOL)	分子の電子との各種衝突過程	1956-2008	3,765
CHART MOL (CMOL)			
SPUTY	固体のスputタリングイールド	1931-2000	1,241
BACKS	固体表面での後方散乱係数	1976-2002	396
(AM Bibliographic database)			
ORNL	ORNL (USA) で作成した原子衝突過程に関する文献データベース	1959-2008	77,714

AMOL 分子の電子衝突過程

- 分子の電子衝突による各種反応過程の断面積、速度係数
- 分子名(化学式、英語名)や反応過程などで検索できる。
- CMOL(分子の原始衝突による各種反応過程)も同様

AMDIS MOLECULE Visitors counting: 000801 since 2008/06/18

[Help]

Search Data Form Clear

Initial State : Molecular formula * : CH4 or
Molecular name * : or
Ionic State :

Final State * : and or

Process :

Data Type : Cross Section Rate coefficient Other

Theoretical Experimental Evaluated

Author(s) * :

Year of Publication : From : To : (YYYY)

Additional conditions for search:

Incident Energy Region (eV) From : To :

SQL

SORT KEY

total scattering
elastic scattering / momentum transfer
excitation
ionization
dissociation
attachment
recombination

AMOL: 例 O₂

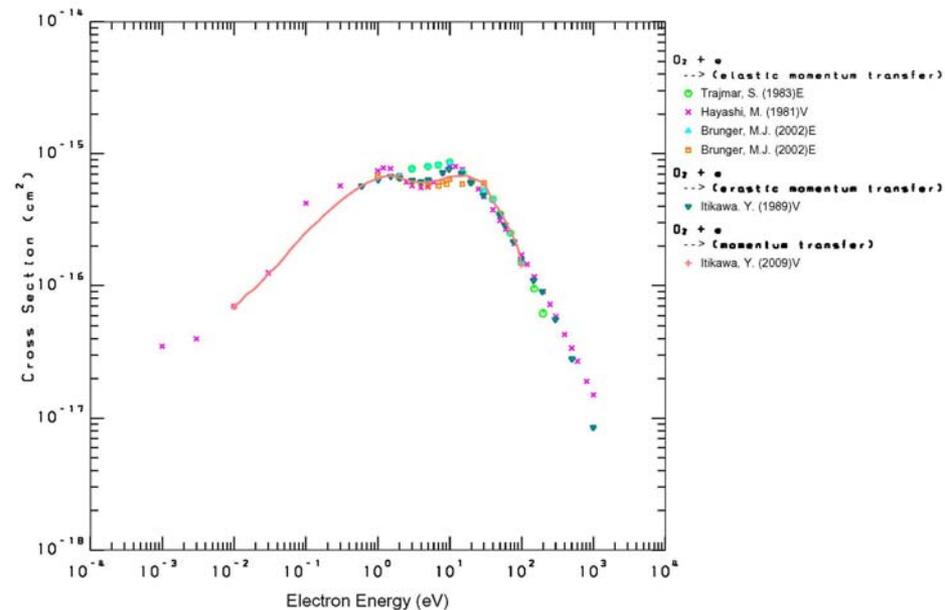
衝突過程ごとに分類したリスト。

Found Result in AMDIS MOLECULE

Found 130 Title(s)

<input checked="" type="checkbox"/> All Data List	130 records found
<input type="checkbox"/> O ₂ + e → (SR continuum)	2 records found
<input type="checkbox"/> O ₂ + e → (W=9.7-12.1eV)	1 records found
<input type="checkbox"/> O ₂ + e → (dissociative electron attachment)	1 records found
<input type="checkbox"/> O ₂ + e → (elastic momentum transfer)	4 records found
<input type="checkbox"/> O ₂ + e → (elastic scattering)	9 records found
<input type="checkbox"/> O ₂ + e → (elastic)	1 records found
<input type="checkbox"/> O ₂ + e → (erastic momentum transfer)	1 records found
<input type="checkbox"/> O ₂ + e → (erastic scattering)	1 records found
<input type="checkbox"/> O ₂ + e → (ionization)	1 records found
<input type="checkbox"/> O ₂ + e → (longest band)	1 records found
<input type="checkbox"/> O ₂ + e → (momentum transfer)	1 records found
<input type="checkbox"/> O ₂ + e → (second band)	1 records found
<input type="checkbox"/> O ₂ + e → (the longest band)	1 records found
<input type="checkbox"/> O ₂ + e → (the second band)	1 records found
<input type="checkbox"/> O ₂ + e → (total dissociation)	1 records found
<input type="checkbox"/> O ₂ + e → (total double ionization)	1 records found
<input type="checkbox"/> O ₂ + e → (total ionization)	1 records found
<input type="checkbox"/> O ₂ + e → (total scattering)	12 records found
<input type="checkbox"/> O ₂ + e → (total single ionization)	1 records found
<input type="checkbox"/> O ₂ + e → A ³ Σ+C ³ Δ+c ¹ Σ	1 records found
<input type="checkbox"/> O ₂ + e → A ³ Σ+C ³ Δ+c ¹ Σ	1 records found

Momentum transfer
断面積。
市川の評価データ
(2009)を実線で表示



CMOL: 分子の重粒子衝突過程

CHART MOLECULE Visitors counting: 000623 since 2008/06/18 [\[Help\]](#)

Initial

Element A : Element/Molecular formula * or
Atomic number
Molecular name * or
Charge state
Excited state

Element B : Molecular formula *
Molecular name * or
Charge state:
Excited state

Final

Products Element/Molecular formula *
 and or

Element/Molecular name *
 and or

Process

Data Type Cross Section Rate coefficient Other

Theoretical Experimental Evaluated

Author(s) * :

Year of Publication : From : To : (YYYY)

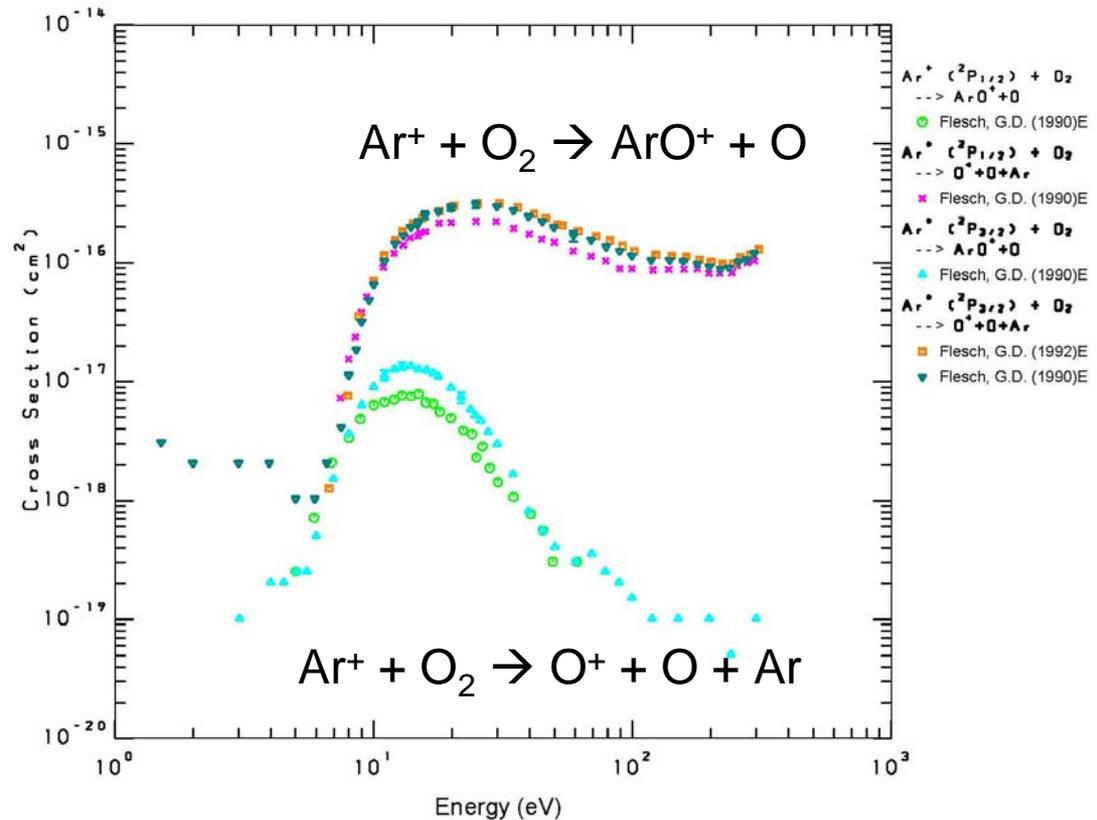
- 入射イオン、標的分子を指定して検索
- H₂ (D₂), N₂, 炭化水素、CO, CO₂等
が中心。
- データ数はまだあまり多くない。
- 標的O₂は44セット。

CMOL: 例 O₂

Found Result in CHART MOLECULE

Found 44 Title(s)

- All Data List 44 records found
- Ar⁺ (²P_{1/2}) + O₂ → ArO⁺+O 1 records found
 - Ar⁺ (²P_{1/2}) + O₂ → O⁺+O+Ar 1 records found
 - Ar⁺ (²P_{3/2}) + O₂ → ArO⁺+O 1 records found
 - Ar⁺ (²P_{3/2}) + O₂ → O⁺+O+Ar 2 records found
 - C⁺ (²P) + O₂ → C 1 records found
 - C⁺ + O₂ → C+O₂⁺ 1 records found
 - H + O₂ → H⁺ 1 records found
 - H⁺ + O₂ (1s) → H(n=1)+O₂⁺ 1 records found
 - H⁺ + O₂ → H 1 records found
 - H⁺ + O₂ → H+O₂⁺ 2 records found
 - He + O₂ → He⁺ 1 records found
 - He + O₂ → He⁺ (CS) 1 records found
 - He + O₂ → He²⁺ 2 records found
 - He + O₂ → He²⁺ (CS) 3 records found
 - He⁺ + O₂ (1s) → He(n=1)+O₂⁺ 1 records found
 - He⁺ + O₂ → He 2 records found
 - He⁺ + O₂ → He (CS) 1 records found
 - He⁺ + O₂ → He+O₂⁺ 1 records found
 - He⁺ + O₂ → He²⁺ 2 records found
 - He⁺ + O₂ → He²⁺ (CS) 1 records found



データ入力・アップデート

- 原子分子過程部門の少人数スタッフ、および、核融合研の共同研究として、原子物理学研究者のボランティアによるデータ収集活動によりデータ入力、アップデートを行っているのが現状。なかなか網羅できない。

2. サテライトデータベース dbshino の表紙にリンク

検索機能のないデータベース。テキストファイル等でデータを公開。
共同研究などの成果の公開

- ALADDIN (電子衝突による電離断面積と励起速度係数) (英語)
- 二重励起状態のデータベース (二重励起状態のエネルギーレベルと二電子性再結合によるサテライト線) (英語)
- 電子衝突による分子の微分断面積データベース (英語)
- 陽子衝突による水素原子の電離微分断面積(英語)
- 水素分子への電子の解離付着係数 (英語)
- 電離平衡時のイオン比表 (英語)
- 固体表面のスパッタリング収率、反射係数、飛程値のデータベース (Eckstein博士の計算による) (英語)
- PWI計算コードライブラリー
- 原子・分子の電子衝突断面積の推奨データセット(電気学会提供)
- 光吸収 (英語)

故 林先生の原子分子文献・数値データベース

- 林先生(故人)によって、67の原子分子の文献及び断面積データの収集が行なわれたが、文献データベースはほとんどが未発表
- 以下の18の原子・分子の文献データ(20世紀に出版された文献情報)が、NIFS-DATAとして2003-2004年に出版されているが、のこりはまだ。その中に、O₂も含まれる。

NIFS-DATA-72 (Ar),
 NIFS-DATA-74 (CO₂),
 NIFS-DATA-76 (SF₆),
 NIFS-DATA-77 (N₂),
 NIFS-DATA-79 (Xe),
 NIFS-DATA-80 (F₂, Cl₂, Br₂, I₂),
 NIFS-DATA-81 (水蒸気),
 NIFS-DATA-82 (H₂),
 NIFS-DATA-83 (HF, HCl, HBr, HI),
 NIFS-DATA-87 (NH₃, PH₃),
 NIFS-DATA-90 (CH₄)

CH₄

Table QT-1. Summary of the experimental study of grand total cross section Q_T for CH₄.

Author	year	ϵ (eV)	error (%)
Brode	1925	1.5 - 320	
Bruche	1927	1 - 44	
Bruche	1929	1 - 50	
Ramsauer	1929	0.2 - 1.3	
Ramsauer	1931		
Barbarito	1979	0.1 - 16	
Hasted	1979	(0.3 - 5)	
Bonham	1980	(0.5 - 100)	
Griffith	1982	5 - 400	
* Perch	1985	0.085 - 12	1 - 4
Floeder	1985	5 - 400	
* Jones	1985	1.3 - 50	3 - 8
* Lohmann	1986	0.1 - 20	3 - 5
* Sueoka	1986	1 - 400	4 - 5
* Dababneh	1988	4.5 - 500	
* Nishimura	1991	5 - 500	13
* Zecca	1991	0.9 - 4000	6.5 - 8
* Kanik	1992	4 - 300	
* Garcia	1998	400 - 5000	3

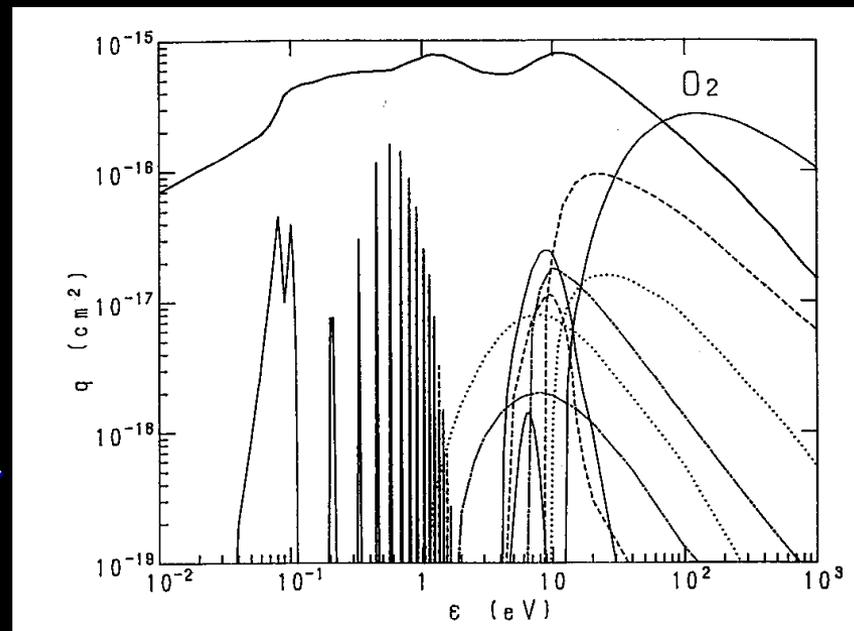
() The data are not available.

* These data are shown in the tables.

(from NIFS-DATA-90)

故 林先生のデータベースとしての整備・出版

- 林先生が評価された断面積データは、36の原子分子が、「プラズマ材料科学ハンドブック」(1992)に図として掲載されている。
- 未発表のデータを電気学会の放電委員会の協力のもとで、整備。
- 未発表の4原子分子 (Cd, NO, CCl₂F₂, CCl₄) の断面積をデータベースとして整備中。
- 文献データもデータベースとして整備中。



「プラズマ材料科学ハンドブック」に掲載されているO₂の電子衝突断面積

3 世界にある原子分子データベース

- インターネットでアクセスできる原子分子データベースは「プラズマ原子分子過程ハンドブック」17章で紹介。
- リンクリスト(上記の一部は未掲載)
<http://dpc.nifs.ac.jp/dblinks1.html>
- 応用分野ごとのコミュニティでデータベースが作られて公開されている
- 分子の衝突過程データベースはあまり多くない

韓国NFRIの原子分子データベース

- 韓国のNFRIが、独自にプラズマ応用のための原子分子データベースを作成。原著論文の調査および独自のデータ評価を行っている。表示は韓国語。シミュレーションコードも別途開発
- 分子：
http://plasma.kisti.re.kr/web/property/property_molecule.jsp



<http://plasma.kisti.re.kr/>

NFRI (韓国) のデータベース

Plasma Property Database

플라즈마 물성정보 시스템 | 플라즈마 소개 | 물성정보 조회 | 플라즈마 시뮬레이션 | 정보마당

플라즈마 물성정보 DB Atomic and Molecular Database for Industrial Plasma

분자

단원자 분자

Br ₂	C ₂	Cl ₂	D ₂	F ₂	H ₂	He ₂	I ₂
K ₂	Li ₂	N ₂	Na ₂	O ₂	S ₂		

이원자 분자

BrCl	BrO	CD	ClH	ClO	CO	CS	CsCl
DCI	DH	FeO	GeH	HBr	HCl	HD	HF
HI	LiBr	NH	NO	OH	TiCl		

삼원자 분자

CCl ₂	CD ₂	ClO ₂	CO ₂	COS	CS ₂	D ₂ O	DCO
------------------	-----------------	------------------	-----------------	-----	-----------------	------------------	-----

Plasma Property Database

플라즈마 물성정보 시스템 | 플라즈마 소개 | 물성정보 조회 | 플라즈마 시뮬레이션 | 정보마당

플라즈마 물성정보 DB Atomic and Molecular Database for Industrial Plasma

분자

대분류: Collision 데이터 분류: Cross Section 충돌 방식: Electron Impact

입자정보

입자: O₂ 이름:

주프로세스 부프로세스

==전체==
Attachment
Absorption
Charge Transfer
Dissociation

Associative Attachment
Attachment
Total Dissociative Attachment
Dissociative Attachment
Ion Pair Production

조회

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대전시 유성구 유성동 52-11 (305-800) TEL : 042-829-5002
서울시 용산구 방방대로 200-9 (100-761) TEL : 02-3299-6000
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본 사이트는 행정안전부와 한국정보보호진흥원의 지원으로 구축되었습니다.

- 分子種を選んだあと、衝突過程を指定して検索

NFRIのデータベース

분자

홈 -> 플라즈마 특성정보 DB -> 분자

총 8건

부프로세스(반응식)	검증구분	원문	참고문헌
<input type="checkbox"/> Total Ionization $e + O_2$	T	NDSL	Joshiapura, K N; Antony, B K; Vinodkumar, Minaxi. Electron scattering and ionization of ozone, O_2 and O_4 molecules. <i>Journal of physics B, Atomic, molecular, and optical physics</i> , V.35,p4211,(2002)
<input type="checkbox"/> Total Ionization $e + O_2$	T	NDSL	Vandana Saksena, M. S, Kushwaha and S. P. Khare. Electron Impact Ionisation of Molecules at High Energies. <i>International Journal of Mass Spectrometry and Ion Processes</i> , V.171,pL1,(1997)
<input type="checkbox"/> Total Ionization $e + O_2 \rightarrow O_2^+ +$	R	NDSL	Majed, T.; Strickland, D. J.. New Survey of Electron Impact Cross Sections for Photoelectron and Auroral Electron Energy Loss Calculations. <i>Journal of physical and chemical reference data</i> , V.26,p335,(1997)
<input type="checkbox"/> Total Ionization $e + O_2$	R		M. Brunger, R. S. Brusa, S. J. Buckman, M. T. Eloff, Y. Hatano, K. Kameta, G. P. Karwasz, and N. Kouchi, B. G. Lindsay, M. A. Mangan, A. Zecca, and Y. Itikawa, Landolt-Börnstein Numerical Data and Functional Relationships in Science and Technology New Series-Group I: Elementary Particles, Nuclei and Atoms 17C: Interactions of Photons and Electrons with Molecules. <i>null</i> , V.17C,pChap.5.1,(2003)
<input type="checkbox"/> Total Ionization $e + O_2$	E	NDSL	Monthiro Okada;Hisayuki Toku;Yasushi Yamamoto;Kiyoshi Yoshikawa. Characteristics of Hall Accelerator with He, H₂, CH₄, O₂ and Ar Gases. <i>Japanese Journal of Applied Physics</i> , V.33,p4782,(1994)
<input type="checkbox"/> Total Ionization <i>null</i>	E		K. Wakiya. Differential and integral cross sections for the electron impact excitation of O₂ I, Optically allowed transitions from the ground state. <i>Journal of Physics B:Atomic and molecular physics.</i> , V.11,p3913,(1978)
<input type="checkbox"/> Total Ionization <i>null</i>	E		DONALD RAPP;PAULA ENGLANDER-GOLDEN. Total Cross Sections for Ionization and Attachment in Gases by Electron Impact. I. Positive Ionization. <i>THE JOURNAL OF CHEMICAL PHYSICS</i> , V.43,p1464,(1965)
			J. W. McConkey;C. P. Malone;P. V. Johnson;C. Winstead;V. McKoy;I. Kanik.

×축: 에너지 [eV] y축: 산란단면적 1E-16 [cm²] 조회

× 검증구분: E(Experiment), T(Theory), R(Recommendation)

부프로세스(반응식)	검증구분	원문	참고문헌
<input checked="" type="checkbox"/> Total Ionization $e + O_2$	T	NDSL	Joshiapura, K N; Antony, B K; Vinodkumar, Minaxi. Electron scattering and ionization of ozone, O_2 and O_4 molecules. <i>Journal of physics B, Atomic, molecular, and optical physics</i> , V.35,p4211,(2002)

목록보기

- 原著論文ごとに結果が表示。断面積データはグラフ表示できる。

NIST Chemical Kinetics Database

http://kinetics.nist.gov/kinetics/

Kinetics Database Resources

Simple Reaction Search

Search Reaction Database

Search Bibliographic Database

Set Unit Preferences

Feedback

Rate Our Products and Services

Citation

Help

Other Databases

NIST Standard Reference Data Program

NIST Chemistry Web Book

NDRL-NIST Solution Kinetics Database

NIST

National Institute of Standards and Technology

Home ©NIST, 2011 Accessibility information

NIST Chemical Kinetics Database

Standard Reference Database 17, Version 7.0 (Web Version), Release 1.6.3 Data Version 2011.06

A compilation of kinetics data on gas-phase reactions

Reaction Database Quick Search Form

Enter the reactant(s) and/or product(s) in the fields below. Fields may be left blank.

+ → +

If you would like more searching options, try...
[advanced reaction search form](#)
[bibliographic search form](#)

[Welcome](#)
About the database.

[Getting Started](#)
A quick introduction to the database.

[Credits and History](#)
Who created the present version and the earlier versions?

[Feedback](#)
How to report errors or obtain technical assistance.

Kinetics Database Resources

Simple Reaction Search

Search Reaction Database

Search Bibliographic Database

Set Unit Preferences

Feedback

Rate Our Products and Services

Help

Other Databases

NIST Standard Reference Data Program

NIST Chemistry Web Book

NDRL-NIST Solution Kinetics Database

NIST

National Institute of Standards and Technology

Home ©NIST, 2011 Accessibility information

Search Results

Click on a link in the table below to see detail on the selected reaction.

	Records	Reaction
Simple Reaction Search	1 record matched	CH ₄ + FCGeH → Products
Search Reaction Database	1 record matched	CH ₄ + ClCGeH → Products
Search Bibliographic Database	1 record matched	CH ₄ + HCCGeCl → Products
Set Unit Preferences	1 record matched	CH ₄ + HCCGeF → Products
Feedback	2 records matched	CH ₄ + HCCGeH → Products
Rate Our Products and Services	1 record matched	CH ₄ + FC(O)O → Products
Help	1 record matched	CH ₄ + Rhodium carbonyl (5-2,4-cyclopentadien-1-yl)- → Adduct
Other Databases	1 record matched	CH ₄ + Al(CH ₃) ₃ → AlH(CH ₃) ₂
	1 record matched	CH ₄ + (CH ₃) ₂ Ge → (CH ₃) ₃ GeH
	2 records matched	CH ₄ + CCCN → HCCCN + ·CH ₃
	3 records matched	CH ₄ + ·CH ₂ → ·CH ₃ + ·CH ₃
	1 record matched	CH ₄ + ·CH ₂ → C ₂ H ₆
	1 record matched	CH ₄ + HCSiH → Products
	1 record matched	CH ₄ + CF ₃ CF → ·CH ₃ + CF ₃ CHF
	1 record matched	CH ₄ + (CH ₃) ₂ C → iso-C ₄ H ₁₀
	1 record matched	CH ₄ + CH ₃ SCH ₂ → (CH ₃) ₂ S + ·CH ₃
	1 record matched	CH ₄ + CH ₃ Sn(CH ₃) ₃ → (CH ₃) ₃ SnH
	95 records matched	CH ₄ + Cl → ·CH ₃ + HCl
	2 records matched	CH ₄ + NCO → Products
	14 records matched	CH ₄ + CF ₃ O → CF ₃ OH + ·CH ₃
	1 record matched	CH ₄ + CF ₃ O → Products
	1 record matched	CH ₄ + N → CH ₃ NH
	4 records matched	CH ₄ + N → HCN + H ₂ + H·
	2 records matched	CH ₄ + N → Products

- 化学反応式に分子記号等を入れて、データを検索

NIST Chemical Kinetics Database

Kinetics Database Home ©NIST, 2000
Accessibility information

Search Results

CH₄ + O₂ → ·CH₃ + HO₂

Rate expression: $k(T) = A (T/298 \text{ K})^n e^{-E_a/RT}$
 Rate expression units:
 First order: s⁻¹
 Second order: cm³/molecule s
 Third order: cm⁶/molecule² s
 R = 8.314472E-03 kJ / mole K

Energy Units	kJ	Molecular Units	Molecule
Pressure Units	Pa	Temperature Units	K
Base Volume Unit	cm	Reference Temperature	298.0
Evaluation Temperature	298.0		

Use the Plot checkboxes to select data for plotting. Plot selected data using the "Create Plot" button. Click the squib to see extra information about a particular rate constant. Additional help is available.

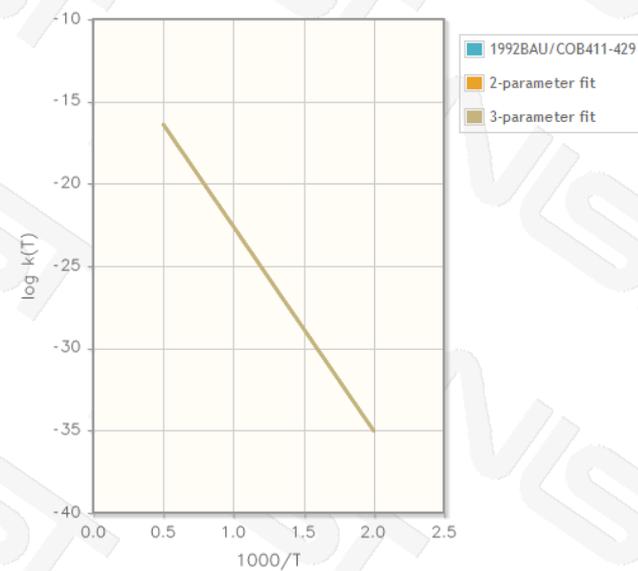
Plot Squib	Temp [K]	A	n	Ea [kJ]	k(298.00 K)	Order
<input type="checkbox"/> 1992BAU/COB411-429	500 - 2000	6.59E-11	238			2
<input type="checkbox"/> 1986TSA/HAM1087	300 - 2500	6.71E-11	238			2
Experiment						
<input type="checkbox"/> 1961FAL/KNO782-791	830	<0.36				2
Reference reaction: C ₂ H ₆ + O ₂ → ·C ₂ H ₅ + HO ₂						

Theory

Kinetics Database Resources

- Simple Reaction Search
- Search Reaction Database
- Search Bibliographic Database
- Set Unit Preferences
- Feedback
- Rate Our Products and Services
- Citation
- Help

Rate Constant Plot



Other Databases

- NIST Standard Reference Data Program
- NIST Chemistry Web Book
- NDRL-NIST Solution Kinetics Database
- NIST Computational Chemistry

Fit of Arrhenius parameters to set:

Temperature range: 500 - 2000 K

Two-parameter fit:

$$k(T) = A \exp(-E_a/RT)$$

$A = 6.59 \times 10^{-11} \text{ [cm}^3/\text{molecule s]}$
 $E_a = 238 \text{ [kJ]}$
 RMSD = 0.0

Three-parameter fit:

$$k(T) = A(T/T_{ref})^n \exp(-E_a/RT)$$

$A = 6.59 \times 10^{-11} \text{ [cm}^3/\text{molecule s]}$
 $n = 0.0$
 $T_{ref} = 298 \text{ [K]}$
 $E_a = 238 \text{ [kJ]}$
 RMSD = 0.0

NIST Chemistry Webbook

<http://webbook.nist.gov/chemistry>

NIST Chemistry WebBook

NIST Standard Reference Database Number 69

View: [Search Options](#), [Models and Tools](#), [Documentation](#), [Changes](#), [Notes](#)

[Show Credits](#)

NIST reserves the right to charge for access to this database in the future.

Search Options [top](#)

General Searches

- [Formula](#)
- [Name](#)
- [IUPAC identifier](#)
- [CAS registry number](#)
- [Reaction](#)
- [Author](#)
- [Structure](#)

Physical Property Based Searches

- [Ion energetics properties](#)
- [Vibrational and electronic energies](#)
- [Molecular weight](#)

Models and Tools [top](#)

- [Thermophysical Properties of Fluid Systems](#) High accuracy data for a select group of fluids.
- [Group Additivity Based Estimates](#) Estimates of gas phase thermodynamic properties based on a submitted structure.
- [Formula Browser](#) Locates chemical species by building up a chemical formula in Hill order.

Documentation [top](#)

- [Frequently asked questions](#)
- [Version history](#)
- [A Guide to the NIST Chemistry WebBook](#) A guide to this site and the data available from it.

- 原子分子の化学的性質を網羅したハンドブック
- 分子構造や、気相反応などのエンタルピー、エントロピー、自由エネルギーなど、電離ポテンシャル、解離イオン種の appearance energy などのデータとそのリファレンスなどが調べられる。

NIST Chemistry Webbook

Oxygen

- **Formula:** O₂
- **Molecular weight:** 31.9988
- **IUPAC Standard InChI:**
 - InChI=1S/O2/c1-2
 - [Download the identifier in a file.](#)
- **IUPAC Standard InChIKey:** MYMOFI2GZYHOMD-UHFFFAOYSA-N
- **CAS Registry Number:** 7782-44-7
- **Chemical structure:** O=O

This structure is also available as a [2d Mol file](#).

- **Other names:** Molecular oxygen; Oxygen molecule; Pure oxygen; O₂; Liquid-oxygen-; UN 1072; UN 1073; Dioxygen
- **Permanent link** for this species. Use this link for bookmarking this species for future reference.
- **Information on this page:**
 - [Gas phase thermochemistry data](#)
 - [Reaction thermochemistry data \(reactions 1 to 50\)](#)
 - [Gas phase ion energetics data](#)
 - [Ion clustering data](#)
 - [References](#)
 - [Notes / Error Report](#)
- **Other data available:**
 - [Phase change data](#)
 - [Reaction thermochemistry data: reactions 51 to 68](#)
 - [Henry's Law data](#)
 - [Mass spectrum \(electron ionization\)](#)
 - [Constants of diatomic molecules](#)
 - [Fluid Properties](#)
- **Data at other public NIST sites:**
 - [Microwave spectra \(on physics lab web site\)](#)
 - [Electron-Impact Ionization Cross Sections \(on physics web site\)](#)
 - [Computational Chemistry Comparison and Benchmark Database](#)
 - [Gas Phase Kinetics Database](#)
- **Options:**
 - [Switch to calorie-based units](#)

Data at NIST subscription sites:

Reaction thermochemistry data

Go To: [Top](#), [Gas phase thermochemistry data](#), [Gas phase ion energetics data](#), [Ion clustering data](#), [References](#), [Notes / Error Report](#)

Data compilation [copyright](#) by the U.S. Secretary of Commerce on behalf of the U.S.A. All rights reserved.

Data compiled as indicated in comments:

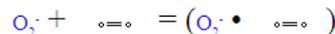
B - J.E. Bartmess

M - M.M. Meot-Ner (Mautner) and S. G. Lias

ALS - H.Y. Afeefy, J.F. Liebman, and S.E. Stein

Note: Please consider using the [reaction search](#) for this species. This page allows searching of all reactions involving this species. A general reaction search form is [also available](#). Future versions of this site may rely on reaction search pages in place of the enumerated reaction displays seen below.

Reactions 1 to 50



By formula: $\text{O}_2 + \text{O} = (\text{O}_2 \cdot \text{O})$

Quantity	Value	Units	Method	Reference	Comment
$\Delta_f H^\circ$	48. ± 20.	kJ/mol	AVG	N/A	Average of 5 out of 7 values; Individual data points
Quantity	Value	Units	Method	Reference	Comment
$\Delta_f S^\circ$	102.	J/mol*K	PHPMS	Hiraoka, 1988	gas phase; <i>M</i>
$\Delta_f S^\circ$	130.	J/mol*K	PHPMS	Conway and Nesbit, 1968	gas phase; <i>M</i>
Quantity	Value	Units	Method	Reference	Comment
$\Delta_f G^\circ$	13. ± 4.6	kJ/mol	TDA	Hiraoka, 1988	gas phase; see also Sherwood, Hanold, et al., 1996 . Aquino, Taylor, et al., 2001 calns indicate rectangular anion; <i>B</i>
$\Delta_f G^\circ$	16. ± 4.2	kJ/mol	TDA	Conway and Nesbit, 1968	gas phase; <i>B</i>
$\Delta_f G^\circ$	23. ± 4.2	kJ/mol	IMRE	Payzant J.D. and Kebarle, 1972	gas phase; <i>B</i>
$\Delta_f G^\circ$	13. ± 4.2	kJ/mol	IMRE	Pack and Phelps, 1971	gas phase; <i>B</i>

Enthalpy

Entropy

Free energy

UMIST database for Astrochemistry

<http://www.udfa.net/>

- Astron. & Astrophys., 466, 1197–1204 (2007)
- 2体衝突 速度係数のフィッティング関数
 $k = \alpha (T/300)^\beta \exp(-\gamma/T) \text{ cm}^3 \text{ s}^{-1}$

udfa⁶

C2H4

Search

or

Select a species...

or

Download UDfA...

Found 122 'C2H4' reactions, showing 1 - 50 next 50

Reaction	α	β	γ	$T_1 - T_0$ (K)	Accuracy	Source
1 C + C ₂ H ₄ → C ₃ H ₃ + H	3.00E-10	-0.11	0.0	15 - 300	within 25%	Measurement
2 C ⁺ + C ₂ H ₄ → C ₃ H ₂ ⁺ + H ₂	3.40E-10	0.00	0.0	10 - 41000	within 25%	Measurement
3 C ⁺ + C ₂ H ₄ → C ₃ H ⁺ + H ₂ + H	8.50E-11	0.00	0.0	10 - 41000	within 25%	Measurement
4 C ⁺ + C ₂ H ₄ → C ₂ H ₄ ⁺ + C	1.70E-11	0.00	0.0	10 - 41000	within 25%	Measurement
5 C ⁺ + C ₂ H ₄ → C ₂ H ₃ ⁺ + CH	8.50E-11	0.00	0.0	10 - 41000	within 25%	Measurement
6 C ⁺ + C ₂ H ₄ → H ₂ C ₃ H ⁺ + H	1.02E-09	0.00	0.0	10 - 41000	within 25%	Measurement
7 C ₂ + C ₂ H ₄ → C ₄ H ₃ + H	3.50E-10	0.00	0.0	24 - 300	within 50%	Measurement
8 C ₂ H ₂ ⁺ + C ₂ H ₄ → C ₄ H ₅ ⁺ + H	3.17E-10	0.00	0.0	10 - 41000	within 25%	Lit. Search
9 C ₂ H ₂ ⁺ + C ₂ H ₄ → C ₂ H ₄ ⁺ + C ₂ H ₂	4.14E-10	0.00	0.0	10 - 41000	within 25%	Lit. Search
10 C ₂ H ₂ ⁺ + C ₂ H ₄ → H ₂ C ₃ H ⁺ + CH ₃	6.62E-10	0.00	0.0	10 - 41000	within 25%	Lit. Search
11 C ₂ H ₂ ⁺ + CH ₃ CH ₃ → C ₂ H ₄ ⁺ + C ₂ H ₄	2.48E-10	0.00	0.0	10 - 41000	within 25%	Measurement
12 C ₂ H ₂ ⁺ + SiH ₄ → Si ⁺ + C ₂ H ₄ + H ₂	6.60E-11	0.00	0.0	10 - 41000	within 50%	Measurement
13 C ₂ H ₂ ⁺ + SiH ₄ → SiH ₂ ⁺ + C ₂ H ₄	1.65E-10	0.00	0.0	10 - 41000	within 50%	Measurement
14 C ₂ H ₃ + C ₂ H ₄ ⁺ → C ₂ H ₄ + C ₂ H ₃ ⁺	5.00E-10	0.00 / -0.50	0.0	10 - 41000	factor 2	Lit. Search
15 C ₂ H ₃ ⁺ + C ₂ H ₄ → C ₂ H ₅ ⁺ + C ₂ H ₂	8.90E-10	0.00	0.0	10 - 41000	within 25%	Measurement
16 C ₂ H ₃ ⁺ + CH ₃ CH ₃ → C ₂ H ₅ ⁺ + C ₂ H ₄	2.91E-10	0.00	0.0	10 - 41000	within 25%	Measurement

IUPAC Evaluated Kinetic Data

<http://www.iupac-kinetic.ch.cam.ac.uk/>

- 大気化学のための、原子分子反応、原子分子と固体や液体との評価済み反応速度係数等のデータ表。

The screenshot shows the homepage of the IUPAC Subcommittee for Gas Kinetic Data Evaluation. The header features the IUPAC logo and the text "IUPAC Subcommittee for Gas Kinetic Data Evaluation" and "International Union of Pure and Applied Chemistry (IUPAC)". Below the header, there is a navigation menu with links for Home Page, Recent changes, Committee members, Email list, Publications, IUPAC home page, Related web sites, Research projects, and RSS feed. The main content area is titled "Evaluated Kinetic Data" and includes a description of the website's purpose, a "Summary tables" section with links to various reaction categories (Gas phase, Heterogeneous reactions on ice surfaces, Heterogeneous reactions on mineral dust), and a "Datasheets" section with a search function and filters for different reaction types (Gas-phase reactions, Photolysis reactions, Heterogeneous reactions on solids, Heterogeneous reactions on liquids). The footer includes the logo of the Natural Environment Research Council.

IUPAC Evaluated Kinetic Data



IUPAC Subcommittee for Gas Kinetic Data Evaluation

International Union of Pure and Applied Chemistry (IUPAC)

Providing evaluated kinetic data on the web since 1999.

[Home Page](#)

[Recent changes](#)

[Committee members](#)

[Email list](#)

[Publications](#)

[IUPAC home page](#)

[Related web sites](#)

[MCM-IUPAC project](#)

 [RSS feed](#)

Use Firefox for best results
when viewing XHTML files.

Data sheets for gas phase reactions of Ox species

To cite material from the datasheets below we suggest "R. Atkinson, D. L. Baulch, R. A. Cox, J. N. Crowley, R. F. Hampson, R. G. Hynes, M. E. Jenkin, M. J. Rossi, and J. Troe, *Atmos. Chem. Phys.*, 4, 1461-1738 (2004); IUPAC Subcommittee for Gas Kinetic Data Evaluation, <http://www.iupac-kinetic.ch.cam.ac.uk>" [Vol 1](#)

A zip file containing all of the PDF format datasheets for this category is available : [iupac_ox_gasphase.zip](#). Please do not redistribute these datasheets or zipfile. They are for personal use only.

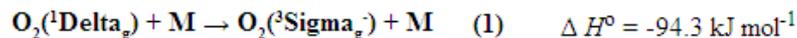
Our ID ACP ID	Reactants	Products	Formats	Last change in preferred values	Last evaluated
Ox1	$O + O_2 + M$	→	PDF Word XML XHTML	2002-03-09	2002-03-09
Ox2	$O + O_3$	→	PDF Word XML XHTML	2001-10-02	2001-10-02
Ox3	$O(^1D) + O_2$	→	PDF Word XML XHTML	2001-10-02	2001-10-02
Ox4	$O(^1D) + O_3$	→	PDF Word XML XHTML	2001-10-02	2001-10-02
Ox5	$O_2^* + O_3$	→	PDF Word XML XHTML	2001-10-02	2001-10-02
Ox6	$O_2(^3\Sigma_g^- \nu) + M$	→	PDF Word XML XHTML	2001-10-02	2001-10-02
Ox7	$O_2(^1\Delta_g) + M$	→	PDF Word XML XHTML	2001-10-02	2001-10-02
Ox8	$O_2(^1\Delta_g) + O_3$	→	PDF Word XML XHTML	2001-10-02	2001-10-02
Ox9	$O_2(^1\Sigma_g^+) + M$	→	PDF Word XML XHTML	2001-10-02	2001-10-02
Ox10	$O_2(^1\Sigma_g^+) + O_3$	→	PDF Word XML XHTML	2001-10-02	2001-10-02

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IUPAC Subcommittee on Gas Kinetic Data Evaluation

Website: <http://www.iupac-kinetic.ch.cam.ac.uk/> See website for latest evaluated data. Datasheets can be downloaded for personal use only and must not be retransmitted or disseminated either electronically or in hardcopy without explicit written permission.

This datasheet last evaluated: 2001-10-02 ; last change in preferred values: 2001-10-02 ; last peer-reviewed publication: 2004-03-09



Rate Coefficient Data

Absolute Rate Coefficients

Rate Coefficient (k) / cm ³ molecule ⁻¹ s ⁻¹	Third Body	Unknown / UNKNOWN	Reference	Techniques and Comments
$(1.51 \pm 0.05) \times 10^{-18}$	O2	298	Borrell et al., 1977	DF-CL (a)
$(1.47 \pm 0.05) \times 10^{-18}$	O2	298	Leiss et al., 1978	(b)
$(1.65 \pm 0.07) \times 10^{-18}$	O2	298	Raja et al., 1986	DF-CL (a)
$3.15 \times 10^{-18} \exp(-205/T)$	O2	100–450	Billington and Borrell, 1986	DF-CL (a)
1.57×10^{-18}		298		
1.4×10^{-19}	N2	300	Collins et al., 1973	FP-VUVA (c)
5.6×10^{-18}	H2O	298	Findlay and Snelling, 1971	(d)
$< 1.5 \times 10^{-20}$	CO2	298		
$(4 \pm 1) \times 10^{-18}$	H2O	298	Becker et al., 1971	(e)

Comments

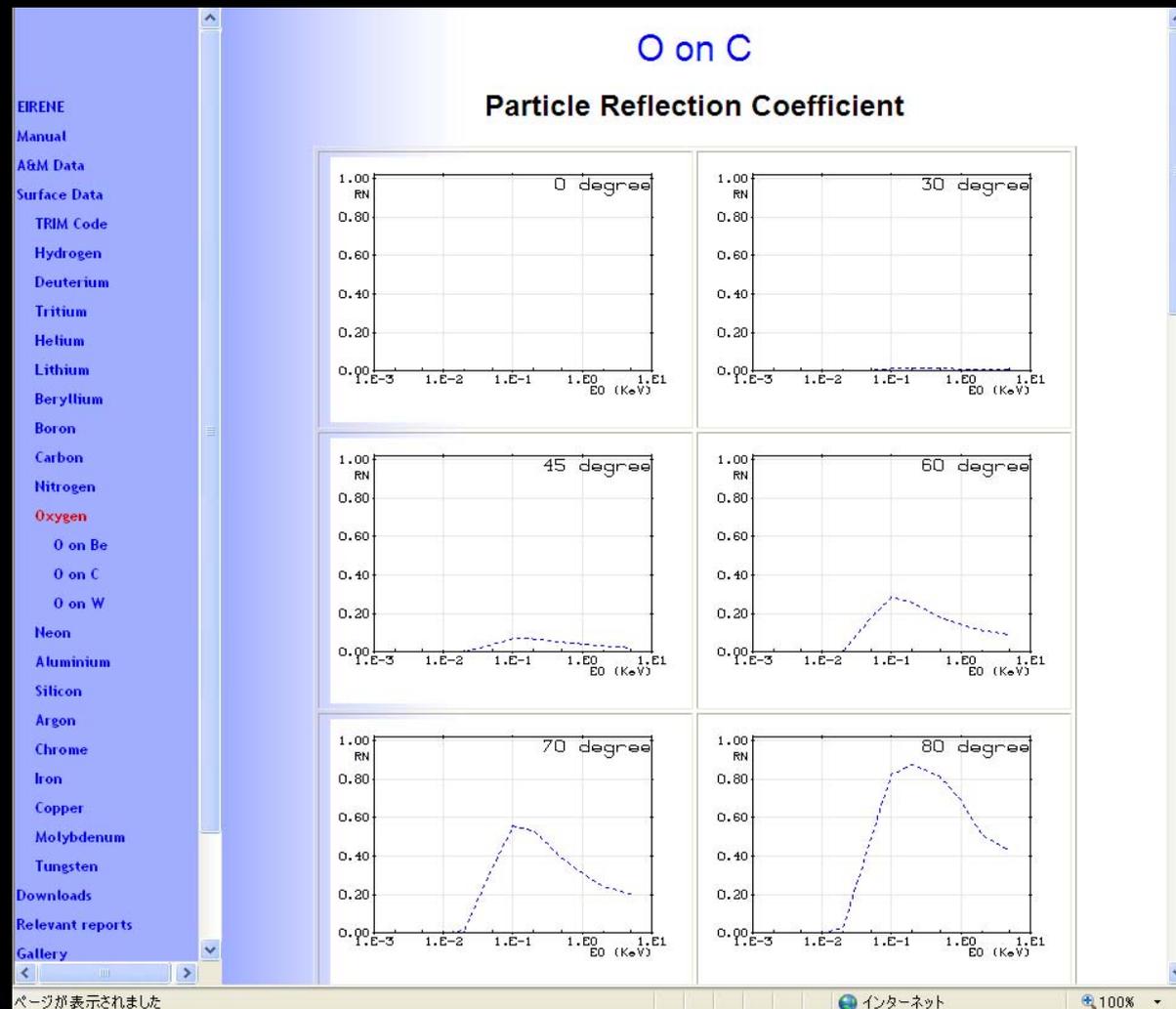
(a) Discharge flow system. O₂ (¹Δ) was monitored by dimol emission at 634 nm or from O₂ (¹Σ) emission at 762 nm.

(b) Large static reactor. O₂ (¹Δ) was monitored by emission at 1.27 μm.

(c) O₂ (¹Δ) was detected by time-resolved absorption at 144 nm.

Surface Interaction Database / TRIM code

- TRIMコードでの計算結果(粒子反射係数、エネルギー反射係数、運動量反射係数の角度依存性)の図を表示。
- Online database?
- $E < 100\text{eV}$ は精度が悪い



Online calculation sites & open atomic codes

- ハンドブックに記載した、オンライン計算サイト、及び公開している原子コードは、基本的に原子、原子イオンの原子データに関するものばかり。

- 分子の電子衝突電離断面積：NIST BEB法による経験式

<http://physics.nist.gov/PhysRefData/Ionization/Xsection.html>

経験式の中で用いる係数は、原子・分子コードでの計算が必要。

燃焼化学関係のデータベース

- プラズマ支援燃焼: 例: I. N. Kosarev et al., Combustion and Flame 154 (2008) 569.
- 点火過程のkinetics=RAMEC:
E.L. Petersen, D.F. Davidson, R.K. Hanson, Combust. Flame 117 (1999) 272–290.
- GMI-Mech 1.2 (35種の分子・原子, 190反応過程)
M. Frenklach, H. Wang, M. Goldenberg, G.P. Smith, D.M. Golden, C.T. Bowman, R.K. Hanson, W.C. Gardiner, V. Lissianski, in: GRI, Topical Report No. GRI-95/0058, 1995.
<http://www.me.berkeley.edu/gri-mech/>

GRI-Mech

<http://www.me.berkeley.edu/gri-mech/>

● 例：炭化水素とOHの 反応データ

Number	Reaction	Rate Coefficient $A T^n \exp(-E/RT)$			Served as Optimization Variable in GRI-Mech Releases
		A (mol,cm ³ ,s)	n (T in K)	E (cal/mol)	
11	O + CH4 -> OH + CH3	1.02E+09	1.5	8600	1.2; 2.1; 3.0
52	H + CH3 (+M) -> CH4 (+M)	pressure dependent			3.0
53	H + CH4 -> CH3 + H2	6.60E+08	1.6	10840	1.1; 1.2; 2.1; 3.0
98	OH + CH4 -> CH3 + H2O	1.00E+08	1.6	3120	1.1; 1.2; 2.1; 3.0
118	HO2 + CH3 -> O2 + CH4	1.00E+12			1.1; 1.2; 2.1; 3.0
130	CH + CH4 -> H + C2H4	6.00E+13			
139	CH2 + CH4 -> CH3 + CH3	2.46E+06	2.0	8270	3.0
150	CH2(S) + CH4 -> CH3 + CH3	1.60E+13		-570	3.0
157	CH3 + H2O2 -> HO2 + CH4	2.45E+04	2.5	5180	
160	CH3 + HCO -> CH4 + CO	2.65E+13			1.1; 1.2; 2.1
161	CH3 + CH2O -> HCO + CH4	3.32E+03	2.8	5860	
162	CH3 + CH3OH -> CH2OH + CH4	3.00E+07	1.5	9940	
163	CH3 + CH3OH -> CH3O + CH4	1.00E+07	1.5	9940	
164	CH3 + C2H4 -> C2H3 + CH4	2.27E+05	2.0	9200	
165	CH3 + C2H6 -> C2H5 + CH4	6.14E+06	1.7	10450	3.0
211	NNH + CH3 -> CH4 + N2	2.50E+13			
303	CH3 + CH3CHO -> CH3 + CH4 + CO	2.72E+06	1.8	5920	
317	CH3 + C3H8 -> C3H7 + CH4	9.03E-01	3.6	7154	

CH4 only Find Reactions Instructions

ページが表示されました インターネ



$$k = 1.02\text{E}+09 T^{1.5} \exp(-8600 \text{ cal/mol} / RT) \text{ cm}^3/\text{mol s}$$

SOURCE:

Tsang, W., and Hampson, R.F. (1986) *J. Phys. Chem. Ref. Data* 15, 1087.

COMMENTS:

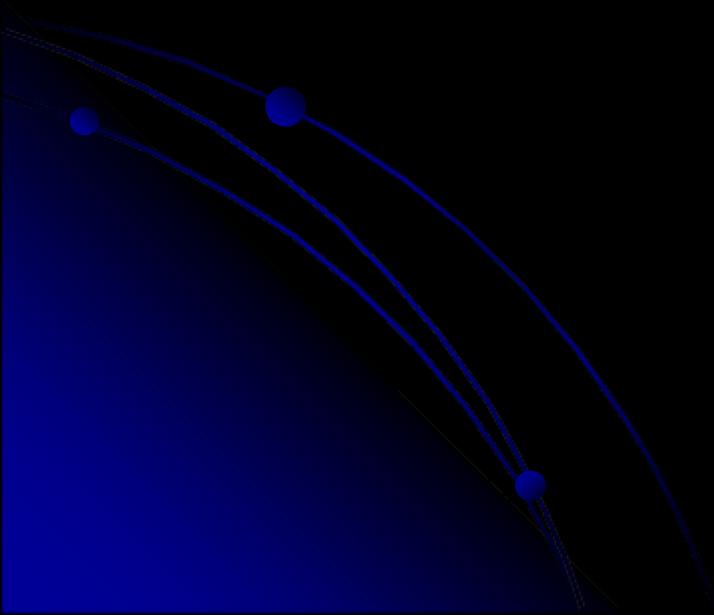
Served as an optimization variable in GRI-Mech 1.2, 2.1 and 3.0 releases. The rate coefficient was not changed.

Temp (K)	delta-S (cal/mol K)	delta-H (kcal/mol)	kf ---- (mol, cm ³ , s) ----	kr	Req
300	7.3	2.8	2.88E+06	8.08E+06	3.56E-01
500	8.4	3.2	1.98E+09	7.50E+08	2.65E+00
1000	8.6	3.3	4.26E+11	2.97E+10	1.43E+01
1500	7.8	2.3	3.31E+12	1.42E+11	2.33E+01
2000	7.0	.9	1.05E+13	3.89E+11	2.70E+01
2500	6.3	-.8	2.26E+13	8.30E+11	2.72E+01
3000	5.6	-2.7	3.96E+13	1.54E+12	2.57E+01

[[Rate coefficient format](#) | [Chemkin file](#) | [Thermo data](#) | [Main menu](#)]

最近のデータベース情勢

- ヨーロッパにおけるVAMDC (Virtual Atomic and Molecular Data Center) プロジェクト



さいごに

- 原子分子データベースの維持、アップデートは、専門家の強力とともに、ユーザーのサポートも大切

