

## Atomic–Molecular Ionization by Electron Scattering

For analyzing the physical aspects of electron collisions with atoms and molecules, an understanding of cross sections, especially of the ionization cross sections, for the impacting electrons is necessary. Providing a detailed and up-to-date discussion to the theory and applications of electron scattering, this text equips readers with the basic concepts of quantum scattering theories, including complex scattering potential method, cross section results for atoms including those of inert gases, atomic oxygen, nitrogen, and carbon, and also for the less explored atomic systems.

Study of electron scattering phenomena for diatomic and common molecules, polyatomic molecules, and radicals including hydrocarbons, fluorocarbons, and other larger molecules, together with relevant radical species, is discussed in detail. This book discusses applications of electron impact ionization and excitation in gaseous or plasma and condensed matter. Recent advances in the field of electron molecule scattering and ionization for polyatomic molecules are covered extensively.

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# Atomic–Molecular Ionization by Electron Scattering

*Theory and Applications*

K. N. Joshipura  
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CAMBRIDGE  
UNIVERSITY PRESS

Cambridge University Press  
978-1-108-49890-6 — Atomic-Molecular Ionization by Electron Scattering  
K. N. Joshipura , Nigel Mason  
Frontmatter  
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## CAMBRIDGE UNIVERSITY PRESS

University Printing House, Cambridge CB2 8BS, United Kingdom

One Liberty Plaza, 20th Floor, New York, NY 10006, USA

477 Williamstown Road, Port Melbourne, vic 3207, Australia

314 to 321, 3rd Floor, Plot No.3, Splendor Forum, Jasola District Centre, New Delhi 110025, India

79 Anson Road, #06-04/06, Singapore 079906

Cambridge University Press is part of the University of Cambridge.

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[www.cambridge.org](http://www.cambridge.org)

Information on this title: [www.cambridge.org/9781108498906](http://www.cambridge.org/9781108498906)

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First published 2019

Printed in India

*A catalogue record for this publication is available from the British Library*

ISBN 978-1-108-49890-6 Hardback

Additional resources for this publication at [www.cambridge.org/9781108498906](http://www.cambridge.org/9781108498906)

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Cambridge University Press  
978-1-108-49890-6 — Atomic-Molecular Ionization by Electron Scattering  
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*To our teachers and students ...*

# CONTENTS

<i>List of Figures</i>	<i>ix</i>
<i>List of Tables</i>	<i>xxi</i>
<i>Foreword I</i>	<i>xxiii</i>
<i>Foreword II</i>	<i>xxv</i>
<i>Preface</i>	<i>xxvii</i>
<i>Acknowledgments</i>	<i>xxxix</i>
<b>1. Atoms and Molecules as Bound Quantum Systems</b>	<b>1</b>
1.1 Introduction – A Brief History of the Study of Electron Scattering	1
1.2 The Hydrogen Atom and Multi-Electron Atoms	6
1.3 Atomic Properties – Atomic Radii	9
1.4 Molecular Structure and Properties	11
<b>2. Quantum Scattering Theories</b>	<b>14</b>
2.1 Definition of Electron Scattering Cross Sections	14
2.2 Description of Experimental Measurements	16
2.3 High Energy Electron Scattering	25
2.4 Partial Wave Complex Potential Formalism	27
2.5 Scattering from Atomic and Molecular Hydrogen	30
2.6 Conclusions	45
<b>3. Electron Atom Scattering and Ionization</b>	<b>46</b>
3.1 Introduction	46
3.2 Inert Gas Atoms	48
3.3 Oxygen, Nitrogen, and Carbon	58
3.4 Other Atomic Targets	64
3.5 Metastable Atomic Species	73
3.6 General Trends and Correlations in Electron–Atom Scattering	80
<b>4. Electron Molecule Scattering and Ionization – I: Small Molecules and Radicals</b>	<b>83</b>
4.1 The Nitrogen Molecule	84
4.2 Other Diatomic and Well-Known Targets	89

4.3	The Water Molecule, Its Derivatives OH, HO <sub>2</sub> , H <sub>2</sub> O <sub>2</sub> , and the Water Dimer (H <sub>2</sub> O) <sub>2</sub>	105
4.4	Methane, CH <sub>4</sub> , and the Radicals CH <sub>x</sub> (x = 1, 2, and 3)	114
4.5	Other Common Molecules and Their Radicals	119
4.6	Reactive Species CN, C <sub>2</sub> N <sub>2</sub> , HCN, and HNC; BF	123
4.7	Metastable Species of Molecular Hydrogen and Nitrogen	126
4.8	General Trends and Correlations	128
<b>5.</b>	<b>Electron Molecule Scattering and Ionization – II: Other Polyatomic Molecules and Radicals</b>	<b>130</b>
5.1	Small Polyatomic Molecules	131
5.2	Two-center Systems, Small Hydrocarbons, etc.	140
5.3	Larger Tetrahedral and Other Molecules	147
5.4	Heavier Polyatomics	159
5.5	Larger Hydrocarbons and Fluorocarbons	165
5.6	Molecules of Biological Interest	172
5.7	General Trends and Correlations	175
<b>6.</b>	<b>Applications of Electron Scattering</b>	<b>177</b>
6.1	Electron Scattering Processes in Nature and Technology	178
6.2	Electron Scattering in Different Phases of Matter	180
6.3	The Terrestrial Atmosphere	188
6.4	The Role of Electron Collisions in Planetary Atmospheres and Comets	190
6.5	The Role of Electrons in Astrophysics and Astrochemistry	198
6.6	Electrons and Nanotechnology	202
6.7	Scattering under External Plasma Confinements	206
6.8	Biomolecular Targets and Radiation Damage	208
6.9	Positron Atom/Molecule Scattering	212
6.10	Conclusions: the Future of Electron Scattering	217
	<b>Bibliography</b>	<b>219</b>
	<b>Index</b>	<b>249</b>

## FIGURES

1.1	The typical Franck–Hertz electron curve showing the presence of a series of peaks separated by 4.9 eV (254 nm) characteristic of the excitation energy of the first electronic state of mercury	2
1.2	(a) The Ramsauer apparatus used to measure low energy scattering from atoms and molecules, revealing (b) the Ramsauer–Townsend minimum in the total and elastic scattering cross section of the rare gases	3
1.3	The first observation of an electron scattering resonance in helium (Schulz 1963)	4
1.4	Energy levels of the Hydrogen atom, from equation (1.2)	7
1.5	Linear correlation of $\alpha_d$ against $1/I^3$ for the inert-gas atoms and halogens with correlation coefficient $R^2 = 0.99446$ and $0.98975$ respectively	10
1.6	The four different radii $r_p$ , $\langle r \rangle$ , $R_W$ and $R_{pol}$ of atoms across the periodic table (Joshipura 2013)	11
2.1	Schematic diagram of a scattering experiment; scattering angle $\theta$ is as shown here; the corresponding angle $\phi$ , not shown, is the azimuthal angle formed in the XY plane	16
2.2	Apparatus used to measure electron impact ionization cross sections (Krishnakumar and Srivastava 1988)	19
2.3	A typical electron scattering spectrometer (Allan 2007, 2010)	21
2.4	Electron Energy Loss spectra for (a) the Argon atom (Khakoo et al. 2004) and (b) the Water molecule (Thorn et al. 2007)	22
2.5	A schematic of the Dissociative Electron Attachment Process (DEA) with an illustration of the potential energy surfaces of neutral and temporary negative ionic states	24
2.6	Bar chart showing the percentage contribution of various scattering processes in $e-H$ collisions at the $Q_{ion}$ peak of 60 eV, relative to experimental $Q_T$ data (Zhou et al. 1997); $Q_{el}$ from the sum-check in equation (2.19); the $Q_{ion}$ , excitation TCS $Q_{1s \rightarrow 2p}$ , and $Q_{exc}$ ( $n > 2$ ) from (NIST database)	33

x	<i>Figures</i>	
2.7	Major TCS ( $\text{\AA}^2$ ) of $e$ - $H$ scattering; uppermost curve: $Q_T$ based on the measurements (Zhou et al. 1997) joined with the EBS values; next two curves: $Q_{el}$ calculated in PWA and in DWBA (Benda and Karel 2014); lower three curves: $Q_{ion}$ , $Q_{1s \rightarrow 2p}$ , and $Q_{exc}(n > 2)$ from the NIST database	34
2.8	Electron scattering cross sections ( $\text{\AA}^2$ ) with $H_2$ molecules; $Q_{TOT}$ , <i>solid line</i> : CSP-ic; (Joshipura et al. 2010); <i>solid dash dot line with squares</i> : recommended data (Yoon et al. 2008); <i>solid triangles</i> : Hoffman et al. (1982); $Q_{el}$ , <i>solid line</i> : CSP-ic; <i>open triangles</i> : Khakoo and Trajmar (1986); <i>dots</i> : Yoon et al. (2008); $Q_{inel}$ , <i>solid line</i> : CSP-ic; <i>dash</i> reference data-set; $Q_{ion}$ , <i>'dash double dot'</i> : CSP-ic; <i>crosses</i> : measured data – Straub et al. (1996); $\Sigma Q_{exc}$ , <i>dots</i> : CSP-ic and <i>open circles</i> : from the reference data-set	42
2.9	Total ionization cross sections in $e$ - $H_2$ scattering; CSP-ic results compared with the recommended data (Yoon et al. 2008), BEB theory (NIST database), and CCC theory (Zammit et al. 2016)	43
3.1	Various TCS of $e$ -He scattering (Vinodkumar et al. 2007), along with compared data	52
3.2	Various TCS of $e$ -Ne scattering (Vinodkumar et al. 2007) along with compared data	53
3.3	TCS for $e$ -Ar scattering (Vinodkumar et al. 2007)	54
3.4	Bar-chart showing the relative contribution of various scattering processes with argon near the ionization peak, 125 eV (Vinodkumar et al. 2007)	55
3.5	TCS for $e$ -Kr scattering (Vinodkumar et al. 2007)	56
3.6	TCS for $e$ -Xe scattering (Vinodkumar et al. 2007)	56
3.7	Cross sections of $e$ -O collisions (Joshipura et al. 2006); <i>topmost curve</i> : calculated $Q_{inel}$ by the CSP-ic method; $Q_{ion}$ <i>continuous curve</i> : measured $Q_{ion}$ data (Thompson et al. 1995); $\star$ : $Q_{ion}$ DM formula (Deutsch et al. 2001); $-\cdot-\cdot-$ ; <i>the lowest two curves</i> : calculated $\Sigma Q_{exc}$ , the excitation-sum from two data-sets $-\cdot-\cdot-$ and $\bullet$ by Johnson et al. (2003)	59
3.8	A bar-chart of relative contributions of 100 eV TCS ( $\text{\AA}^2$ ) for atomic oxygen (Joshipura et al. 2006)	61
3.9	Various total cross sections of $e$ -N atom collisions (Joshipura et al. 2009)	62
3.10	Ionization and cumulative excitation in $e$ -N scattering (Joshipura et al. 2009); Cross section $Q_{ion}$ ; continuous curve CSP-ic, dash dot BEB of Kim and Desclaux (2002), measured data; circle and box – two data sets by Brook et al. (1978), $Q_{ion}(N_2/2)$ IAM, lowest curve $\Sigma Q_{exc}$ CSP-ic	62
3.11	TCS of $e$ -C scattering (Pandya 2013) along with comparisons; from top: $-\bullet-$ ( $Q_{el} + Q_{inel}$ ) Joshipura and Patel (1994), next two curves CSP-ic, $-\cdot-\cdot-$ $Q_T$ and $-\cdot-\cdot-$ $Q_{el}$ ; lower four curves, $Q_{ion}$ as indicated inside	64



Figures

xi

3.12	TCS plot of e–Be collisions evaluated using the CSP-ic method (Chaudhari et al. 2015)	65
3.13	Electron collisional ionization of Be atoms; continuous curve CSP-ic by Chaudhari et al. (2015) and other results	66
3.14	Electron collisional ionization of Boron atoms, CSP-ic by Chaudhari et al. (2015) and other results	66
3.15	Electron scattering with the Lithium atom; Upper curve $Q_{exc}$ (2s → 2p) BEf-scaled excitation cross section (NIST database), Lower curve $Q_{ion}$ BEB ionization data (Irikura 2017)	67
3.16	Total ionization cross sections of Fluorine atoms; continuous curve from Joshipura and Limbachiya (2002); ★ experimental data from Hayes et al. (1987), DM formula from Margreiter et al. (1994)	68
3.17	CSP-ic total ionization cross sections of halogen atoms I, Br, Cl, and F from top to bottom	69
3.18	Electron ionization of Si atoms; $Q_{ion}$ : CSP-ic: <i>continuous curve</i> : Gangopadhyay (2008); <i>dots</i> : DM (Margreiter et al. 1994); <i>dashes</i> : Bartlett and Stelbovics (2004); <i>stars</i> : experimental data Freund et al. (1990); $\Sigma Q_{exc}$ : <i>lowest curve</i> : CSP-ic	70
3.19	$Q_{ion}$ for C, Si, and Ge atomic targets calculated in CSP-ic (Patel 2017)	71
3.20	Electron scattering from Aluminium (Joshipura et al. 2006); <i>top-most curve</i> : $Q_{inel}$ ; <i>continuous curve</i> : $Q_{ion}$ , by CSP-ic; <i>dash-dot curve</i> : $Q_{ion}$ , by DM (Deutsch et al. 2001); <i>dotted curve</i> : $Q_{ion}$ by BEB (Kim and Stone 2001); <i>lower chain curve</i> : $Q_{ion}$ by Bartlett and Stelbovics (2002); ★: $Q_{ion}$ , measured data (Freund et al. 1990); <i>the lowest curve</i> : $\Sigma Q_{exc}$ by CSP-ic	72
3.21	Electron scattering from copper atoms (Joshipura et al. 2006); <i>top-most curve</i> : $Q_{inel}$ ; <i>continuous curve</i> : $Q_{ion}$ , by CSP-ic; measured data, star by Freund et al. (1990) and bullet by Bolorizadeh (1994); <i>the lowest curve</i> $\Sigma Q_{exc}$ in CSP-ic	73
3.22	Comparisons of the ionization cross sections of the metastable species H*(2s) measured by Defrance et al. (1981); H(1s), BEB from the NIST data-base; H(1s) measured data of Shah et al. (1987); es-1 and es-2 estimates	76
3.23	Electron impact ionization cross sections for the metastable species He*(2 <sup>3</sup> S); <i>dotted curve with data points</i> : Dixon et al. (1976); He(GS) BEB values (NIST database), He(GS); <i>single-point</i> : measured data from Shah et al. (1988)	77
3.24	Ionization cross sections of the GS and metastable N*( <sup>2</sup> P), N*( <sup>2</sup> D) states of N atoms CSP-ic (Pandya and Joshipura 2014), compared with the BEB data (Kim and Desclaux 2002)	78
3.25	CSP-ic ionization cross sections of the GS and EMS of atomic oxygen (Pandya and Joshipura 2014)	79
3.26	Maximum TCS $\sigma_{max}$ as a function of $\sqrt{(\alpha_d/I)}$ for inert gas atoms, extrapolated to Rn atom	81

xii	<i>Figures</i>	
4.1	Total cross sections of e–N <sub>2</sub> collisions, for references (Joshipura et al. 2009)	87
4.2	$Q_{\text{ion}}$ and electronic-sum $\Sigma Q_{\text{exc}}$ for the N <sub>2</sub> molecule (Joshipura et al. 2009)	88
4.3	Cumulative total neutral dissociation cross section of N <sub>2</sub> ; continuous curve-effective $Q_{\text{NDiss}}$ and ‘corrected’ $\Sigma Q_{\text{exc}}$ (Pandya and Joshipura 2010, 2014); <i>squares</i> – Winters (1966); <i>bullets and triangles</i> – original and recommended data Cosby (1993)	89
4.4	$Q_T$ for the target sequence O, O <sub>2</sub> , O <sub>3</sub> , and O <sub>4</sub> from bottom to top; for O <sub>2</sub> the measured data are from Dababneh et al. (1988) and Dalba et al. (1980); for O <sub>3</sub> the measurements are from Pablos et al. (2002).	91
4.5	Ionization cross sections of O–O <sub>2</sub> –O <sub>3</sub> –O <sub>4</sub> sequence from bottom to top (Joshipura et al. 2002); atomic O, <i>dot</i> : CSP-ic, experimental data Thompson et al. (1995); <i>middle curves</i> O <sub>2</sub> , <i>dash-dot</i> : CSP-ic; <i>dot</i> : Kim et al. (1997), <i>inverted triangles</i> : measured data – Krishnakumar and Srivastava (1992); for O <sub>3</sub> <i>continuous curve</i> : CSP-ic, <i>open circle</i> : measurements - Newson et al. (1995); <i>uppermost curve</i> : O <sub>4</sub>	92
4.6	Total (complete) and ionization cross sections for ozone molecule; $Q_{\text{TOT}}$ <i>uppermost curve</i> CSP-ic; <i>stars</i> : Pablos et al. (2002); $Q_{\text{ion}}$ , <i>dots</i> : CSP-ic, <i>dashes</i> : BEB (Kim et al. 1997, see also NIST database), <i>diamonds</i> : Newson et al. (1995)	93
4.7(a)	Bar chart showing the relative contribution of various electron collision processes in O <sub>2</sub> at the maximum of $Q_{\text{ion}}$ , 100 eV (Joshipura et al. 2002)	93
4.7(b)	Bar chart showing the relative contribution of various electron collision processes in O <sub>3</sub> at the maximum of $Q_{\text{ion}}$ , 100 eV (Joshipura et al. 2002)	94
4.8	TCS plot for e–CO scattering (Pandya 2013)	95
4.9	$Q_{\text{ion}}$ in e–CO <sub>2</sub> scattering, compared with BEB calculations (Hwang et al. 1997) and measured data of Straub et al. (1996)	96
4.10	Electron collision cross sections with the NO molecule adopted from Joshipura et al. (2007)	97
4.11	Relative contribution of various TCS in e–NO collisions at 100 eV (Joshipura et al. 2007)	98
4.12	Ionization cross sections of NO, N <sub>2</sub> O, and NO <sub>2</sub> molecules, adapted from Joshipura et al. (2007)	99
4.13	Comparison of the calculated $Q_{\text{ion}}$ of well-known light atoms and molecules from Haider et al. (2012)	100
4.14	Electron impact ionization cross section of F <sub>2</sub> (Joshipura and Limbachiya 2002)	101
4.15	Electron impact ionization of Cl <sub>2</sub> (Joshipura and Limbachiya 2002)	101
4.16	Electron impact ionization cross section for Br <sub>2</sub> (Joshipura and Limbachiya 2002)	102
4.17	Electron impact ionization of I <sub>2</sub> (Joshipura and Limbachiya 2002)	103
4.18	$Q_T$ for e–LiH scattering (Shelat et al. 2011)	104

*Figures*

xiii

4.19	Various cross sections of e–H <sub>2</sub> O scattering (Joshipura et al. 2017)	107
4.20	Ionization cross sections $Q_{\text{ion}}$ (upper curves) of the water molecule compared with various other data (Joshipura et al. 2017)	108
4.21	Various cross sections of electron collisions with OH radical (Joshipura et al. 2017)	109
4.22	Calculated total cross sections of HO <sub>2</sub> (Joshipura et al. 2017); BEB $Q_{\text{ion}}$ (NIST database)	111
4.23	Theoretical TCS for electron scattering from the H <sub>2</sub> O <sub>2</sub> molecule (Joshipura et al. 2017)	112
4.24	Theoretical TCS for electron scattering from the water dimer (Joshipura et al. 2017)	113
4.25	CSP-ic results along with comparisons on e–CH <sub>4</sub> scattering from Joshipura et al. (2004)	114
4.26	A bar-chart showing TCS of e–CH <sub>4</sub> scattering at 70 eV (Joshipura et al. 2004); cross section $Q_T$ is shown by the first bar; $Q_{\text{el}}$ and $Q_{\text{inel}}$ are 52.5% and 47.5% of $Q_T$ respectively; $Q_{\text{ion}}$ and $\Sigma Q_{\text{exc}}$ are 83% and 17% of $Q_{\text{inel}}$ respectively	116
4.27	Total elastic cross sections for electron–methane scattering from very low to high energies; continuous black curve: quantemol-N results; and dashed curve: SCOP results, merging near the ionization threshold ~15 eV, Vinodkumar et al. (2011)	116
4.28	Electron scattering from the CH radical (Vinodkumar et al. 2006)	117
4.29	Electron scattering from the CH <sub>2</sub> radical (Vinodkumar et al. 2006)	118
4.30	Electron scattering from the CH <sub>3</sub> radical (Vinodkumar et al. 2006)	118
4.31	Electron impact ionization cross sections for the NH <sub>3</sub> molecule and its radicals; NH <sub>3</sub> , CSP-ic <i>continuous curve</i> : Joshipura et al. (2001); <i>dashes</i> : BEB (NIST database); <i>stars</i> : experimental data Rao and Srivastava (1992); NH <sub>2</sub> <i>topmost chain curve</i> and NH <i>lowest chain curve</i> : Joshipura et al. (2001); NH experimental data <i>diamonds</i> Tarnovsky et al. (1997)	119
4.32	Cross sections $Q_{\text{el}}$ , $Q_{\text{rot}}$ , $Q_{\text{inel}}$ , and $Q_{\text{ion}}$ for SO radical (Joshipura et al. 2008)	121
4.33	Electron scattering from the SO <sub>2</sub> molecule (Joshipura et al. 2008)	121
4.34	Total ionization cross sections of H <sub>2</sub> S molecule – Vinodkumar et al. (2011); from top down, $Q_{\text{inel}}$ , <i>dashed curve</i> : CSP-ic; <i>continuous curve</i> : ICSP-ic, BEB (NIST database); <i>open circle</i> : measurements by Belic and Kurepa (1985); <i>star</i> : Lindsay et al. (2002); <i>filled squares</i> : Rao and Srivastava (1993), <i>open triangles</i> : Otvos and Stevenson (1956)	122
4.35	Electron impact ionization cross sections of CN (lowest curve), C <sub>2</sub> N <sub>2</sub> and CNCN (upper most curve); CSP-ic and AR (Pandya et al. 2012) compared with experimental results of Smith (1983) for C <sub>2</sub> N <sub>2</sub> and BEB calculation for C <sub>2</sub> N <sub>2</sub>	123
4.36	Electron impact ionization of HCN and HNC (Pandya et al. 2012)	124
4.37	Ionization cross sections for BF (Pandya et al. 2012)	125

xiv	<i>Figures</i>	
4.38	$Q_{\text{ion}}$ of five iso-electronic molecular systems, and a 13-electron target CN (Pandya et al. 2012); <i>square</i> : measurements of $N_2$ (Straub et al. 1996); <i>triangle</i> : measurements of CO (Orient and Srivastava 1987); <i>circle</i> : measurements of $C_2H_2$ (Hayashi et al. 1990); CSP-ic results; continuous <i>curve</i> : for CN; dash dot: for HCN; <i>dot</i> : for BF	125
4.39	Ionization cross sections of electron impact on $H_2^*(c^3\Pi_u)$ , Joshipura et al. (2010) lowest dashed curve, $H_2$ ground-state	127
4.40	TCS for electron impact on $N_2^*(A^3\Sigma_u^+)$ , $Q_{\text{ion}}$ of $N_2$ (GS) also included; Joshipura et al. (2009)	128
4.41	Linear correlation of $\sigma_{\text{max}}$ as a function of $\sqrt{(\alpha_0/I)}$ for a variety of ground-state molecular targets	129
5.1	Calculated TCS of $NF_3$ from Rahman et al. (2012), <i>filled circles</i> : $Q_T$ in CSP-ic; <i>open circles</i> : measured $Q_T$ data of Szymkowski et al. (2004); other CSP-ic results – <i>triangles</i> : $Q_{\text{el}}$ ; <i>stars</i> : $Q_{\text{ion}}$ ; <i>squares</i> : $\Sigma Q_{\text{exc}}$	132
5.2	Ionization cross sections of $NF_3$ ; <i>squares</i> : Tarnovsky et al. (1994); <i>triangles</i> : Haaland et al. (2001); <i>filled circles</i> : measurements, Rahman et al. (2012); <i>solid line</i> : CSP-ic theory, Rahman et al. (2012); <i>dashed line</i> : BEB values, Szymkowski et al. (2004), <i>dash-dotted line</i> : DM, Deutsch et al. (1994)	133
5.3	Electron scattering cross sections $Q_{\text{ion}}$ with $NF$ ; <i>solid line</i> : CSP-ic, Limbachiya (2016); <i>dash</i> : DM formula, Deutsch et al. (1994); <i>dash dot dot</i> : theory, Huo et al. (2002); <i>star</i> : measured data of Tarnovsky et al. (1994)	134
5.4	Electron scattering cross sections $Q_{\text{ion}}$ with $NF_2$ ; <i>solid line</i> : CSP-ic, Limbachiya (2016); <i>dash</i> : – DM formula, Deutsch et al. (1994); <i>dash dot dot</i> : theory, Huo et al. (2002); <i>star</i> : measured data of Tarnovsky et al. (1994)	134
5.5	Total ionization cross sections of $CF_4$ ; <i>solid curve</i> : CSP-ic, Antony et al. (2005), <i>dash</i> : BEB (NIST database); <i>dash-dot</i> : Christophorou and Olthoff (1999); <i>star</i> : experimental data, Poll et al. (1992); <i>filled circle</i> : Nishimura et al. (1999)	136
5.6	Total ionization cross sections of the $CF_2$ radical; <i>solid curve</i> : CSP-ic (Antony et al. 2005); <i>dashes</i> : BEB (NIST database); <i>dash-dots</i> : DM (Deutsch et al. 2000); <i>stars</i> : experimental data (Huo et al. 2002); <i>dots</i> : siBED model (Huo et al. 2002)	136
5.7	Theoretical cross sections $Q_{\text{TOT}}$ , $Q_{\text{rot}}$ , and $Q_{\text{ion}}$ for $H_2CO$ .	138
5.8	Total ionization cross sections of $H_2CO$ ; <i>continuous curve</i> : ICSP-ic (Vinodkumar et al. 2011); <i>dash-dots</i> : CSP-ic (Vinodkumar et al. 2006); <i>dashes</i> : BEB (NIST database); <i>bullets</i> : experimental data (Vacher et al. 2009)	138

*Figures*

xv

- |      |  |     |
|------|--|-----|
| 5.9  | Total cross sections of the CHO radical; CSP-ic results (Vinodkumar et al. 2006) are augmented with the Born-dipole $Q_{\text{rot}}$ (Joshi 2017) to obtain $Q_{\text{TOT}}$ ; $Q_{\text{ion}}$ is that of Vinodkumar et al. (2006)  | 139 |
| 5.10 | TCS of $e\text{-C}_2\text{H}_2$ scattering; <i>upper curves</i> : $Q_T$ , continuous CSP-ic (Vinodkumar et al. 2006); <i>dashes</i> : theory, Jain and Baluja (1992); <i>stars</i> : experimental $Q_T$ , Ariyasinghe (2002); <i>bullets</i> : Sueoka and Mori (1989); $Q_{\text{ion}}$ ; <i>lower dotted curve</i> : CSP-ic Vinodkumar et al. (2006); <i>dash dots</i> : BEB (NIST database); <i>inverted triangles</i> : Hayashi (1990); <i>boxes</i> : Gaudin and Hagemann (1967)   | 141 |
| 5.11 | TCS for $e\text{-C}_2\text{H}_4$ scattering; <i>upper curves</i> : $-Q_T$ , continuous CSP-ic (Vinodkumar et al. 2006); <i>dashes</i> : theoretical results (Brescansin et al. 2004); <i>stars</i> : experimental $Q_T$ , (Ariyasinghe and Powers 2002); <i>bullets</i> : Sueoka and Mori (1989); <i>lower plots</i> : $Q_{\text{ion}}$ ; <i>dotted curve</i> : CSP-ic, (Vinodkumar et al. 2006); <i>dash-dots</i> : BEB (NIST database); <i>inverted triangles</i> : Hayashi (1990); <i>squares</i> : Nishimura and Tawara (1994) | 142 |
| 5.12 | TCS of $e\text{-C}_2\text{H}_6$ scattering; <i>upper curve</i> : $Q_T$ , CSP-ic (Vinodkumar et al. 2006); <i>bullets</i> : Sueoka and Mori (1986); <i>stars</i> : Ariyasinghe and Powers (2002); <i>lower curves</i> : $Q_{\text{ion}}$ , <i>dotted curve</i> : CSP-ic Vinodkumar et al. (2006); <i>dash-dots</i> : BEB (NIST database); <i>inverted triangles</i> : Hayashi (1990); <i>squares</i> : Nishimura and Tawara (1994); <i>triangles</i> : Chatham et al. (1984)  | 143 |
| 5.13 | Ionization cross sections of $\text{C}_2\text{F}_4$ ; <i>solid curve</i> : CSP-ic (Antony et al. 2005); <i>single bullet</i> : BEB (NIST database); <i>single square</i> : DM from Bart et al. (2001); <i>stars</i> : experimental data, Bart et al. (2001)  | 145 |
| 5.14 | Ionization TCS of $e\text{-C}_2\text{F}_6$ ; <i>continuous curve</i> : CSP-ic (Antony et al. 2005); <i>dashes</i> : BEB (NIST database); <i>stars</i> : Experimental data – Nishimura et al. (2003); <i>bullets</i> : Poll et al. (1992); <i>dash-dots</i> , Christophorou and Olthoff (1998)  | 145 |
| 5.15 | Total ionization cross sections of $e\text{-CF}_3\text{I}$ scattering; <i>solid curve</i> : CSP-ic (Antony et al. 2005); <i>dashes</i> : DM (Onthong et al. 2002); <i>stars</i> : experimental (Jiao et al. 2001)  | 147 |
| 5.16 | Total (complete) cross sections $Q_T$ of silane; <i>line</i> : theory; continuous curve CSP-ic of Vinodkumar et al. (2008); <i>dash</i> : Jain and Baluja (1992); <i>dashed dot line</i> : Jiang et al. (1995); <i>experimental stars</i> : Zecca et al. (1992); <i>triangles</i> : Szmytkowski et al. (1995); <i>open circles</i> : Sueoka et al. (1994)  | 148 |
| 5.17 | Ionization cross sections of $\text{SiH}_4$ ; <i>continuous curve</i> : theory, CSP-ic (Vinodkumar et al. 2008), <i>dashes</i> : BEB, (Ali et al. 1997); <i>chain curve</i> : Malcolm et al. (2000); <i>stars</i> : experimental, Basner et al. (1997); <i>triangles</i> : Chatham et al. (1984); <i>open circles</i> : Krishnakumar and Srivastava (1995)   | 149 |
| 5.18 | $Q_{\text{ion}}$ of $\text{SiH}$ ; <i>continuous curve</i> : CSP-ic, Vinodkumar et al. (2008); <i>dashes</i> : BEB, (Ali et al. 1997); <i>dash-dots</i> : Malcolm and Yeanger (2000); <i>stars</i> : experimental data, Tarnovsky et al. (1997)  | 150 |

xvi	<u>Figures</u>	
5.19	Set of cross sections for e–SiF <sub>4</sub> scattering; <i>upper curve</i> ; $Q_T$ ; <i>lower curve</i> : $Q_{\text{ion}}$ (Joshipura et al. 2004); <i>stars</i> : $Q_{\text{ion}}$ experimental, Basner et al. (2001); <i>lowest curve</i> : $\Sigma Q_{\text{exc}}$	151
5.20	Ionization in e–GeH <sub>4</sub> scattering; theory, <i>full line curve</i> : CSP-ic (Vinodkumar et al. 2008); <i>dashes</i> : BEB (Ali et al. 1997); <i>dash-dots</i> : DM (Probst et al. 2001); <i>dots</i> : estimated $Q_{\text{ion}}$ (Szymtkowski and Denga 2001); <i>star</i> : experimental, Perrin and Aarts (1983)	152
5.21	Total ionization cross sections of GeH; CSP-ic Vinodkumar et al. (2008); <i>dash curve</i> : BEB (Ali et al. 1997); <i>dash-dots</i> : DM (Probst et al. 2001)	153
5.22	Cross sections for e–CCl <sub>4</sub> scattering; $Q_T$ – <i>uppermost continuous curve</i> : CSP-ic (Joshipura et al. 2004); <i>dashes</i> : AR Jiang et al. (1995); <i>bullets</i> : experimental data Zecca et al. (1991,1992); <i>lower curves</i> : $Q_{\text{ion}}$ – <i>continuous curve</i> : CSP-ic (Joshipura et al. 2004); <i>stars</i> : experimental data, Hudson et al. (2001); <i>lowest curve</i> : $\Sigma Q_{\text{exc}}$	154
5.23	All TCS of SiCl <sub>4</sub> ; $Q_T$ – <i>uppermost continuous curve</i> : CSP-ic (Kothari et al. 2011); <i>open circles</i> : experimental Mozejko et al. (1999); $Q_{\text{el}}$ – <i>dashes</i> : CSP-ic (Kothari et al. 2011); <i>dash-double-dots</i> : Mozejko et al. (2002); <i>lower curves</i> : <i>dash dots</i> and <i>dots</i> : $Q_{\text{ion}}$ and $\Sigma Q_{\text{exc}}$ in CSP-ic	155
5.24	Electron impact ionization cross sections of SiCl <sub>4</sub> ; theory, <i>dash-dots</i> CSP-ic (Kothari et al. 2011), <i>dots</i> DM Basner et al. (2005), <i>dashes</i> DM Deutsch et al. (1997); experiment – <i>bullet</i> , Basner et al. (2005), <i>triangle</i> , PICS of King and Price (2011); <i>star</i> , measured data on CCl <sub>4</sub> molecule (Hudson et al. 2001)	156
5.25	Ionization cross sections of SiCl <sub>3</sub> radical; <i>uppermost continuous curve</i> : theory-CSP-ic, Kothari et al. (2011); <i>dash-dots</i> : DM Deutsch et al. (1997); <i>dash-double-dots</i> : DM Gutkin et al. (2009); <i>bullets</i> : experimental data, Gutkin et al. (2009)	156
5.26(a)	Ionization cross sections of Si <sub>2</sub> H <sub>6</sub> ; <i>continuous curve</i> : theory, CSP-ic (Vinodkumar et al. 2008), <i>dashes</i> : BEB Ali et al. (1997); <i>dash-dots</i> : DM Deutsch et al. (1998); measurements, <i>stars</i> : Chatham et al. (1984); <i>circles</i> : Krishnakumar and Srivastava (1995)	157
5.26(b)	Total ionization cross sections of Ge <sub>2</sub> H <sub>6</sub> ; <i>solid line</i> : CSP-ic, Vinodkumar et al. (2008); <i>dash</i> : BEB $Q_{\text{ion}}$ , Ali et al. (1997)	158
5.27	Electron collisions with Si(CH <sub>3</sub> ) <sub>4</sub> ; $Q_{\text{ion}}$ theory, <i>continuous curve</i> : CSP-ic (Joshipura et al. 2007); <i>dash-dots</i> : BEB (Ali et al. 1997); <i>bullets</i> : experimental data (Basner et al. 1996); <i>dotted curve</i> : CSP-ic $\Sigma Q_{\text{exc}}$	159
5.28	Electron scattering with SO <sub>2</sub> Cl <sub>2</sub> ; $Q_{\text{TOT}}$ – <i>uppermost dash-double dot curve</i> : CSP-ic (Joshipura and Gangopadhyay 2008); <i>stars</i> : experimental data (Szymtkowski et al. 2006), $Q_T$ – <i>solid curve</i> : CSP-ic; $Q_{\text{el}}$ – <i>dash-dot curve</i> : CSP-ic; <i>dotted curve</i> : IAM (Szymtkowski et al. 2006); <i>lower curves</i> : $Q_{\text{ion}}$ ; <i>lower peak</i> : CSP-ic, <i>dash</i> : BEB (Szymtkowski et al. 2006)	160

Figures

xvii

- |      |   |     |
|------|---|-----|
| 5.29 | Electron scattering with SO <sub>2</sub> ClF; <i>uppermost curves</i> : $Q_{TOT}$ and $Q_T$ CSP-ic (Joshipura and Gangopadhyay 2008); $Q_{TOT}$ , <i>star</i> : measured data (Szmytkowski et al. 2005); $Q_{el}$ <i>middle curve</i> : CSP-ic; <i>dotted curve</i> : $Q_{el}$ IAM (Szmytkowski et al. 2005); $Q_{ion}$ , <i>lower curve</i> : CSP-ic; <i>dash</i> : BEB (Szmytkowski et al. 2005)                  | 161 |
| 5.30 | Electron scattering with SO <sub>2</sub> F <sub>2</sub> ; <i>upper curves</i> : $Q_{TOT}$ and $Q_T$ CSP-ic (Joshipura and Gangopadhyay 2008); $Q_T$ , <i>uppermost dashed curve (ICS + ECS)</i> : Szmytkowski et al. (2006), $Q_{el}$ , <i>chain curve</i> : CSP-ic; <i>middle dotted curve</i> : Szmytkowski et al. (2006); $Q_{ion}$ : <i>faint dash</i> CSP-ic; <i>dash</i> BEB of Szmytkowski et al. (2006)     | 161 |
| 5.31 | Electron scattering from SF <sub>6</sub> ; $Q_T$ <i>upper curves</i> : <i>continuous</i> : CSP-ic (Joshipura et al. 2004), <i>dash</i> : AR, Jiang et al. (1995); <i>stars</i> : experimental data Debabneh et al. (1985); <i>lower curves</i> : $Q_{ion}$ <i>short dash</i> : CSP-ic, <i>dash-dot</i> : BEB (NIST database), experimental Rapp and Englander-Golden (1965); <i>lowest curve</i> : $\Sigma Q_{exc}$ | 163 |
| 5.32 | $Q_{ion}$ of H <sub>3</sub> PO <sub>4</sub> molecule by two different theories  | 164 |
| 5.33 | TCS of C <sub>3</sub> H <sub>8</sub> ; $Q_T$ <i>upper curve</i> : CSP-ic (Vinodkumar et al. 2006); <i>stars</i> : measured data, Tanaka et al. (1999); <i>bullets</i> : Floeder et al. (1985); $Q_{ion}$ <i>lower curve</i> : CSP-ic and BEB (NIST database); <i>inverted triangle</i> : measured data, Nishimura and Tawara (1994) and <i>square</i> : Schram et al. (1966)  | 166 |
| 5.34 | $Q_{ion}$ for C <sub>4</sub> H <sub>6</sub> (1, 3 butadiene); <i>continuous curves</i> : CSP-ic (Patel et al. 2014), BEB (Kim and Irikura 2000); experimental data from Kwitnewski et al. (2003)  | 168 |
| 5.35 | $Q_{ion}$ for C <sub>4</sub> H <sub>6</sub> (2 butyne); <i>continuous curve</i> : CSP-ic (Patel et al. 2014); experimental data from Kwitnewski et al. (2003)   | 168 |
| 5.36 | $Q_{ion}$ for C <sub>4</sub> F <sub>6</sub> (Perfluorobutadiene 1,3); CSP-ic calculations (Patel et al. 2014) with two values of ionization threshold; experimental data – Bart et al. (2001)   | 169 |
| 5.37 | $Q_{ion}$ for C <sub>4</sub> H <sub>8</sub> 1 Butene; <i>upper curve</i> CSP-ic Patel et al. (2014); <i>lower curve</i> Kim and Irikura (2000)  | 170 |
| 5.38 | $Q_{ion}$ for C <sub>4</sub> H <sub>8</sub> 2-Butene; CSP-ic (Patel et al. 2014); BEB – Kim and Irikura (2000)  | 170 |
| 5.39 | CSP-ic ionization cross sections for the three isomers of C <sub>4</sub> H <sub>8</sub> (Patel et al. 2014), the <i>lowest curve</i> showing c-C <sub>4</sub> H <sub>8</sub>  | 171 |
| 5.40 | Ionization cross sections for c-C <sub>4</sub> F <sub>8</sub> ; <i>continuous curve</i> : CSP-ic (Patel et al. 2014); recommended data (Christophorou and Olthoff 2001); <i>triangle</i> : experimental data, Toyoda et al. (1997); <i>inverted triangle</i> : Jiao et al. (1998); <i>star</i> : at 70 eV, Beran and Kevan (1969)   | 172 |
| 5.41 | CSP-ic $Q_{ion}$ for furan, THF, and DMF along with measured data on furan (Swadia 2017)  | 173 |
| 5.42 | Linear correlation of $\sigma_{max}$ as a function of $\sqrt{(\alpha_0/I)}$ , for a set of 11 molecules   | 176 |
| 6.1  | Total elastic scattering cross section $\sigma_{elast}$ for Argon and the corresponding rate constant $k = \sigma_{elast} \bar{X} \langle v_e \rangle$ (Franz 2009)   | 183 |

xviii	<i>Figures</i>	
6.2	Inelastic mean free path $\lambda_{\text{IMFP}}$ of electrons in silicon; <i>continuous curve</i> : Pandya et al. (2012) merged smoothly with a universal curve data-point; <i>bullets</i> : Rhodin and Gadzuk (1979); <i>dashes</i> : Lesiak et al. (1996); <i>crosses</i> : Gergely (1997); <i>dash-dots</i> : Gries (1996); <i>vertical line</i> : Koch (1996); <i>short dashes</i> : Tanuma et al. (1988); <i>dots</i> : Tung et al. (1979)	184
6.3	Comparison of the calculated IMFP for three solids Si, SiO, and SiO <sub>2</sub> (Pandya et al. 2012)	185
6.4	Electron mean free paths in H <sub>2</sub> O liquid and ice forms (Joshipura et al. 2007)	187
6.5	Electron concentration and temperature profiles of the terrestrial ionosphere, showing its different regions	189
6.6(a)	Pictures of aurora: Earth (from <a href="https://pl.pinterest.com/pin/312859505342271390/?lp=true">https://pl.pinterest.com/pin/312859505342271390/?lp=true</a> )	191
6.6(b)	Pictures of aurora: Jupiter (from <a href="https://www.nasa.gov/feature/goddard/2016/hubble-captures-vivid-auroras-in-jupiter-s-atmosphere">https://www.nasa.gov/feature/goddard/2016/hubble-captures-vivid-auroras-in-jupiter-s-atmosphere</a> )	191
6.6(c)	Pictures of aurora: Saturn ( <a href="https://commons.wikimedia.org/wiki/Aurora#Other_Planets">https://commons.wikimedia.org/wiki/Aurora#Other_Planets</a> )	191
6.7	The anion spectrum of Titan's atmosphere recorded by the Cassini-Huygens mission at an altitude of 953 km (Coates et al. 2007)	193
6.8	MFPs $\Lambda_{\text{ion}}$ (in m) our ionosphere at 80 km (Lat. 70° N, Long. 100° W); from Pandya et al. (2010)	194
6.9	Effective collision frequency $\nu_{\text{N-diss}}$ (in s <sup>-1</sup> ) for neutral dissociation of H <sub>2</sub> in Jovian atmosphere (Pandya 2013)	195
6.10	Effective collision frequency $\nu_{\text{N-diss}}$ (in s <sup>-1</sup> ) for neutral dissociation of N <sub>2</sub> on Titan, at two altitudes (Pandya et al. 2010)	195
6.11	Ionizing collision frequency $\nu_{\text{ic}}$ (in s <sup>-1</sup> ) as a function of electron energy and temperature, for N <sub>2</sub> in the earth's ionosphere (Lat. 70° N, Long. 100° W); upper curve 80 km, lower curve 100 km	196
6.12	A schematic diagram of molecular synthesis on dust grains in the Inter-Stellar Medium	200
6.13	Schematic diagram showing the expected secondary electron energy distribution from cosmic ray impact on a dust grain compared with typical product yields induced by dissociative ionization and dissociative excitation and the resonant driven process of Dissociative Electron Attachment (DEA), Boyer et al. (2016)	201
6.14	A 'virtual factory' is a computerized simulation of a fabrication facility; reproduced from SIA Semiconductor Industry Association Roadmap (1994)	203
6.15	Principles of (a) Focused Electron Beam Induced Deposition (FEBID) 1 and (b) Extreme Ultraviolet Lithography (EUVL); from Mackus et al. (2014)	204



Figures

xix

6.16	Electron induced damage in DNA showing production of Single Strand Breaks (SSB), Double Strand Breaks (DSB), and loss of supercoiled DNA for electron energies between 3 and 20 eV spanning the ionization energy of DNA constituent molecules (Boudaïffa et al. 2000)	209
6.17	Schematic diagram showing direct and indirect radiation damage	210
6.18	Schematic showing the dose deposition by X-rays and Carbon-ion beams; note the concentration of dose deposition in the so-called Bragg Peak by carbon ions	211
6.19	Total scattering cross section in Argon using electrons and positrons; the two cross sections merge at high energies (>200 eV) (Karwasz 2002)	213
6.20	Positron scattering from molecular oxygen showing data of Singh and Antony (2017) using a modified spherical complex optical potential formalism, compared to a range of experimental data	214
6.21	Various total cross sections of positron–neon scattering (Kothari and Joshipura 2010); $Q_T$ : <i>dotted curve</i> : CSP-ic; <i>continuous</i> : Dewangan and Walters (1977); measured $Q_T$ : <i>stars</i> : Kauppila et al. (1981); <i>triangles</i> : Tsai (1976); <i>bullets</i> : Griffith et al. (1979); Lower data-sets $Q_{ion}$ : <i>dashed curve</i> : CSP-ic; <i>faint curve</i> : Campeanu et al. (2001); <i>triangles</i> : Jacobsen et al. (1995); <i>faint stars</i> : Knudsen et al. (1990); <i>circles</i> : Kara et al. (1997); <i>diamonds</i> : Marler et al. (2005); <i>squares</i> : average experimental $Q_{ion}$ for electrons, Krishnakumar and Srivastava (1988); $Q_{el}$ : <i>dash-dots</i> : CSP-ic; $Q_{ps}$ : <i>inverted triangle</i> : Marler et al. (2005); $\Sigma Q_{exc}$ : <i>dash-dots</i> : CSP-ic, + $Q_{exc}$ by Mori and Sueoka (1994)	215
6.22	A composite bar-chart showing all the TCS of positron scattering with $N_2$ and CO at 100 eV (Kothari and Joshipura 2011)	216

## TABLES

1.1	Structural properties of a few common and small molecules (CCCBDB)	12
2.1	Total (complete) cross sections $Q_T$ (in $\text{\AA}^2$ ) of $e$ -H collisions at three energies, showing results of the EBS (Byron and Joachain 1977); the Unitarized EBS or UEBS (Byron et al. 1982); and the Schwinger Variational Principle – SVP	32
2.2	Cross sections $Q_T$ (in $\text{\AA}^2$ ) of $e$ -H <sub>2</sub> collisions at three energies, showing (a) modified AR as in equation (2.22), (b) the molecular EBS calculations (Khare 2001), (c) experimental data of Zhou et al. (1997), and (d) recommended data of Yoon et al. (2008)	36
2.3	The first few electronic states and their respective excitation thresholds of H <sub>2</sub> (Yoon et al. 2008); except for the data* for $b\ \Sigma_u^+$ , which is from Anzai et al. (2012)	39
2.4	Properties and CSP-ic parameters of H <sub>2</sub> (Joshipura et al. 2010)	42
3.1	Dimensionless CSP-ic parameters for $e$ -He scattering	51
3.2	Comparison of $e$ -He TCS (in $\text{\AA}^2$ ) at the inelastic peak $E_p = 100$ eV, (a) Vinodkumar et al. (2007); (b) data compiled from NIST database	52
3.3	A comparative study of theoretical results (Vinodkumar et al. 2007) on inert-gas atoms, at their respective peaks of $Q_{\text{inel}}$	57
3.4	Fitting parameters A and B of the formula (3.7)	58
3.5	Properties of a few selected light atoms in their excited metastable states (Pandya and Joshipura 2014, and references therein)	75
3.6	Impact energy at peak position, and maximum ionization cross sections of the N and O atomic species (Pandya and Joshipura 2014)	79
3.7	Peak cross section ratio compared with the $P_A$ ratio for metastable oxygen	80
4.1	Dimensionless parameters $a$ , $C_1$ , and $C_2$ for nitrogen molecule	85

- 4.2 100 eV cross sections (in  $\text{\AA}^2$ ) for  $\text{O}_2$  molecule; (a) recommended data: 92  
 Itikawa (2009), (b) Joshipura et al. (2002), (c) BEB (NIST database)
- 4.3 CSP-ic TCS (in  $\text{\AA}^2$ ) of e-NO scattering, at 100 eV, with the corresponding 99  
 data from Itikawa (2016) given in brackets
- 4.4  $Q_{\text{ion}}$  (in  $\text{\AA}^2$ ) for the two diatomic halogens, in CSP-ic and in BEB (Ali and 102  
 Kim 2008) at 60 eV energy
- 4.5 Structural properties of the present sequence of targets (from the 105  
 CCCBDB database)
- 4.6 Maximum  $Q_{\text{ion}}$  and corresponding peak position (Joshipura et al. 2017) 113
- 4.7 TCS ( $\text{\AA}^2$ ) of methane at 100 eV incident energy; CSP-ic of Joshipura 115  
 et al. (2004) are compared with the recommended data of Song et al.  
 (2015); \*the  $Q_{\text{inel}}$  of Song et al. are calculated from their ( $Q_T - Q_{\text{el}}$ )
- 4.8 Properties of  $\text{H}_2$  (GS) and  $\text{H}_2^*$  (Joshipura et al. 2010, +Branchett et al. 126  
 1990)
- 4.9 Properties of  $\text{N}_2$  (GS) and  $\text{N}_2^*$ , see Joshipura et al. (2009) 127
- 5.1 Bond lengths in two-center hydrocarbon targets (CCCBDB database) 140
- 5.2 TCS  $Q_T$ ,  $Q_{\text{el}}$ , and  $Q_{\text{ion}}$  of  $\text{C}_2\text{H}_2$  all in  $\text{\AA}^2$ ; (a) recommended data, Song et 142  
 al. (2017) with uncertainties in the bracket each, (b) CSP-ic results  
 (Vinodkumar et al. 2006)
- 5.3 Bond lengths in the two-center fluorocarbon targets (CCCBDB 144  
 database)
- 5.4 Various theoretical TCS (in  $\text{\AA}^2$ ) for  $\text{SiH}_4$  (a) Gangopadhyay (2008) 149  
 (b) Vinodkumar et al. (2008) (c) Verma et al. (2017) (d) BEB (NIST  
 database)
- 5.5 Various theoretical TCS (in  $\text{\AA}^2$ ) for silane and germane at 100 eV, 152  
 compiled from Vinodkumar et al. (2008).
- 5.6 (a) Ionization cross sections (in  $\text{\AA}^2$ ) of  $\text{SF}$ ,  $\text{SF}_2$ , and  $\text{SF}_3$  radicals at 100 eV (a) 163  
 CSP-ic Gangopadhyay (2008), (b) BEB (NIST database)
- 5.6 (b) 100 eV cross sections (in  $\text{\AA}^2$ ) of  $\text{SF}_4$ ,  $\text{SF}_5$ , and  $\text{SF}_6$ ; (a) CSP-ic (b) BEB 163  
 (NIST database), and (c) Christophorou and Olthoff (2004);  $Q_T$  and  $Q_{\text{el}}$  of  
 $\text{SF}_6$  (Gangopadhyay 2008)
- 5.7 100 eV theoretical cross sections (in  $\text{\AA}^2$ ) for electron scattering from 164  
 $\text{H}_3\text{PO}_4$ ; (a) Mozejko and Sanche (2005), (b) CSP-ic Bhowmik (2012);  $Q_T$   
 in (a) is the sum of the corresponding  $Q_{\text{el}}$  and  $Q_{\text{ion}}$  (in BEB)
- 5.8 Peak  $Q_{\text{ion}}$  values (in  $\text{\AA}^2$ ) of  $\text{C}_3\text{H}_4$ ,  $\text{C}_3\text{H}_6$ , and  $\text{C}_3\text{H}_8$  at broadly around 80 eV 166  
 (a) CSP-ic, Vinodkumar et al. (2006); (b) BEB (NIST database)
- 5.9 Peak  $Q_{\text{ion}}$  and peak  $\Sigma Q_{\text{exc}}$  values in CSP-ic; \* from Limbachiya et al. 175  
 (2015), \*\* from Bhowmik (2012)
- 6.1 Structural properties of  $\text{H}_2\text{O}$  in three phases (Joshipura et al. 2007, and 186  
 references therein); \* from Timneanu et al. (2004)

## FOREWORD I

Electron collisions with atoms and molecules are commonplace. In the natural world they occur in lightning strikes, aurorae, and the Earth's ionosphere in general; outside our planet they are important for similar processes in other planets. The glow of Jupiter's aurora can clearly be seen using telescopes from the Earth. Electron collisions also form a primary process in cometary tails that are bathed in the solar wind, and in many other astrophysical processes. Plasma is the fourth state of matter which involves partial ionization of the atomic and molecular components. Plasmas occur naturally in flames, stars, and elsewhere. Humankind has increasingly harnessed the power of electron collisions in many ways: to start cars with spark plugs, in the traditional light bulb, and in many lasers. Much of modern industry is driven by the use of electron collisions to create plasmas which etch silicon and other materials into ever more complex structures or to provide surface coatings to alter, enhance, or protect the properties of materials. The quest to harness the Sun's power on Earth via fusion involves making a vast hot plasma with a wealth of electron collision processes requiring detailed study. In the current century it has also been realized that the damage experienced by bio-systems as a consequence of all types of high energy particles and radiation is predominantly caused by collisions involving secondary electrons. These electrons are created by the ionizing effect of the original high-energy collision particle independent of the nature of the colliding species. In medical applications these collisions can be harmful, causing double strand breaks of DNA, or beneficial as in radiation therapy, which is widely used to exorcize malignant tumours.

Electrons colliding with atoms and particularly molecules can initiate a variety of processes. Probably the most important of these is the creation of ions (charged species) either through impact ionization or by electron attachment leading to positively and negatively charged ions respectively. These ionized species are chemically active and act as initiators of many of the processes mentioned above.

Understanding, controlling, and utilizing the full power of the collisions of electrons with atoms and molecules has thus become a major objective of many physical scientists but with benefits and applications well beyond the field of physical science. However, electron collisions with atoms and molecules are governed by the laws of quantum

mechanics. This means that the collisions do not obey the everyday laws of collisions such as those found on the billiard table but instead behave in subtle ways which require understanding of the physics at the atomic level. It is just over a hundred years since Franck and Hertz famously demonstrated that the energy levels of the mercury atom were quantized (i.e. discrete), by studying the effects of electron collisions. Since then our understanding of such processes and our ability to control and harness them has made huge progress. This progress has been achieved through the combined application of greatly improved measurement techniques and enhanced theoretical methods, fortified by the power of modern computers. Of course electron collisions also provide fundamental insights into the nature of the collision partner. There is thus now a wealth of knowledge on the processes that follow electron collisions with atoms and molecules as captured both in data sets that can form the input to detailed models of electron collisions and through general principles of what drives these processes.

I therefore welcome this book. It is written by two physicists who have studied electron collision physics over many decades, gaining important insights into ionization and other processes through applications of novel theoretical and experimental methods. The book places their years of experience in a single volume in an easy and accessible manner for the education and enjoyment of the reader.

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## FOREWORD II

To study any system, an interaction with the system is essential. For microscopic objects and systems, which cannot be seen by the naked eye, usually the electron (or photon) beam, with known characteristics, acts as the probe. At a micro-distance, the projectile particles interact/collide with the object and subsequently they are scattered in all possible directions. The scattered particles, electrons in our case, carry the signature of interaction with the object (target). Hence, the measurement of the differential cross sections,  $I(\theta, \phi)$  over all possible directions, yields the total collisional cross section  $\sigma(E_i)$  as a function of the incident energy  $E_i$  of the electrons. For the atomic targets, the collisions are elastic as well as inelastic, including ionization. For the molecules, the additional processes like dissociation and the dissociative ionization, etc., are also possible. Besides, the dissociative components may be in the excited state. Myriad phenomena arising out of electron scattering make the study very interesting from the manifold view-points of theory, experiment, as well as applications.

In the present book, written by Professors K. N. Joshipura and Nigel Mason, collisions of electrons with atoms are briefly discussed initially. In the greater part of the book, molecules are considered as targets. The study is extended to the radicals and the metastable molecules, while a few molecules of biological interest are also considered. The applications of various scattering cross sections to diverse fields like astrophysics, astrochemistry, nanotechnology, etc., are described in the last chapter.

Both the authors are experienced players in the field of electron–atom–molecule collisions. They have a good number of publications to their credit. From the theory as well as application point of view the present book should be quite useful.

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## PREFACE

Electrons are ubiquitous in nature and throughout modern industry, and therefore there are varieties of situations in which electrons interact with atoms and molecules producing diverse physical and chemical phenomena. Extensive studies, both experimental and theoretical, have been carried out on the interactions of electrons with different atomic and molecular targets; indeed the last few decades have witnessed rapid developments in the techniques and methodology for exploring electron–atom/molecule scattering. The wider recognition of the role of fundamental electron interactions in natural phenomena (for example, the observation of aurorae on other planets and the contribution of electron interactions in astrochemistry), in underpinning novel technologies such as Focussed Electron Beam Induced Deposition (FEBID), and as a major source of radiation damage by ionizing radiation has led to an increase in the size of the international community studying electron collisions in all phases of matter.

In this book, our aim is to provide an overview of the field with a focus on theoretical methods used to describe the collisions of intermediate to high energy (exceeding about 15 eV) electrons. The book has six chapters and begins with a discussion of the subject by outlining the necessary textbook background on atoms, molecules, and quantum scattering theories. Attention has been devoted (in Chapter 1) to atomic sizes or ‘radii’ – something that is normally missing in most books and reviews of this kind. A brief survey of atomic radii, running across the periodic table of elements, is outlined.

The major part of this monograph provides an up-to-date review of electron scattering from atoms and molecules, summarizing recent publications. Although the title of the present book mentions ionization specifically, the contents are comprehensive in that we highlight several important inelastic processes occurring in the background of elastic scattering. For many atoms and a large number of molecules, recent theoretical results are discussed along with experimental and other data, and wherever possible recommended data are presented to provide the user with data sets for models and simulations of processes in which electron interactions play a significant role.

The book also provides a summary of basic and most used electron scattering theories and, in particular, discusses an approximate theoretical formalism, called ‘Complex Scattering Potential – ionization contribution’ method, developed by the authors to derive ionization cross sections for a large variety of atomic and molecular systems typically from the first ionization energy onwards, up to 2000 eV or so.

Results for common/atmospheric atoms and molecules are presented in Chapters 2 to 4, while results for polyatomic and/or exotic molecules, including hydrocarbons, fluorocarbons, and biomolecules, etc., are presented in Chapter 5. Of particular interest are the reactive radicals and long-lived metastable species for which experiments are scarce or non-existent and hence the theoretical cross section data hold more significance to the user community. Attempts have also been made, separately for atoms and molecules, to correlate the dynamic quantities, i.e., total cross sections, with some of the static properties of a variety of atomic and molecular systems.

The final chapter, Chapter 6, discusses many fields of science and technology where electron interactions with atoms and molecules play a prominent role. Nature provides large veritable laboratories in the form of the atmospheres of Earth, Mars, Venus, Jupiter, Saturn, etc., and their satellites to explore the role of electron interactions with atoms and molecules whilst their importance has also been revealed recently in comets and other astronomical systems, including the atmospheres of exoplanets.

Electron scattering is a dominant process in many technological fields such as gaseous electronics and electrical discharges, mass spectrometry, lasers and plasma systems, etc. Indeed many of the plasma and related nano-fabrication techniques such as the emerging FEBID and EUV lithography are governed by electron induced processing and scattering. We briefly discuss the role of electron scattering in regulating plasma confinement in fusion plasmas. We also briefly discuss the interaction of electrons with larger biomolecular systems, since it is now recognized that secondary electron emission, and subsequent electron regulated damage to cellular DNA, is a determining factor in radiation damage and, if controlled, may provide new treatment processes in clinical radiotherapy.

For completeness we also discuss electron scattering in the condensed phase of matter and consider scattering by the electron anti-particle, the positron. Scattering of positrons with several atomic and molecular targets is reviewed, mainly in the spirit of providing a comparison with electron scattering.

Thus, in essence, our plan in this work is to place before the scientific community an updated overview of the status of electron interactions with atoms and molecules and the current theoretical methods for exploring such effects. Whilst we emphasize high energy theoretical research, we provide the reader with a comprehensive set of references from which they can explore the field further. We have also demonstrated the wide range of applications of electron scattering from atoms and molecules and



*Preface*

xxix

hope the data compilation will be of use to these communities whilst providing them with a description of the underlying physics. We recognize that we may have missed some results and as new data are being published all the time this book will need updating. Suggestions and comments are most welcome in this regard.

June 2018

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