Lecture Notes in Chemistry 60

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Relativistic Theory of Atoms and Molecules II

A Bibliography 1986-1992

Springer-Verlag
Berlin Heidelberg New York
London Paris Tokyo
Hong Kong Barcelona
Budapest

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Relativistic Theory of Atoms and Molecules. A Bibliography 1916-1985
(Lecture Notes in Chemistry Vol. 41, ISBN 3-540-17167-3) Springer-Verlag 1986

ISBN 978-3-540-57219-0 ISBN 978-3-642-51488-3 (eBook)
DOI 10.1007/978-3-642-51488-3

Library of Congress Cataloging-in-Publication Data
Pyykkö, Pekka, 1941- . Relativistic theory of atoms and molecules II : a bibliography, 1986-1992 / P. Pyykkö. p. cm. – (Lectures notes in chemistry; 60)

1. Atomic theory–Bibliography. 2. Molecular theory–Bibliography. I. Title. II. Series. Z5524.A6P99 1993 [QD461] 016.5412–dc20 93-31082 CIP

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Typesetting: Camera ready by author
52/3140 - 5 4 3 2 1 0 - Printed on acid-free paper

PREFACE

Seven years have elapsed since "RTAM I" was published. It contained 3119 references from the years 1916 to 1985. The present volume covers the years 1986 - 1992 and also contains a number of references previously missed or now purposely inserted. The pre-1986 references are marked with a "*". The running numbers in the present Bibliography begin from 3120 and end at 6577.

A source book like this, is inevitably very superficial and could be characterized by the Chinese expression "to watch flowers riding a horse" [走马观花]. It's virtue, if any, lies in being reasonably complete.

A further problem may be in recovering the information on a particular subject. To find the calculations on a particular molecule, the Quantum Chemistry Literature Data Base (QCLDB) is recommended as a companion. To facilitate finding the references by a given author or with a given title, the combined reference files of RTAM I-II will be made available on a diskette through Springer-Verlag.

We apologise for any inadvertent omissions or characterisations that the author would not find fitting. No legal responsibility is accepted in such cases.

Thanks are due to colleagues who have contributed material. Mr. Chen Jing gave most helpful practical assistance, the text part was typed by Monika Holmberg, Susanne Lundberg and Johan Sandberg. The project received support from Finska Vetenskaps-Societeten.

I also thank the Chemistry Editor of Springer-Verlag, Dr. Rainer Stumpe, for constructive cooperation during the past years.

Helsinki, 4th June, 1993

Pekka Pyykkö

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1. INTRODUCTION

The area of the relativistic theory of atoms and molecules, with its contacts "upstream" to relativistic quantum mechanics and QED, and "downstream" to atomic and molecular physics and all branches of heavy-element chemistry, has now become so vast that a detailed exposition of the entire domain by the same author is hardly thinkable. The purpose of the present compilation is to make available the comprehensive bibliography, assembled by the author over the years, on the art of solving the Dirac equation, or approximations thereof, for atoms and molecules.

Most of the material is given in tabular form. After the general references in ch. 1., the ch. 2 covers the relativistic single-particle wave functions. Ch. 3 gives some references on QED aspects. The methods for multielectron atoms are discussed in ch. 4 and the available results in ch. 5. Symmetry aspects are covered in ch. 6. Molecular calculations are reviewed in ch. 7, with a slightly more detailed analysis than in other areas. Some solid-state problems and band-structure calculations are mentioned in ch. 8. Chapter 9 summarises the subject of "relativity and the periodic system", and the various molecular properties.

The fringe areas where no complete coverage was attempted, include elementary particle models (included in Table 2.4.), Breit-Pauli perturbation calculations on atoms and molecules (Tables 4.11. and 7.9., respectively), the large area of relativistic nuclear calculations (Table 4.13.), band-structure calculations (Tables 8.1-2.), or otherwise excellent review articles with a very slight 'relativistic' content. In each of these cases it was thought useful to give an idea of current acitivity, however.

The 3458 new references are given in the Bibliography. No "distinctions" are awarded in it. Thus, in the present, tabular form of organizing the material, central contributions and small curiosities receive the same amount of attention. We apologize for any inadvertent omissions, or summaries that the author would not find fitting.

Table 1.1. gives a list of treatises and other general references.

Table 1.1. Monographs and other general references.

Reference	Area
Kramers (1957)	Foundations of quantum theory. Translation of Kramers (1938). Chapter on relativistic theories.
Green (1965)	Book on QM, including Dirac theory.
Hestenes (1966)	Space-time algebra.
Aitchison (1972)	Relativistic QM.
Flügge (1974)	Properties of the Dirac equation.
Pilkuhn (1979)	Relativistic particle physics.
Altmann (1986)	Quaternions and double groups.
Dyall (1986)	Review on relativistic atomic and molecular calculations.
Grant (1986b)	Review on relativistic atomic and molecular calculations.
Pyykkö (1986a)	Part I of the present bibliography.
Safronova (1986b)	Relativistic and correlation effects in atoms and ions. Symposium proceedings.
Sokolov and Ternov (1986)	Radiation from relativistic electrons.
Sucher (1986, 1987, 1989ab)	Reviews on QED in atomic physics.
Greiner (1987)	Physics of strong fields.
Karazija (1987)	Theory of x-ray and electronic spectra of free atoms. An introduction.
Kutzelnigg (1987)	The relativistic many-body problem in molecular theory: a review.
Lindgren (1987a)	Relativistic many-body problems: Proceedings of Trieste, 1986.
Schwarz (1987, 1990)	Reviews on relativistic molecular calculations.
Englert (1988)	Semiclassical theory of atoms.
Ermler et al. (1988a)	Review on SO coupling and other relativistic effects in atoms and molecules.
Grant (1988a)	High-Z atoms.
Grant (1988b)	Review on atoms.
Grant and Quiney (1988)	Foundations of relativistic atomic and molecular theory.
L. N. Ivanov et al. (1988)	Multicharged ions.
Johnson (1988)	Review on RRPA.
Khriplovich (1988, 1991)	Book on PNC in atoms.
Levitan and Sargsyan (1988, 1991)	Book on Sturm-Liouville and Dirac operators.
Malli (1988)	Review on relativistic quantum chemistry.
Pyykkö (1988a)	Relativistic effects in structural chemistry.
Quiney (1988)	Relativistic MBPT.
Teitelboim (1988)	QM of fundamental systems.
Wilson (1988)	Edited volume on atomic and molecular calculations. Reviews by Grant, Gropen, Pyykkö, Quiney and Wilson.

Table 1.1. (continued).

Johnson et al. (1989b)	Relativistic, QED and PNC effects in atoms (Santa Barbara 1988).
Kiselev and Lyaptsev (1989)	Diagrammatic PT, including QR corrections.
Malli (1989)	Review on 5d and 5f elements.
Mårtensson-Pendrill (1989ab)	Reviews on relativistic pair-correlation methods for atoms.
Bagrov and Gitman (1990)	Exact solutions of relativistic wave equations.
Greiner (1990)	Relativistic QM : wave equations.
Y.-K. Kim (1990)	Relativistic and QED effects in highly-charged ions.
Kinoshita (ed.)(1990)	Precision tests on QED.
Landau (1990)	Book on QM. §13-18: Relativistic QM.
Dreizler and Gross (1990)	Density functional theory. Book.
Migdalek (1990)	Book on model potentials for atoms.
Moiseiwitsch (1990)	Electron capture at relativistic energies.
Quiney (1990ab, 1991)	Relativistic finite-basis calculations.
Koga and Morokuma (1991)	Homogeneous catalysis by transition-metal complexes.
Schmutzer (1991)	Textbook on relativistic QM.
Wilson et al. (1991)	Relativistic effects in atoms, molecules and solids. Proceedings of the Abingdon 1990 conference.
Bransden and McDowell (1992)	Charge exchange in ion-atom collisions.
Connerade (1992)	Review on cooperative effects in atomic physics, especially "giant resonances".
Grant (1992)	Review on atomic theory.
Greiner and Reinhardt (1992)	Book on QED.
Jones (1992)	Lecture notes on R QM, QED and QCD.
Szász (1992)	Book on HF-level theory of atoms.
Thaller (1992)	Book on the Dirac equation.
Wilson (1992ab)	Relativistic MBPT for atoms and molecules.

2. ONE-PARTICLE PROBLEMS

This chapter gives the references to the one-particle Dirac equation. Occasional references to other relativistic equations are included.

For detailed solutions of the Dirac equation, or for further details on its mathematical properties, we recommend the recent monographs by Bagrov and Gitman (1990) and by Thaller (1992).

Table 2.1. The Dirac equation: interpretative studies, symmetry properties and non-relativistic limits. For literature on the Klein paradox, see Table 2.4.

Reference	Comments
Kudar (1926)	A further original discovery of the "Klein-Gordon" equation, besides Fock, Gordon, Klein and Schrödinger.
Breit (1931c)	Interpretation of Dirac's $\boldsymbol{\alpha}$-matrices.
Hönl and Papapetrou (1940)	Interpretation of the Dirac equation.
Tani (1949, 1951)	Physical interpretation of the Dirac equation.
Foldy (1956)	Synthesis of covariant particle equations (Dirac, KG, Proca) from the Lorentz group.
Gürsey (1957)	Relativistic kinematics of a classical point particle in spinor form.
Kramers (1957)	Translation of Kramers (1938). Chapter on relativistic theory.
Moses (1959)	Maxwell equations in a spinor notation.
Hilgevoord and Wouthuysen (1963)	Covariant splitting of $\mathbf{j}$ into $\mathbf{l}$ and $\mathbf{s}$ for a spin-½ particle.
Barthélémy (1967)	Levinson theorem for Dirac.
Forman (1968)	History of the relativistic doublet problem around 1924.
Dittrich (1970)	Equivalence of the Dirac equation to a subclass of Feynman diagrams.
Lévy-Leblond (1974)	Group theory in QM. Spin obtained already in NR theory. Criticises several textbooks.
Perkins (1976)	Direction of Zitterbewegung.
Ni (1979)	Levinson theorem for Dirac and KG.
Berthier and Georgescu (1980)	Unique continuation for a Dirac operator.
Klaus (1980a)	Number of discrete Dirac eigenvalues for a potential τV, $V \leq 0$, is proportional to τ^3.
Barut and Bracken (1981)	Zitterbewegung and the internal geometry of the electron.

Table 2.1. (continued).

Hostler (1982)	An SL(2,C)-invariant representation of the Dirac equation.
Bessis et al. (1984)	Atomic fine structure in curved space.
Biedenharn and Horwitz (1984)	Chiral two-component spinors and the factorization of Kramers' equation.
Biedenharn et al. (1984)	Spinorial relativistic rotator.
Grosse (1984, 1986)	Solitons connected to the 1D Dirac equation.
Blockley and Stedman (1985)	Supersymmetry: the 2D Pauli equation and a Dirac particle in constant **B**.
Gesztesy et al. (1985)	Mathematical properties of the Pauli Hamiltonian.
Hostler (1985c)	Scalar formalism for QED.
Shirokov (1985)	Irreducible representations of the inhomogeneous Lorentz group as basis of relativistic QM.
Belloni and Reina (1986)	Sommerfeld's (1931) way to the Thomas precession.
Bismut and Freed (1986)	Eta invariants and the holonomy theorem for Dirac operators.
Chang et al. (1986)	Two-component Pauli-like effective Hamiltonians in Dirac theory. H-like tests, Z = 1-100. Rare-gas SCF tests.
Chatterjee (1986)	Large-D solution of the KG equation in spherical potentials , including Coulomb.
Cohen and Mustafa (1986)	Classical (non-quantum) special relativity can give g-factors > 1.
Fanchi (1986)	Time parameters in relativistic QM: Galilean time, Minkowski time and historical time.
Gough (1986)	Analysis of spin and spin-orbit effects using quaternionic algebra.
Gross (1986)	Relativistic equations for nucleon systems.
Hostler (1986)	Scalar formalism for non-Abelian gauge theory.
Keller (1986)	Generalized Dirac equation admitting isospin and color symmetries.
Z.-Q. Ma (1986)	Levinson's theorem for potentials with attractive or repulsive Coulomb tails.
Morita (1986)	Role of quaternions in Dirac theory.
Qian et al. (1986)	Double wave description for a single relativistic free electron.
Rudra (1986)	Maximal symmetry groups of quantum relativistic equations.
Sallhofer (1986)	Elementary derivation of the Dirac equation.
Takahashi and Ropchan (1986)	First-order Schrödinger equation. Includes SO.
Szwed (1986)	'Square root' of the Dirac equation within supersymmetry.

Table 2.1. (continued)

Talman (1986)	Minimax principle for the Dirac equation.
Haar and Curtis (1987)	The Thomas procession gives g_e-1, not $g_e/2$.
Hall (1987)	"Dirac spinor orbits". L^2 orbits with eigenvalue return to origin.
Hokkyo (1987)	Zitterbewegung and mass formulas
Ichinose and Tamura (1987)	The Zitterbewegung of a Dirac particle in a 1+1 D space-time.
Lipkin (1987)	Criticizes C.-Y. Wong (1986).
Malvetti (1987)	Recoil corrections to M1 hfs, including the anomalous magnetic moment of the proton.
Marshakov and Fainberg (1987)	Representation of a Dirac particle as a sum over paths.
Moore et al. (1987, 1988)	Relativistic, many-particle Lagrangian for EM interactions.
Polyzou (1987)	Numerical methods for the discrete states of the squareroot operator $h = (-\frac{1}{2}\nabla^2 + m^2)^{\frac{1}{2}} + V$.
Arodz and Ruijgrok (1988)	Classical limit of the Dirac eq. with an external EM field.
Bessis and Bessis (1988)	Space-curvature effects in atomic and molecular calculations: a review.
Cannata and Ferrari (1988)	"Hausdorff dimension of trajectory" for a spin-1/2 particle in a FW representation.
Cooper et al. (1988)	Supersymmetry as guide for exact solutions for the Dirac equation. Chiral fields. 2D, 4D fields.
Hinton et al. (1988)	Levinson's theorem and Titchmarsh-Weyl theory.
Ionescu et al. (1988)	Nonlinear extensions of the Dirac equation.
Katz (1988)	Semiclassical (h->0) limit of the Dirac equation and the g-2 experiment.
Levitan and Sargsyan (1988)	Book on Sturm-Liouville and Dirac operators.
Ley-Koo and Wang (1988)	Dirac equation in orthogonal curvilinear coordinates.
Lieb and Yau (1988)	Discuss $Z\alpha$-related instabilities for point-nucleus atoms, described by "relativistic Schrödinger" equations. For the many-electron case, a bound on α only is obtained.
Z.-Q. Ma and A.-Y. Dai (1988)	Integral equations with symmetrical kernel applied to a system with a Dirac-type spectrum.
Moore and Scott (1988, 1989)	A class of physically acceptable, classical, relativistic many-particle Lagrangians.
Rastall (1988)	New form of the Dirac equation: wave function a 2 x 2 matrix.

Table 2.1. (continued).

Sherry (1988)	Zitterbewegung. See Epstein (1989) for comments.
Teitelboim (1988)	Quaternionic quantum field theory.
Anghel (1989)	L^2-index theorems for perturbed Dirac operators.
Batenburg and Schakel (1989)	A geometrical interpretation of spin.
Belov and Maslov (1989)	Semiclassical path-coherent states of a Dirac operator with an anomalous Pauli interaction.
Berezin et al. (1989)	Quaternions in relativistic physics. Book, 155 references.
Epstein (1989)	Points out an error in Sherry's (1988) discussion of Zitterbewegung.
Good (1989)	Relativistic particles in EM fields.
Gough (1989)	Probability density of a relativistic free electron.
Grigore et al. (1989)	NR limit of h_D.
Gulmaro Corona (1989)	A one-parameter family of approximations to the initial Cauchy problem for the Dirac equation, see Suárez (1984).
Hillion (1989)	"Front form" of electromagnetism.
Kutzelnigg (1989ab)	NR limit: a Lévy-Leblond (1967, 1970) equation. nth-order PT derived.
Kutzelnigg (1989c)	Relativistic version of Kato's cusp condition.
Okun (1989ab)	Discusses the concept of mass in relativistic theory. Criticizes some interpretations of $E=mc^2$.
Omote et al. (1989)	Galilean covariance leads to the Schrödinger equation.
Pan and Zhao (1989)	The usual mass-velocity term h_m is OK in 1st-order PT, contrary to claims of Farazdel and Smith (1986).
Percoco and Villalba (1989a)	Aharonov-Bohm effect [of potentials in regions where they vanish] on Dirac electrons: solution along a line of magnetic flux.
Polyzou (1989)	Relativistic two-body models.
Sherry (1989)	Pseudo-classical phase space description of the relativistic eletron.
Sokalski (1989)	2D Dirac equation has no magnetic moment. The $+\frac{1}{2}$ and $-\frac{1}{2}$ solutions are separated by $2\ mc^2$.
Ungar (1989)	Relativistic velocity composition paradox and the Thomas rotation.
White (1989)	NR limit of the Dirac operator.
Ambjørn et al. (1990)	Random walk representation of the Dirac propagator.
Baerends et al. (1990)	Suggest the use of different radii, r and r_{FW} (Foldy-Wouthuysen) for discussing relativistic orbital contraction.

Table 2.1. (continued).

Benítez et al. (1990)	Solution and hidden supersymmetry of a Dirac oscillator.
Chatterjee (1990)	Review on large-D expansions for Dirac and KG equations.
Cho et al. (1990)	A Clifford algebra quantization of Dirac's electron-positron field. Free particle.
Clemence (1990)	Levinson's theorem for a Dirac system.
Davies (1990)	Quaternionic Dirac equation.
Dieks and Nienhuis (1990)	Relativistic aspects of NR QM.
Dreitlein and Sauer (1990)	Manipulation of spinors and the group SL(2,C) using te language C++.
Ferrarese et al. (1990)	Interpretation of Thomas precession.
Ferrari and Russo (1990)	"Zitterbewegung" and localization for a NR two-band system in solids.
Greiner (1990)	Book on relativistic wave equations.
Hestenes (1990)	Zitterbewegung attributed, not necessarily to E>0 and E<0 interference, but to a complex phase factor in the Dirac equation.
Keller and Rodriguez-Romo (1990)	A "multivectorial Dirac equation".
Ketov and Prager (1990ab)	Square root of the Dirac equation within extended supersymmetry.
Klaus (1990)	Levinson theorem for the Dirac equation. Connects the number of bound states to phase shifts of continuum functions.
Kutzelnigg (1990)	A PT-based analysis and classification of relativistic approaches.
Rumrich et al. (1990)	Basis-set truncation violates gauge invariance in the coupled-channel representation of the Dirac equation.
Vonsovskii et al. (1990)	Zitterbewegung of a band electron.
Al-Jaber et al. (1991)	NR derivation of SO coupling.
Bordovitsyn and Ternov (1991)	Zitterbewegung with definite parity operators.
Crawford (1991)	Clifford algebra.
Domingos and Caldeira (1991)	Localisation of relativistic quantum particles is not in conflict with causality.
Evans (1991)	Klein's paradox for a modified, "4-space" Dirac equation.
Gilbert and Murray (1991)	Clifford algebras and Dirac operators in harmonic analysis.
Hamacher and Hinze (1991)	"Finite-volume variational method" for the Dirac equation. No applications reported.
Hartley and Tucker (1991)	Classical relativistic motion of a charged particle with spin in an external EM field.
Hestenes (1991)	The electron, new theory and experiment.

Table 2.1. (continued).

Hinton et al. (1991)	Inverse scattering in 1D.
Jackiw and Nair (1991)	Relativistic wave equation for anyons in 2+1 D.
Jaroszewicz and Kurzepa (1991)	Dirac propagator in nD represented as a random walk.
Kato and Yajima (1991)	A time-dependent Dirac equation for moving nuclei.
Kijowski (1991)	Lattice approximation of the Dirac equation.
Kostin (1991)	Linearized relativistic wave equations: Dirac, Feshbach-Villars and others.
Martínez y Romero et al. (1991)	Supersymmetric properties and stability of the Dirac sea.
Mathur (1991)	Thomas precession, SO interaction and Berry's phase.
Moshinsky et al. (1991)	A "many-body Dirac oscillator" basis for the Poincaré group.
Mustafa and Sever (1991)	Shifted 1/D expansion for the KG equation with vector and scalar potentials (D = number of dimensions).
Parisse (1991, 1992)	'Resonances of the Dirac operator' (Kramers degeneracy etc.)
Pavsic (1991)	Interpretation of R QM with invariant evolution parameter.
Sandin (1991)	Interpretation of $E = mc^2$
Simulik (1991)	Connection between the symmetry properties of teh Dirac and Maxwell equations. Conservation laws.
Sonego (1991)	Quasiprobabilities and explicitly covariant QT.
Todorov (1991)	Position-velocity coexistence in a 'minimal' statistical interpretation of the Dirac electron states.
Ungar (1991)	Thomas precession and the associated grouplike structure.
Yamasaki (1991)	Relativistic composition of velocities and the Thomas precession.
Arik and Mungan (1992)	q-oscillators and relativistic position operators.
Baylis (1992)	Classical (non-quantum) eigenspinors and the Dirac equation (cp. Gürsey (1957).
Baylis et al. (1992)	Pauli algebra and $i = (-1)^{1/2}$ in physics.
Beckers et al. (1992a)	Extended symmetries and hidden supersymmetry of the free Dirac equation.
Beckers et al. (1992bc)	Lie extended symmetries for spin 0, 1/2 or 1 particles with non-zero rest mass.
Buenker (1992a)	"Photons with zero kinetic energy".
Bulla et al. (1992)	Holomorphy of Dirac scattering matrix with respect to c^{-2}.
de la Jara and Tabensky (1992)	Spinor operators.

Table 2.1. (continued).

Domínguez-Adame (1992)	A relativistic interaction without Klein paradox.
Gudder (1992)	Discretized Schrödinger and Dirac quantum random walks.
Hegerfeldt et al. (1992)	Quantization may break down the relativistic invariance of wave equations.
Hillion (1992)	Nondispersive solutions of the KG equation.
Holladay (1992)	Derivation of relativistic energy from Lorentz gamma.
Holland (1992)	Dirac equation in the de Broglie-Bohm theory of motion.
Keller and Rodriguez (1992)	Geometric superalgebra and the Dirac equation.
Littlejohn and Flynn (1992)	Semiclassical theory of SO coupling.
Lozada (1992)	Equations of motion for an arbitrary multipole point particle in an external EM field.
McKeon and Ord (1992)	1+1 D Dirac equation obtained from a stochastic process.
Menon (1992)	Although $[h_D, \mathbf{s}] \neq 0$ in Dirac theory, the expectation value $\langle \mathbf{s}(t) \rangle$ is constant.
Muller (1992)	Thomas precession: where is the torque?
Plyushchay (1992)	Free relativistic particle with fractional spin.
Rawnsley (1992)	Exact symplectic structures and a classical model for the Dirac electron.
Schulman (1992)	Optimum two-time localization for massive, free relativistic particles.
Stepanov and Tutik (1992)	1/D expansion of the Dirac equation via an $\hbar$ expansion.
Thaller (1992)	The Dirac equation. Book. 506 references.
Ungar (1992)	The abstract Lorentz transformation group.

Table 2.2. The Dirac equation: further transformations

Reference	Comments
Tani (1949, 1951)	FW-like transformations discovered independently.
Eriksen (1958)	FW transformations for two-particle problems.
Eriksen and Kolsrud (1960)	Canonical transformation of Dirac's equation to even forms. Expansion in terms of the external fields.
McVoy and van Hove (1962)	Formulae for electron-scattering from "FW" nucleons.
Brodsky and Primack (1968)	Electromagnetic interactions of composite systems: not equal to sum of the individual FW transformations.
Chiu (1968)	Dirac and Pauli-level operators for radiative transitions of molecules.
Tsai (1973)	Uses a FW transformation to diagonalise a spin-($\frac{1}{2}$) particle with an anomalous magnetic moment in **B**.
Moss and Okninski (1976)	Diagonal forms of the free-particle Dirac Hamiltonian.
Saroja et al. (1978)	The Cini-Touschek transformation of a free Dirac particle expressed as product of two FW transformations.
Gesztesy et al. (1985b)	Selfadjointness of Dirac operators with anomalous magnetic moment.
Baretty et al. (1986)	A "no pair" equation in momentum space. Tested on H-like 1s states.
Ch. Chang et al. (1986)	A variational 2-component approximation without projection operators.
Durand (1986b)	Transformation to a Pauli Hamiltonian.
Farazdel and Smith (1986)	Claims that the mass-velocity term h_m would be incorrect. See Pan and Zhao (1989).
Hess (1986)	A 1-component "no-pair" Hamiltonian for variational calculations. Good up to order $(\alpha Z)^3$ for H-like atoms.
Heully et al. (1986a)	Transformed 1- and 2-electron Dirac Hamiltonians for MB calculations.
Heully et al. (1986b)	Comment on Hardekopf's and Sucher's (1984) projection operators for 1-electron atoms.
Jarvis and Stedman (1986)	Supersymmetry in 2nd-order Dirac-Coulomb equations.
Jaskolski and Karwowski (1986)	QR approach to low-energy electron scattering from closed-shell atoms.
Karwowski and Kobus (1986)	A new QR equation, tested on a Th model potential. Beats Barthelat et al. (1980).
Kobus (1986)	Argues that the Cowan-Griffin Hamiltonian requires non-orthogonal orbitals for closer parallelism with the exact Dirac solution.

Table 2.2. (continued).

Rutkowski (1986ab, 1988)	A new perturbative approach to relativistic effects. Applied on H using GTOs.
Rutkowski (1986c)	New PT approach for two-electron atoms.
Goldberg and Pratt (1987a); Goldberg et al. (1989)	A 2nd-order Dirac equation derived for screened Coulomb potentials, used in single-channel quantum defect theory.
Hardekopf (1987)	Relativistic momentum-space equations with application to atomic physics. See Heully et al. (1986b) for comments.
Jankowski and Rutkowski (1987)	Double PT for relativity and correlation. He-like ground states, Z=2...30, as example.
Kobus and Jaskólski (1987)	Comparisons between the QR Cowan-Griffin and full Dirac solutions for total and orbital energies and $\langle r^n \rangle$. Low-energy positron scattering from Hg.
Kobus et al. (1987)	H-like $\langle r^n \rangle$ as tests between the QR and Dirac approaches.
Kutzelnigg (1987)	Reviews transformed Dirac equations for molecular work.
Mohanty and Sampson (1987, 1988)	H-like E1 TP as tests of various QR approximations.
Rutkowski and Rutkowska (1987)	H_2^+ using a new PT approach. Terms of order c^n, n = 2, 4, 6 obtained.
Thakur (1987)	Semiclassical approximation for massless particles, with a non-local kinetic energy, in relativistic potentials.
Baretty and Garcia (1988)	A modified Darwin term proposed for variational calculations.
Bel and Ruiz (1988)	Relativistic Schrödinger equations.
Delgado-Barrio et al. (1988)	QR HF model for Ne solved at SZ level.
Karwowski et al. (1988)	Improve the QR method of Karwowski and Kobus (1985) for transition probabilities. See also Mohanty and Sampson (1987, 1988).
Katsuki and Huzinaga (1988)	Variational use of h_p <u>or</u> h_{CG} is possible if the innermost GTOs are contracted to act as a boundary condition (H-like 1s, 2p states, Z= 1-100.
Kissel-Phillip and Schwarz (1988)	Relativistically corrected Schrödinger equation: A relativistic kinetic energy $(m^2c^4+p^2c^2)^{\frac{1}{2}}$ combined with a simulated Zitterbewegung potential and a V_{SO}.
Rustgi et al. (1988a)	Limitations of semirelativistic approaches in the Thomas-Reiche-Kuhn sum rule.

Table 2.2. (continued).

Thaller (1988)	Unitary transformations of the Dirac operator into an "even" form. Applications to scattering theory.
Baylis and Jones (1989ab)	A Pauli-algebra simplification of the Clifford algebra.
Cortona (1989)	Transforms the relativistic spin-polarized atomic equations of Doniach and Sommers (1981) to two uncoupled Dirac equations.
Hostler (1989)	FW-type reduction of the 2nd-order Dirac equation
Jankowski and Rutkowski (1989)	Double-PT for relativity and correlation.
Jansen and Hess (1989a)	Revision of the transformation of Douglas and Kroll (1974) to the form of Hess (1986).
Jaskolski (1989)	QR approach to electron-scattering from atoms.
Kutzelnigg (1989ab)	PT of the Dirac equation, starting from a Lévy-Leblond equation.
Beckers and Debergh (1990)	FW transformations and supersymmetry applied on oscillators.
Goldman (1990)	Shows that the squared Dirac Hamiltonian of Volkov (1989) gives no advantages.
Moreno et al. (1990)	Supersymmetry, FW transformation and stability of the Dirac sea.
Ternov (1990)	Spin of a relativistic electron in the Heisenberg represenation.
Karwowski and Martin (1991); Martin and Karwowski (1991)	QR formulation of the quantum-defect-orbital method.
Kosaka and Yonei (1991ab)	WKB method for an electron in screened Coulomb potentials.
Kosik (1991)	Approximate Dirac-Coulomb radial integrals.
Layton and Chu (1991)	A variational, Fourier-grid approach to the Dirac equation.
Weigel et al. (1991)	Semiclassical expansions in nuclear DF theory.
Adler and Martin (1992)	The electron g = 2 derived for a Pauli equation.
Arredondo Ruiz (1992)	A KG equation with indefinite form.
Buenker (1992b)	'Exponentially damped BP hamiltonian' and positronium decay.
Cardoso (1992)	Bessel function expressions for Dirac fields.
Clerk and McKellar (1992)	Scalar symmetry of the massless Dirac equation.
DeAngelis and Serva (1992)	Probabilistic, Brownian path integral approach to the FW transformation.
Lucha et al. (1992); Lucha and Schöberl (1992)	Breit Hamiltonian for quark-antiquark pairs. A new semirelativistic equation.

Table 2.2. (continued).

Malik et al. (1992)	Relativistic terms in the reduction of the Bethe-Salpeter equation.
Mourad and Vashakidze (1992)	A relativistic Schrödinger equation with SO interaction: $h = \boldsymbol{\alpha}\cdot\mathbf{p} + \beta m + V(1+\beta)/2$.
D.-D. Wu (1992)	Ambiguity of perturbative Dirac theory.

Table 2.3. The Dirac equation: solutions for hydrogen-like system.

Reference	Comments
Sommerfeld (1915)	FS of H-like atoms. Precursor of Sommerfeld (1916).
Rozhanskii and Frenkel' (1938)	Connections between the Sommerfeld and Dirac theories. Points out the equivalence with a NR potential $V= -Z/r-a/r^2$.
Bethe (1948)	Virial theorems and momentum space eigenfunctions for the Dirac-Coulomb case.
Infeld and Hull (1951)	Dirac-Coulomb radial functions from a factorization method. Matrix elements of V(r) for bound and continuum states.
Salpeter (1958)	Dirac-Coulomb problem for an electron with an electric dipole moment.
Epstein and Epstein (1962)	Hypervirial theorems involving α, ß and r^n.
Armstrong (1963)	Anomalous solutions with j=0 to the Dirac-Coulomb problem.
Rosen (1963)	Relativistic Coulomb scattering.
Pratt et al. (1964)	K-shell photoionization cross sections.
Green (1965)	Applies the factorisation technique to the 2nd-order radial Dirac-Coulomb problem.
Dollard and Velo (1966)	Asymptotic ($r \to \infty$) behaviour of a Dirac particle scattered by a Coulomb field.
Bacry and Richard (1967)	Group theory of the KG Coulomb problem.
Kiefer and Fradkin (1969)	Noninvariance group for the Dirac-Coulomb problem.
Dittrich (1970, 1974)	Feynman diagrams of the Dirac-Coulomb problem.
Hojman (1971)	Algebraic method for the Dirac-Coulomb problem.
Johnson (1972)	2s lifetime of H-like atoms, Z = 1-92.
Lin and Feinberg (1974)	M1 decays of 2s in H-like ions.
Narnhofer (1974)	The KG and Dirac-Coulomb problems. The former leads to r^{-2} Schrödinger terms. Analytical properties as function of Z.
Cizek and Paldus (1977)	D-dimensional KG and Dirac hydrogen.
Friar (1979b)	Analytical solution on finite-nucleus contributions to order $(\alpha Z)^6$.
Nieto (1979)	KG hydrogen solved in D dimensions. The unphysical V=-1/r used for all D.
Mil'shtein and Strakhovenko (1982)	O(2,1) algebra and the Dirac-Coulomb Green function.
Durand and Durand (1983)	Analytic s-state solution for the "relativistic Schrödinger equation", $T = (p^2 + m^2)^{\frac{1}{2}} - m$.
Castorina et al. 1984)	Partial-wave analysis for potentials $\lim_{r \to 0} V(r)=-\alpha/r$. WKB fits.

Table 2.3. (continued).

Friar and Tomusiak (1984)	Alternative analytic s-state solution for the "relativistic Schrödinger equation".
Miramontes and Pajares (1984)	D-dimensional KG and Dirac H-like atoms.
Borisoglebskii and Yakimovich (1985)	Nuclear-quadrupole-moment-induced $\Delta L = \pm 3$ TP for hydrogen-like atoms.
Thaler (1985)	Relativistic effects in protonium ($p\bar{p}$). (Strong-interaction effects with relativistic wave functions.)
Wong and Yeh (1985)	Dirac-Coulomb Green function and its application to Raleigh scattering.
Aerts and Nieuwpoort (1986)	GTO solutions for 1s-3d* with $Z \leq 92$.
Ayres (1986)	Fermion-antifermion bound states.
Bruce (1986)	2D Dirac-Coulomb problem.
Chang et al. (1986)	Two-component Pauli-like effective Hamiltonian in Dirac theory.
Chatterjee (1986)	Large-D solution of the KG equation.
Durand (1986b)	Transformation from Dirac to Pauli. Variational.
Dutta et al. (1986)	Compton profiles of Kr-Rn using screened hydrogenic functions.
Emss and Thaller (1986)	Dirac-Coulomb scattering asymptotics.
Garcia (1986)	Classical (non-quantum) limit of the Dirac-Coulomb problem.
Hall (1986)	Eigenvalues of screened Coulomb potentials related to the screening function.
Hegarty (1986); Hegarty and Aerts (1987)	Discusses conditions for finite-basis solution of the Dirac equation. Example: U^{91+}.
Hess (1986)	"No-pair" formalism tested on the 1s state.
Heully et al. (1986b)	Explain the deviation of the H-like results of Hardekopf and Sucher (1984) from Dirac-Coulomb ones by negative-energy-state contamination.
Indelicato (1986)	Binding energies, Z=100...170 for finite-nucleus 1s levels.
Jarvis and Stedman (1986)	Supersymmetry in 2nd-order Dirac-Coulomb equations. 1D and 3D. Also KG 1D and 3D.
Krause (1986)	He-like systems treated variationally using a screened H-like basis.
Z.-Q. Ma (1986)	Levinson's theorem for potentials with (attractive or repulsive) Coulomb tails.
Moore and Scott (1986)	An α expansion for general V(r), tested on H.
Mukoyama (1986)	Excitation of H-like atoms by heavy charged particles.
Papp (1986a)	Ground-state energy of relativistic two-body Hamiltonians with a Coulomb potential.

Table 2.3. (continued).

Rutkowski (1986ab)	A new PT approach tested using GTOs.
Talman (1986)	The H-like $2p_{\frac{1}{2}}$ energy for Z = 92 as test of a new "minimax" method.
Thaller and Enss (1986)	Asymptotic observables and Coulomb scattering of the Dirac equation.
M.K.F. Wong (1986)	Infeld-Hull factorisation and the simplified solution of the Dirac-Coulomb equation.
Bhattacharya et al. (1987)	Uses screened Dirac-Coulomb functions to discuss M-shell vacancy effects on L-shell x-ray spectra.
Eichler (1987)	Relativistic charge exchange with Coulomb boundary conditions.
Grosse (1987)	Perturbed Dirac-Coulomb problem: order of split levels related to sign of $\nabla^2 V_{pert}$.
Hall (1987)	"Dirac spinor orbits" for the large versus the small component.
Hostler (1987a)	Self-energy operator for an electron in an external Coulomb potential.
Hostler (1987b)	Calculates the required matrix elements using the Green function of a 2nd-order Dirac equation.
Ishikawa and Quiney (1987)	Finite-nucleus GTO solution for 1s and $2p_{1/2}$ of Hg^{79+}.
Ishikawa et al. (1987)	O^{7+} using momentum-space GTOs.
Kobus et al. (1987)	$\langle r^n \rangle$ as test between QR and Dirac wave functions.
Malvetti (1987)	M1 hfs of H atoms, including recoil corrections and proton anomalous magnetic moment.
Manakov et al. (1987)	Sturm expansion of the Coulomb Green function in QED. Photon scattering by a bound electron.
Moss (1987)	D-dimensional hydrogen, V=-Z/r. KG and Dirac.
Mrówczynski (1987)	Interaction of relativistic, Coulomb bound states (positronium, pionium etc.) with matter. Part II: Denisenko and Mrówczynski (1987).
Pilkuhn (1987)	See Yelkhovsky (1987).
Stepanovskij (1987)	H-like atom in external **E** or **B**.
Syros (1987)	Non-perturbative evolution operator for the relativistic H atom.
Visser et al. (1987)	H-like atoms with Gaussian nuclear charge distributions solved using GTO:s.
S. Wilson (1987)	Basis sets tested on Dirac H atoms. Also PT using "wrong nuclear charge".
M.K.F. Wong (1987)	Values of the Dirac-Coulomb wave function at origin. (for Lamb shift or positronium decay). The 1s correction factor 1.000 118, 2s only 1.000 004 1.

Table 2.3. (continued).

J.-S. Wu et al. (1987)	Group-theory for scattering S matrix.
Yelkhovsky (1987)	The nuclear magnetic moment-induced atomic quadrupole moment for the 1s, F=3/2 state of hydrogen by Pilkuhn (1984) is correct, after all. See Pilkuhn (1987).
Yin and Pratt (1987b)	Point-Coulomb relativistic Cooper minima in photoionization.
Yoshida (1987, 1988)	Rotating Laplace-Runge-Lenz vector for the relativistic Coulomb problem.
Zimmermann (1987)	Uses Dirac-Coulomb wavefunctions to discuss ns-state hfs.
Zygelman and Dalgarno (1987)	Electron and proton impact excitation of the H-like n = 2 FS levels.
Barut and Salamin (1988)	Spontaneous 2p-1s and 2s-1s emission in hydrogen and muonium.
Carson (1988)	Dirac-Coulomb bound-bound multipole transitions.
Cheon (1988)	$2S_{1/2}-2P_{1/2}$ energy shift influenced by conducting boundaries, $\Delta\nu$= 0.894 MHz for 1μm separation between plates.
Galić (1988)	1+1D hydrogen, V=|x|, has no bound states. Example on Klein's paradox.
Katsuki and Huzinaga (1988)	1s and 2p energies for Z=1-100 using h_D or h_{CG} variationally with contracted inner GTOs.
Mohanty and Sampson (1988)	H-like E1 TP as tests of various QR approximations. See also Karwowski et al. (1988).
Mukoyama and Sarkadi (1988)	Dirac-Coulomb continuum functions at zero kinetic energy in ion-atom collisions.
Nagiev (1988, 1989)	Dynamical symmetry group of the relativistic Coulomb problem for spinless particles.
Panja and Dutt (1988)	1/N theory for spin-0 and spin-½ particles in a Coulomb potential or in arbitary V(r).
Stahlhofen and Biedenharn (1988)	Supersymmetry and scattering in the Dirac-Coulomb problem.
Struensee and Cohen (1988)	n = 2 FS transitions in H + p collisions.
Arbuzov et al. (1989, 1990ab)	Bound states immersed in the continuum.
Atag (1989)	Large-D solution.
Boschi Filho and Vaidya (1989)	Green function for the KG Coulomb problem.
Bottcher et al. (1989)	A "damped relaxation" method tested.
Darewych and Horbatsch (1989, 1990)	Two-body Coulomb system with spins 0, 1/2. KG and Dirac α^4 limits obeyed, respectively.
de Lange (1989a)	Operator analysis of KG and Dirac Coulomb problems.
de Lange (1989b)	A simple solution for the Dirac Coulomb problem.

Table 2.3. (continued).

Goldman (1989a)	Accurate dipole polarizabilities for Z=1...115 from a gauge-invariance method.
Goldman (1989b)	Laguerre basis functions give superior numerical stability to STO:s. Two-photon decay rates of 2s states calculated for Z=1...100.
Kuten' and Rapoport (1989)	M1-hfs-induced atomic M3 moments in F=3/2 j=1/2 states (1s and $2p_{\frac{1}{2}}$).
Lieber (1989)	The Dirac-Coulomb Green's function.
Matsuoka and Okomura (1989)	Accurately energy-optimized GTO basis for H.
Mrówczynski (1989)	Review on relativistic elementary atoms.
Mukoyama (1989b)	K-shell ionization by protons: screened Coulomb and DS functions compared.
Pekeris and Frankowski (1989)	Hyperfine splitting of muonium, positronium and hydrogen from solutions of the Dirac equation in Kerr-Newman geometry. Curved space introduces a trace of imaginary energy.
S. Rashid (1989)	An H-like atom in an intense laser field.
Ritchie (1989)	Scattering of a continuum electron in a Dirac-Coulomb field of another electron.
T. Roy (1989)	Eigenvalues of a Dirac hydrogen atom.
Talwar and Wright (1989)	Dirac-Coulomb functions used to evaluate the "radiation tail" accompanying electron scattering from an extended nucleus (Z, A).
Volkov (1989)	H-like atom using Laguerre-type basis. See Goldman (1990) for comments.
Yoshida (1989)	KG eigenvalues for a Coulomb potential from a rotating Laplace-Runge-Lenz vector.
Boston and Sandars (1990)	The P-violating, T-invariant L=1, "anapole moment" of hydrogenic atoms.
Dominguez-Adame (1990b)	1D H atom in momentum representation.
Dyall and Faegri (1990)	LCAO solution for $2p_{1/2}$ of Hg^{79+}. Kinetic balance and intruder states discussed.
Florescu et al. (1990)	Low-frequency Rayleigh scattering including spin flip.
Kargabaev et al. (1990)	Dirac-Coulomb Green function for finite nuclei.
Krstic and Mittleman (1990)	Bound states of atomic hydrogen in a laser field.
Matsuoka (1990a)	H-like H, Ag, Hg with STO basis and a new finite nuclear model with constant dV/dr.
Parera López (1990)	Scaled hydrogenic solutions as DF basis for He-like systems.
Reiss (1990)	Dirac hydrogen atom in dominant plane-wave field.

Table 2.3. (continued).

Sallhofer (1990ab, 1992)	The Dirac-Coulomb problem using new operators.
Seke (1990)	Deviations from exponential decay for the $2p_{\frac{1}{2}}$ - $1S_{\frac{1}{2}}$ transition.
Shinada (1990)	H atom in static, uniform **B**.
Tong et al. (1990)	s-s, d-s two-photon decay rates.
M.K.F. Wong (1990)	nD Dirac-Coulomb problem solved.
Aissing (1991)	Monte Carlo variance minimization with STOs.
Bawin and Cugnon (1991)	"Partially screened solutions" for the Dirac equation in $Z>Z_c$ Coulomb fields.
Belinfante (1991)	Continuum functions at larger r by summing divergent terms.
Bosanac (1991)	Scattering of a KG wave packet from a Coulomb potential.
Z-H. Chen and Goldman (1991ab)	H-like atoms in strong **B**, up to 10^{12}G. STO basis.
Eberlein (1991)	Level shifts for a hydrogen atom between two conducting plates. Dirac-Coulomb basis.
Goldman and Chen (1991)	H-like atoms in magnetic fields.
Goodson et al. (1991)	D-dimensional KG or Dirac hydrogenic atoms. Singularity analysis.
Grosse et al. (1991)	Order of KG-Coulomb levels, split by a perturbation, related to the sign of its Laplacian.
S.H. Guo et al. (1991)	2D hydrogen (V=-1/r), with and without Chern-Simons potential.
Hasegawa et al. (1991)	Finite-nucleus solutions for various states of Z=1...92.
Hersbach and Ruijgrok (1991)	A quasipotential theory for a spin-1/2 electron bound to a spinless nucleus of finite mass and charge +Ze. Agrees with Dirac-Coulomb up to order α^4.
Kosik (1991)	Approximate Dirac-Coulomb radial integrals.
Layton and Chu (1991)	Solve the $S_{\frac{1}{2}}$ Dirac-Coulomb eigenstates for Z=2 using a variational Fourier-grid approach. With a 41-point radial grid, 2-3 lowest bound states have accurate E_{rel}.
Legrand et al. (1991)	Dirac-Coulomb basis used to describe L-shell ionization in p + Sm collisions.
Matsuoka et al. (1991)	H-like atoms, Z=1...92, using GTO basis and a uniformly charged, finite nucleus.
Nandi and Shastry (1991)	2D and 3D KG-Coulomb problems. Classical (small-h) limits discussed.
Pyykkö and Zhao (1991d)	Notice that for V =-Z/r, the 2D Dirac and 3D KG eigenvalue expressions are similar.
Schlageter and Pilkuhn (1991)	Relativistic polarizabilities of H-like systems for "electrons" with arbitrary g.

Table 2.3. (continued)

Shabaev (1991a)	Virial relations for M1 and E2 hfs integrals and other integrals.
Smit (1991, 1992)	Light-ion induced K-shell ionization in the adiabatic region. H-like wave function.
Spence and Vary (1991a)	Electron-positron scattering resonances from relativistic two-body wave equations.
Spence and Vary (1991b)	Electron-proton resonances at low energy.
Swainson and Drake (1991a-c)	Unified treatment of R and NR H atom. Green functions.
Visscher et al. (1991ab)	Kinetic balance and basis-set contraction tested on H-like atoms.
Yudin (1991)	Excitation and ionization of H-like atoms by fast, multiply charged ions.
Zapryagaev and Nefedov (1991)	Photoionization of multiply charged H-like ions.
Z.-H. Chen and Goldman (1992)	H atom in **B**. R/NR.
Cheung and Li (1992)	A QR equation for a system consisting of a $S=\frac{1}{2}$ fermion and a S=0 boson.
Datta and Datta (1992)	'Minimax' techniques for LCAO methods tested on the Dirac-Coulomb problem.
de Lange and Welter (1992ab)	'Shape invariance' of the Dirac and KG Coulomb problems.
Goldman (1992)	Fundamentals of a basis-set approach tested on the Dirac-Coulomb case.
Grozdanov et al. (1992)	Microwave excitation of H-like Rydberg states.
Kao et al. (1992)	Electron-impact ionization of H-like atoms, Z = 1...47. R/NR.
Kuchiev et al. (1992)	Atomic quadrupole moment of $ns_{\frac{1}{2}}$(F = 1) states.
Papp (1992)	'Fixed point structure' of the Dirac-Coulomb problem. 1/D approach.
Seke (1992ac)	Non-exponential $2p_{\frac{1}{2}}$-1s decay of Dirac hydrogen.
Shen et al. (1992c)	2D Dirac-Coulomb problem.
Shin et al. (1992)	Wigner formulation for the density matrix of the Dirac-Coulomb problem.
Tutik (1992)	Exact solution of the nD Dirac-Coulomb problem.

Table 2.4. The Dirac equation: solutions for various non-Coulomb fields.

Reference	Comments
Volkov (1937)	Dirac electron in a plane, non-polarised EM wave.
Pomeranchuk and Smorodinsky (1945)	Dirac-Coulomb problem for a charged-shell nuclear model.
Voronkov and Kolesnikov (1960)	ns states for finite nuclei with radius r_0, $V=-Z/r_0$, $r<r_0$.
Roos and Sangren (1962)	Spectral theory of the radial Dirac equation.
Jannussis (1966)	**B** using "Schraubenfunktionen".
Barthélémy (1967)	Central-potential scattering.
Canuto and Chinderi (1969)	**E** $\perp$ **B**.
Lam (1970ab)	**E** $\perp$ **B**.
Lipas (1970)	3D KG harmonic oscillator solved to order α^2.
Steslicka and Davison (1970)	Boundary conditions for the relativistic Kronig-Penney model.
Steslicka et al. (1971a)	1D Kronig-Penney model for impurity states of solids.
Steslicka et al. (1971b)	Kronig-Penney model for heavy diatomic crystals.
Bhagwat and Subramanian (1972)	Impurity states in a relativistic Saxton-Hunter model (chain of δ functions).
Fedorov and Kazakov (1973)	Quantized plane wave, directed along a constant **B**.
Hautot (1973)	Coulomb field + **B**.
Tsai (1973)	Spin-($\frac{1}{2}$) and spin-0 particles with anomalous magnetic moments in **B**.
Wüst (1973, 1975, 1977)	Conditions for selfadjoint Dirac operators with a cut-off potential.
Chodos et al. (1974)	The "bag" model for hadrons. Spurious solutions avoided by the boundary conditions r^x, $x>0$, at $r \to 0$, see Johnson and Sapirstein (1986).
Flügge (1974)	Properties of the Dirac equation.
Sen Gupta (1974)	Monoatomic and diatomic 1D lattices of δ-function potentials.
Gyulassy (1975)	Radial Green functions for finite-nucleus (muonic) atoms.
Bongaarts and Ruijsenaars (1976, 1977)	The Klein paradox analysed.
Moss and Okninski (1976)	Dirac particle with anomalous magnetic moment in **B**.
Friar (1979b)	Analytical evaluation of finite-nucleus effects in hydrogenic atoms through order $(Z\alpha)^6$.
Kaburagi et al. (1980)	$V= -\ln r$ as model for meson spectra. Variational method.
Klaus (1980a)	Asymptotic properties of a Dirac particle in a potential V.

Table 2.4. (continued).

Klaus (1980b)	General properties of Dirac operators with several Coulomb singularities.
Eisenberg (1981)	A relativistic nucleon in scalar and vector potentials.
Shen (1981a)	A semi-infinite 1D Kronig-Penney model with a step-function surface.
Shen (1981b)	Surface states of a semi-infinite, 1D Kronig-Penney model in a constant electric field.
Borie and Rinker (1982)	Muonic atoms.
Rabin (1982)	Solves the lattice fermion doubling problem. 1+1 D.
Silagadze and Khelashvili (1984)	A two-fermion bound state with $V(r) = gr + b$, without a Klein paradox.
Stacey (1982)	Elimination of fermion doubling.
Bergou and Ehlotzky (1983)	Exact solutions for KG or Dirac particles in a plane-wave radiation field, directed along a constant **B**.
Jena (1983)	A power-law, Ar^x, model for meson mass spectra; $x = 0.1$.
Atiyah and Singer (1984)	Dirac eq. coupled to vector potentials.
Fleischer and Soff (1984)	Bound states of KG particles for strong potentials. (Coulomb, Hulthén, Yukawa, exponential, finite nucleus, square well...).
Miramontes and Pajares (1984)	nD KG and Dirac hydrogen.
Nickish et al. (1984)	Numerical solutions for a two-particle problem with $h_i = (-\nabla^2 + m^2)^{\frac{1}{2}}$ and $h_{12} = V(r_{12})$.
Behncke (1985)	Spectral properties of the Dirac equation with anomalous magnetic moment.
Bruce (1986)	2D Dirac-Coulomb problem.
Fröhlich et al. (1986)	H-like atom in **B**.
Hall (1986)	Eigenvalues of screened Coulomb potentials related to the screening function.
Moore and Scott (1986)	A perturbation expansion in α for arbitrary, spherically symmetrical potential $V(r)$. Wave functions to order α^2, energies to α^4 given. Tests on H.
Ni (1986)	Exact solution for a Dirac electron in constant **E**.
Nogami and van Dijk (1986)	Discuss bound and scattering solutions of the Dirac equation in a central field.
Papp (1986a)	Ground-state energies for two-body Hamiltonians with Coulomb and Yukawa potentials.
Papp (1986b)	Quasiclassical ground-state energies for quarkonia potentials: $\ln r$, $r-\alpha/r$, C_n/r^n with $C_n n<0$ etc.
Rosenberg (1986)	Relativistic scattering in a slowly time-dependent **E**.

Table 2.4. (continued).

Rosenberg and Spruch (1986)	Extremum principles for relativistic bound-state energies.
C. L. Roy (1986)	1D disordered system, modelled by rectangular wells. DOS for an approximate Dirac equation.
Roy and Pandey (1986a)	Relativistic Kronig-Penney equation and surface states of a distorted surface.
Ray and Pandey (1986b)	Relativistic surface states of a finite crystal.
Sokolov and Ternov (1986)	Radiation from relativistic electrons.
Su and Ma (1986)	(3+1)D and (1+1)D Dirac equations with both scalar ($\beta\phi$) and vector (V) like potentials. No confinement for $\phi=\pm V$.
Thaller (1986)	Scattering theory for long-range Lorentz scalar potentials $\beta V(\mathbf{x})$, such as $\beta/\lvert\mathbf{x}\rvert$.
Ulehla and Horejsi (1986)	Generalized Prüfer transformation and the eigenvalue problem of radial Dirac equations. $V(r)= -5\ e^{-r}$.
Abe and Fujita (1987)	Approximate analytic solution for a scalar linear potential (see ref. 688): $h_D=\boldsymbol{\alpha}\cdot\mathbf{p} +\beta\mu r$.
Abounadi and Darkhosh (1987)	Dirac wave equations in external fields.
Barut and Pavsic (1987)	A classical Dirac electron in curved space.
Bottcher and Strayer (1987)	Time-dependent fermion problems solved on a collocation lattice using splines. Fermion doubling avoided by different discretisation for G and F (forward and backward, respectively).
Calkin et al. (1987)	Delta-function potential in a 1D Dirac eqn.
Coutinho and Nogami (1987a)	A 1D "DF" model for a 2-electron "atom" with δ-function interactions solved to order α^2 (=NR result).
Coutinho and Nogami (1987b); Coutinho et al. (1988)	Conditions for existence of bound states for 1D Dirac problems.
Dominguez-Adame (1987, 1989)	Relativistic Kronig-Penney model.
Falkensteiner and Grosse (1987)	Quantization of fermions interacting with point-like external fields.
Gesztesy and Seba (1987)	New analytically solvable models of relativistic point interactions.
Hall (1987)	"Dirac spinor orbits" for the large versus the small component.
Karpenko (1987)	Relativistic fermion in a square-well potential.
McKellar and Stephenson (1987)	Klein paradox and the Dirac-Kronig-Penney model.
Misra et al. (1987)	Relativistic effects on meson spectra.
Moss (1987)	D-dimentional hydrogen, $V=-Z/r$, solved for KG and Dirac. No bound states for D=1. Cp. Capri and Ferrari (1985).

Table 2.4. (continued).

Mukoyama and Lin (1987b)	Dirac equation in a DS atomic potential using STOs.
Palladino and Leal Ferreira (1987)	Level order for a Dirac particle in mixed scalar and vector potential, $h=\boldsymbol{\alpha}\cdot\mathbf{p} + \beta m + \frac{1}{2}(1+\beta)V(r)$, without Klein paradox.
Polyzou (1987)	The square-root operator solved for Coulomb, Yukawa and 'confining' ($-C_1/r + C_2 r$) potentials.
Rosenhouse and Katriel (1987)	Isospectral transformations in R and NR mechanics. The C -> ∞ and h -> 0 limits of 1D Dirac equations.
Salvat et al. (1987a)	Numerical solutions of the Dirac equation for a 5- parameter MP for Z = 1-92.
Saritepe and Swamy (1987)	2D Dirac equation for an electron in a helical wiggler magnetic field.
Solovtsov and Chernichenko (1987)	Inverse scattering problem in the relativistic quasiclassical approximation.
Stepanovskij (1987)	H-like atom in external **E** or **B**.
Arshansky and Horwitz (1988)	Relativistic potential scattering.
Barut and Bozic (1988)	Motion of Dirac particles with anomalous magnetic moments through magnetic fields. A magnetic barrier as example.
Bijtebier (1988, 1989b)	Scattering matrix elements for a relativistic bound state.
Borie and Jödicke (1988)	Antiprotonic atom, with the anomalous magnetic moment and vacuum polarization potential. Solved numerically.
Bulla et al. (1988)	Relativistic energy band corrections for periodic potentials.
Bychkov (1988)	Energy spectra of 2D systems with SO interaction in an inclined magnetic field.
Calkin et al. (1988)	Nonlocal separable potential $(\beta g+h)V(x)V(x')$.
Ebert and Gyorffy (1988)	Scattering solutions of the Dirac equation for nonspherical targets.
Galić (1988)	1+1 D hydrogen, V=1+1, $V=\|x\|$, has no bound states. Example on Klein's paradox.
Gjaja and Bhattacharjee (1988)	Dirac theory of the free-electron laser (helical undulator potential). Quantum noise found.
Ixaru and Pantea (1988)	A double square well 1D model for positron creation in superheavy collisions.
Jansen et al. (1988)	Continuum solutions of the KG equation. Point Coulomb, finite nucleus, square well, attractive exponential and 'overcritical' potentials considered. Also homogeneous **B**.
Koller et al. (1988)	Positronium and muonium in strong magnetic fields.

Table 2.4. (continued).

Leal Ferreira (1988)	Two-body Dirac equation with a scalar linear potential.
Mladenov (1988)	Relativistic extension of the Saxon-Hutner theorem: In a 1D Kronig-Penney problem, common energy gaps of A and B are energy gaps of the alloy A+B.
Panja and Dutt (1988)	1/D theory for spin-0 or spin-½ particles in arbitrary V(r). Coulomb case as an example.
C. L. Roy (1988)	A spatially constant solution to the 1D Dirac equation.
Seba (1988)	Absorption of eigenvalues in E>0 or E<0 continuum of 1D and 3D Dirac equations.
Ternov et al. (1988)	Solutions of the KG and Dirac equations for EM fields characteristic for free-electron lasers. Spinors for wigglers.
Tóth et al. (1988)	Two-centre Dirac equation with separable potentials.
Vrscay and Hamidian (1988)	Eigenvalues for a Dirac-Coulomb problem, perturbed by βr^q or r^q, by hypervirial theorems.
Arshansky and Horwitz (1989ac)	Bound states for spherically symmetric O(3,1) potentials: Coulomb, harmonic and square well.
Arshansky and Horwitz (1989b)	Relativistic potential scattering and phase shift analysis. Levinson theorem.
Arshansky et al. (1989)	Bound states and EM interactions.
Atag (1989)	Large-D solutions for spherical potentials.
Bagrov et al. (1989)	Yang-Mills fields.
Bardsley et al. (1989)	Electrons in intense laser fields.
Bijtebier (1989a)	Two spin-less particles bound in a potential.
Bottcher et al. (1989)	A damped relaxation method for bound states. Coulomb, 1D Gaussian and uniformly charged sphere potentials as test cases.
de Frutos (1989); de Frutos and Sanz-Serna (1989)	Numerical integration of non-linear, 1+1D Dirac equations. Split-step FFT found best.
Detcheva et al. (1989ab)	Effective electron masses in the Kronig-Penney model.
Dittrich et al. (1989, 1990)	Spherically symmetric $\delta(r)$ potentials.
Dominguez-Adame and Maciá (1989a)	Harmonic oscillator + a Lorentz scalar delta function.
Dominguez-Adame and Maciá (1989b)	Point interaction potentials and bound states.
Glass and Mendlowitz (1989)	Spin flips in Dirac scattering by a 1D barrier.
Goldberg et al. (1989)	Phase shifts for screened Coulomb potentials from WKB approximation.
Good (1989)	Particles in EM fields.

Table 2.4. (continued).

D.-S. Guo et al. (1989)	Scattering theory of multiphoton ionization in strong fields. Uses a quantized-field Volkov solution.
Hofer and Stocker (1989)	Establishes a formal analogy between the 3D V(r) and V(z) Dirac problems.
Jaffe and Manohar (1989)	Bound states of the Dirac equation outside a hard sphere in 1, 2 and 3D .
Jagannathan et al. (1989)	Magnetic electron lenses.
Kamath (1989)	Dirac-Coulomb problem in 2+1 D. While V=ln r gives no solution due to Klein's paradox, the Chern-Simons potential does.
Krstic and Milosevic (1989)	Scattering of electrons in an elliptically polarized ultra-strong laser pulse.
Lovas and Molnár (1989)	Dirac particle in a vector meson field, periodic in space, constant in time. See Sen Gupta (1992).
Manoukian (1989)	Propagator for a Dirac δ potential.
U.D. Misra et al. (1989)	Sommerfeld's σ_2 parameter for the screened Dirac-Coulomb problem deduced for Z=10-103 using theoretical energies of Huang et al. (1976). (E_{rel} is proportional to $\alpha^4(Z-\sigma_2)^4/n^4$).
Missana (1989)	The Volkov (1935) solution in astrophysics
Mitchell et al. (1989)	An 1D "relativistic HF" model for the deuteron with δ-function attraction.
Mladenov (1989)	Saxon-Hutter theorem in the relativistic domain: gaps common to A and B are gaps of any AB alloy.
Moreno and Zentella (1989)	Covariance, CPT and the FW transformation for the Dirac oscillator.
Moshinsky and Szczepaniak (1989)	"The Dirac oscillator", $h_D = c\,\boldsymbol{\alpha}\cdot(\mathbf{p} - im\,\omega\mathbf{r}\,\beta) + mc^2\beta$. NB:linear in both **p** and **r**. Reduces at NR limit to a harmonic oscillator, $V=m\omega^2r^2/2$, with SO splitting.
Noskov and Shvartsman (1989)	Green's functions for external EM field by the eigenfunction method.
Percoco and Villalba (1989a)	A line of magnetic flux.
Percoco and Villalba (1989b)	1D scalar potentials.
Pimentel (1989)	More solutions for space-times with local rotational symmetry, where the Dirac equation separates.
S. Rashid (1989)	Applies the Volkov solution to a H-like atom in an intense laser field. See Mittleman (1991) for comments.
Raspini (1989)	Relativistic Zeeman effect in positronium, n=2.

Table 2.4. (continued).

C. L. Roy (1989); Roy and Basu (1990)	1D disordered systems modelled by rectangular barriers or wells. R/NR comparison.
Roychoudhury and Varshni (1989)	Relativistic 1/D expansion of the Dirac equation. Solutions for a screened Coulomb potential.
Sahu et al. (1989)	Critical binding ($E \leq 0$) of KG and Dirac particles by δ-function and square-well potentials in 1D...3D.
Seba (1989)	Klein's paradox and the δ-function interaction.
Sen Gupta (1989)	1D Dirac equation in V(x) reduced to a Riccati equation.
Shishkin and Villalba (1989ab)	Dirac equation in external vector fields.
Sitenko (1989)	Zero modes for a 2D Dirac operator on a noncompact singly connected surface in external **B**.
Srivastava (1989)	Solution of the Dirac equation in Kasner's space time.
Thaller (1989)	Dirac particles in magnetic fields.
Volkov (1989)	Confining quark potential ßV(r)= 400rß.
Aly and Barut (1990)	Exact solutions for the E-dependent, 2nd-order Dirac equation.
Anghel (1990b)	2D magnetic field.
Bagrov and Gitman (1990)	Exact solutions: a book.
Beckers and Debergh (1990)	FW transformations and supersymmetry applied on oscillators.
Benítez et al. (1990)	Solution and hidden supersymmetry of a Dirac oscillator, $\boldsymbol{\alpha}\cdot(\mathbf{p}-im\omega ßr)$.
Bernabeu and Garcia Molina (1990)	Finite-nuclear-size effects on leptonic wave functions.
Chatterjee (1990)	Review on large-D expansions for Dirac and KG problems.
Coutinho and Nogami (1990)	New proof that 2D and 3D δ-function potentials give no solutions for the Dirac equation.
Danilov (1990)	Spectrum of the Dirac operator in R^n with a periodic potential.
Detcheva et al. (1990)	Scattering from an interface model with Kronig-Penney potentials separated by a step.
Dominguez-Adame (1990a)	$V=1/\|x\|$.
Dominguez-Adame (1990b)	1D H atom in momentum representation.
Dominguez-Adame (1990c)	Surface δ interactions.
Dominguez-Adame and Gonzáles (1990)	Solvable linear potetials.
Durand and Gara (1990)	Matrix methods for the numerical solution of relativistic wave equations.
Fassari (1990)	Bound states for relativistic Kronig-Penney hamiltonians with impurities.
Goldberg et al. (1990)	A relativistic Fermi-Segre formula for the wave function near the nucleus from the WKB approximation.

Table 2.4. (continued).

Ivanov et al. (1990)	Dirac Green function for non-singular potentials.
Ivrii (1990)	2D Dirac particle in a strong magnetic field.
Jagannathan (1990)	Theory of magnetic electron lenses, based on the Dirac equation.
Kargabaev et al. (1990)	Dirac-Coulomb Green function for finite nuclei.
Koutroulos (1990)	Gaussian potential model for lambda particles in hypernuclei.
Krstic and Mittleman (1990)	Bound states of atomic hydrogen in a laser field.
Loewe and Sanhueza (1990)	In 1D, no diving to the positron-like continuum by attractive δ-function potentials. In 3D, yes.
Panja et al. (1990)	1/D theory for a spin-½ particle in a screened Coulomb potential.
Pratap (1990)	Dirac electron in axial-wiggler fields.
Quesne and Moshinsky (1990)	Symmetry Lie algebra of the Dirac oscillator.
Reiss (1990)	Hydrogen atom in dominant plane-wave field.
B. Roy and Roychoudhury (1990a)	Shifted 1/D expansion for the Dirac equation for equally mixed vector and scalar potentials.
B. Roy and Roychoudhury (1990b)	Dirac equation with Hulthén potential. Energy levels solved.
Shaarawi et al. (1990)	Nondispersive wave packet solutions to KG and Dirac equations.
Shinada (1990)	H atom in static, uniform **B**. Adiabatic approximation.
Villalba (1990)	Dirac equation in parabolic cylinder and elliptical coordinates.
Anders and Kotlyarov (1991)	Characterisation of the scattering data of Schrödinger and Dirac operators.
Anderson (1991)	Exact solutions for $v=-2k\ \mathrm{sech}^2 kx$, $w^1=-k \tanh kx$.
Bassetto and Griguolo (1991)	Eigenfunctions for a Dirac operator of a vortexlike Abelian potential on a 2D sphere.
Bychkov et al. (1991)	Two-dimensional electrons with SO interaction in a tilted magnetic field.
Castaños et al. (1991)	Soluble extensions of the Dirac oscillator with exact and broken supersymmetry.
Z.-H. Chen and Goldman (1991ab)	H-like atoms in strong **B**. STO-basis.
Clerk and McKellar (1991)	Relativistic band gaps in 1D disordered Kronig-Penney models.
Cordova (1991)	Fractional charge in massive fermion systems in 1+1, 2+1 and 3+1 D.
Coutinho et al. (1991)	Existence of bound states of a Dirac particle in 2D and 3D $U(r)=\beta\ S(r)+V(r)$.
Dominguez-Adame (1991)	A perturbed Dirac oscillator.

Table 2.4. (continued).

Dominguez-Adame and Méndez (1991)	A solvable two-body Dirac equation in 1D.
Dominguez-Adame and Sanchez (1991)	Kronig-Penney models for quasiperiodic lattices.
Franosch and Soff (1991)	Finite-nucleus effects in muonic atoms.
Goldman and Chen (1991)	H-like atoms in magnetic fields. Relativistic correction changes sign around $B=10^{11}G$.
Grochmalicki et al. (1991)	Relativistic effects on ionization of atoms in intense laser fields.
D.S. Guo and Åberg (1991)	Orthogonality and completeness of the Volkov solutions (Wolkow 1935).
S.H. Guo et al. (1991)	2D hydrogen ($V=-Z/r$), with and without Chern-Simons potential.
Hinton et al. (1991)	Inverse scattering on the line for a Dirac system.
Hu and Su (1991)	Hulthén-type potentials.
Iyer and Kamran (1991)	Separability of the Dirac equation in metrics with local rotational symmetry.
Klimenko and Klimenko (1991)	Elastic scattering amplitudes for an electron in a plane-wave EM field.
Kosaka and Yonei (1991b)	Bound states in screened Coulomb potentials. WKB.
Koutroulos (1991)	R/NR lambda particle models with $V(r)=-D[\cosh^2(r/R)]^{-1}$. Results compared with Gaussian and Woods-Saxon models.
Kukulin et al. (1991)	Dirac equation with harmonic oscillator and extra SO potentials.
de Lange (1991ab)	The Dirac oscillator of Moshinsky and Szczepaniak (1989).
J.-F. Lu et al. (1991)	Relativistic electrons in high-power laser light.
Maciá and Dominguez-Adame (1991)	Scattering states of relativistic point-interaction potentials.
Méndez and Dominguez-Adame (1991)	Mathieu potential $V(x)=V_0\cos 2x$ as model for 1D band structures.
Mishchenko and Sitenko (1991)	Ground states of a 2D Dirac operator in a magnetic field with non-local boundary conditions.
Mittleman (1991)	Comments on Rashid (1989).
Molnár and Lovas (1991)	Dirac particle in a periodic field.
Ndimubandi and Ntibashirakandi (1991)	Dirac oscillators through supersymmetry and FW transformations.
Papp (1991ab)	1/D solutions for two-body systems with arbitrary vector and scalar potentials.
Quesne (1991)	Supersymmetry and the Dirac oscillator.
C. L. Roy (1991)	Relativistic surface states.
Roy and Basu (1991)	Band gaps in 1D disordered systems.
Sato et al. (1991)	1D bound-state problems.
Sen Gupta (1991)	Exact solution of the Dirac equation for a helical wiggler with a guide field: $\mathbf{B}=B_{\parallel}\mathbf{k}+B_{\perp}(\mathbf{i}\cos kz+\mathbf{j}\sin kz)$.
Shishkin (1991)	Volkov problem generalised for various tensorial fields.

Table 2.4. (continued).

Shishkin and Ali (1991)	Dirac particle in wave fields (generalized Volkov problem).
Shishkin and Cabos (1991)	Separation of variables for a Dirac equation in Cartesian coordinates.
Shishkin and Yasin (1991ab)	Generalized Volkov problem (external wave fields of different tensor structures).
Thompson and McKellar (1991)	High square barrier.
Toyama et al. (1991)	Relation between the bound-state radius and the scattering length for one and two Dirac particles.
Toyama (1991)	Dito. Solution for the non-local potential of Nogami and van Dijk (1986).
Alan and Barut (1992)	Volkov solution for particles with anomalous magnetic moments.
Arbuzov et al. (1992)	$V(r) = \alpha \cos(Er)/r$ and narrow resonances.
Boudjedaa et al. (1992)	Green functions for KG and Dirac particles in an EM wave field.
Z.-H. Chen and Goldman (1992)	H atom in **B**. R/NR. The correction changes sign around $B=10^{11}$G.
Clerk and Davies (1992b)	Inversion of barrier transmission for a 1D Dirac equation.
de Lange and Raab (1992)	Book on operator methods. Solvable 1D and 3D problems included.
de Lange and Welter (1992a)	'Shape invariance' of the Dirac oscillator.
Domínguez-Adame and González (1992)	Generalized Dirac-Kronig-Penney model with non-local separable potentials. 1D.
Dittrich et al. (1992)	Coulomb potential + spherically symmetric contact interaction.
Domínguez-Adame (1992)	A relativistic interaction without Klein paradox.
González et al. (1992)	A (2+1)D Dirac equation on a sphere used as fullerene model.
Grigis and Mohamed (1992)	Gaps in the Dirac spectrum for periodic V and **B**.
Grosse et al. (1992)	Order of energy levels for a pure Coulomb + vector-like field.
Grotch et al. (1992)	E1 transitions of $b\bar{b}$ bound states.
Grozdanov et al. (1992)	H-like atoms in circularly polarised microwave fields.
Hillion (1992b)	Nondispersive solutions of the Dirac equation.
Hoang et al. (1992)	Exact solution for a Coulomb + Aharonov-Bohm + Dirac monopole field.
Kalnins and Miller (1992)	Dirac equation in Kerr-Newman space-time. Flat-space applications to bag models.
Krolikowski (1992ab)	Radial equations for the Dirac two-body problem.
Kukulin et al. (1992)	Oscillator potential + SO-coupling.

Table 2.4. (continued).

Lauwers et al. (1992)	Inversion of the Dirac matrix by parallel transported multigrid in SU(2) lattice gauge theory.
Leal Ferreira and Tomio (1992)	Potential bags with smeared surfaces.
Leutwyler and Smilga (1992)	Spectrum of the Dirac operator in vacuum gauge fields, QCD.
Maier and Dreizler (1992)	Poles of the S-matrix for a Dirac square-well potential.
Martínez-y-Romero and Salas-Brito (1992)	Conformal invariance in a Dirac oscillator.
Matsutani (1992)	Berry phase of Dirac particle in thin rod.
Mendel and Trottier (1992)	Model for $Q\bar{q}$ mesons: analytic small-r solution for a $V(r)=-A/(r \ln r)$. Both Dirac and KG solutions finite at origin.
Méndez and Dominguez-Adame (1992)	Level shifts of Dirac particles under point interaction potentials.
Mohamed and Parisse (1992)	Approximations for some singular perturbations.
Moshinsky et al. (1992)	A 1D particle-antiparticle system with a Dirac oscillator interaction.
Mourad and Vashakidze (1992)	$h=h_D + V(1+\beta)/2$.
Nogami and Toyama (1992)	"Transparent potential" (transmission coefficient=1) constructed for the 1D Dirac equation.
Panja et al. (1992)	Large-D expansion for a spin-½ particle in the presence of scalar and vector potentials.
Papp and Micu (1992)	Two-boson systems with $m_1 \neq m_2$ and $V(x) = -g \exp(-ax)$.
Reiss (1992)	Strong EM fields in quantum optics, a review.
Roy and Basu (1992)	Electrical conduction in a 1D disordered system.
Roy and Khan (1992)	Tunneling through a double, rectangular barrier in 1D.
Schramm et al. (1992)	Exact Dirac propagator for the magnetic field of a peripheral collision, $\mathbf{B}= B\,\delta(z)\,\mathbf{e}_x$.
Semay and Silvestre-Brac (1992)	Two-body Dirac and QR equations for a quarkonium model with a Coulomb + confining power law potential. $h=(\boldsymbol{\alpha}_1-\boldsymbol{\alpha}_2)\cdot\mathbf{p}+\beta_2 m_1+\beta_2 m_2+W$, $W= -a/r+br^c(\beta_1+\beta_2)/2 + d$.
Semenov (1992)	A spin-½ neutral particle with an anomalous magnetic moment in a 2D $\mathbf{E}(x,y)$.
Sen Gupta (1992)	Dirac particle in a spatially periodic $\mathbf{B} = B_0 \sin kz$. Comment on Lovas and Molnár (1989).
Shen and Tao (1992)	Exact solution for a 2D Dirac particle with flux ½.

Table 2.4. (continued).

Shin et al. (1992)	Wigner formulation for spin-½ particles in Coulomb and cavity potentials.
Shishkin and Cabos (1992)	Separation of the Dirac equation in curvilinear coordinates for fields of various tensorial characters.
Stepanov and Tutik (1992b)	1/D expansion for the KG equation.
Tamura (1992)	Relativistic Green function for generally shaped and magnetically polarized cell potentials.
van Dijk (1992)	Exact solution of the Dirac equation for a $\beta V_s + V_v$ potential, containing momentum-space form factors $g_0 = 1/(p^2 + \Gamma^2)$ $g_1 = \Gamma p/(p^2 + \Gamma^2)^2$.
Wells et al. (1992)	3+1 D Dirac equation for lepton-pair production in relativistic heavy-ion collisions solved in a Cartesian lattice using splines. Au+Au at 2-100 GeV/nucleon.
Zhou and Rosenberg (1992)	Relativistic scattering of a charged particle from V(r) in presence of a strong, slowly varying multimode EM field.

Table 2.5. Relativistic virial theorems.

Reference	Comments
Bethe (1948)	Rederives $c\langle\boldsymbol{\alpha}\cdot\mathbf{p}\rangle + \langle V\rangle=0$ (2.11)[a] $E=mc^2\langle\beta\rangle$ (2.12) α^2 limits given.
Epstein and Epstein (1962)	Dirac-Coulomb recursion relations like $s\langle\alpha r^{s-1}\rangle=0$ $2\langle i\alpha\beta r^s\rangle-s\langle r^{s-1}\rangle-2k\langle\beta r^{s-1}\rangle=0$
Albeverio (1972)	VT for Dirac electron in external EM fields.
Kalf (1976)	Derives $\langle\boldsymbol{\alpha}\cdot\mathbf{p}\rangle = \langle r(dV/dr)\rangle$ for a class of potentials, including the Coulomb one, $V(r) = -Z/r,\ Z \leq 137$.
Herbst (1977) (ref. 1386)	A KG VT for a Coulomb field: $\langle V\rangle = \langle\mathbf{p}^2/(\mathbf{p}^2 + m^2)^{\frac{1}{2}}\rangle$. $E = \langle(\mathbf{p}^2 + m^2)^{-\frac{1}{2}}\rangle$.
Papp (1986c)	Quasiclassical approach to the VT.
Goldman (1987)	Use of the VT $E=mc^2\langle\beta\rangle$, (2.12), in variational energy optimization.
Vrscay and Hamidian (1988)	Hypervirial theorems give PT expansions for central-field Dirac problems.
Lucha and Schöberl (1990a)	Relativistic virial theorem for $T=(p^2+m^2)^{\frac{1}{2}}$: $\langle\mathbf{x}\cdot\nabla V\mathbf{x}\rangle=\sum_{i=1}^{2}\langle\mathbf{p}^2/(\mathbf{p}^2+m^2)^{\frac{1}{2}}\rangle$
Lucha and Schöberl (1990b)	Review.
Pyykkö (1991b)	Comments on relativistic virial theorems. Excellent reply by Ishikawa.
Shabaev (1991a)	Virial relations for off-diagonal radial matrix elements for a Dirac equation in a central field (M1 and E2 hfs integrals etc.) Coulomb field special case.
Luo and Qiu (1992)	VT for KG, Kemmer and spin-less Salpeter equations. KG: $\langle\mathbf{p}^2\rangle = \langle(E-V)(\mathbf{r}\cdot\nabla)V\rangle$.

[a]Equation numbers from Part 1.

3. QUANTUM ELECTRODYNAMICAL EFFECTS

Table 3.1. Higher-order corrections: methods.

Reference	Comments
Todorov (1973)	Recoil corrections and reduced mass in relativistic calculations (for antiprotonic atoms). (Borie and Jödicke 1988).
Gyulassy (1975)	Higher-order vacuum polarisation charge density for finite-radius nuclei.
Barbieri and Sucher (1978)	Radiative corrections to one-photon decay of H-like atoms. Example: 2s -1s.
Dubler (1978)	Calculation method for the vacuum polarisation potential of order $\alpha(Z\alpha)$.
Hossein Partovi and Jabbarian-Lotfabadi (1978)	New fermion-antifermion equation for positronium.
Silagadze and Khelashvili (1984)	Solvable relativistic two-fermion bound-state problem. No Klein paradox.
Hostler (1985b)	Scalar formalism for QED.
Shabaev (1985b)	Two fermions of masses m and M in QED. Mass corrections of order m/M for the limit m<<M without αZ expansion.
Au (1986)	Two-photon exchange in electron-atom scattering. R^{-6} changes to R^{-7} at asymptotic distances ($R>a_0/\alpha$).
Barut (1986)	Reply to comments on Barut and van Heule (1985) by Bialynicki-Birula (1986).
Barut and Strobel (1986)	Center-of-mass motion for a system of relativistic Dirac particles. Exact separation for N particles is possible.
Barut and Ünal (1986)	The two-fermion QED problem solved exactly up to order α^4.
Bialynicki-Birula (1986)	Comments on Barut and van Huele (1985).
Borie (1986)	The role of the fine-structure constant in QED.
Caswell and Lepage (1986)	Effective Lagrangians for bound-state problems in QED.
Dietz (1986)	Vacuum-induced Friedel-type oscillations in relativistic atoms.
Feldman and Fulton (1986, 1987)	Derive the DF, 1/Z and RRPA models from QED.
Grant (1986b)	Review on relativistic atomic theory and QED.
Ni (1986)	Exact solution of the Dirac equation in constant **E** and the electron-positron creation rate in vacuum.
Sazdjian (1986, 1987, 1988)	Two-particle wave functions.
Sucher (1986)	QED and relativity in atomic physics.

Table 3.1. (continued).

Van Alstine and Crater (1986)	Exact parapositronium-like solution to two-body Dirac equations.
Weitsman and Hagelstein (1986)	Self-energy in many-electron atoms.
Yilmazer (1986)	Relativistic two-fermion problem with the most general electric and magnetic potentials.
Holz (1987)	Self-energy of electrons in a Coulomb field: Momentum-space method.
Barut (1987)	Non-perturbative treatment of the Möller potential. Covariant equations for positronium and muonium.
Barut and Dowling (1987)	QED based on self energy, without 2nd quantization: Lamb shift and Casimir-Polder forces.
Barut and Pavsic (1987)	A Dirac electron in curved space.
Dietz (1987b)	A "g-Hartree" approach to QED of many-electron atoms.
Geiger et al. (1987)	A relativistic two-body equation for positronium.
Hostler (1987a)	Self-energy operator for an electron in an external Coulomb potential.
Ladányi (1987)	Scalar Bethe-Salpeter equation and relativistic bound states.
Landro et al. (1987ab)	Two-photon processes for relativistic electrons.
Malvetti and Pilkuhn (1987, 1989, 1990)	Atoms with several spinless particles or one spinless particle among electrons.
Mandelzweig and Wallace (1987)	QED-based two-body Dirac equation.
B. Müller (1987)	The many facets of the Dirac vacuum.
Pacher et al. (1987)	Retardation effects in radiative electron capture.
Sapirstein (1987)	QED of many-electron atoms: a Furry picture based on the many-electron field.
Srivastava and Widom (1987)	QED processes in electrical engineering circuits.
Su and Eberly (1987)	"Essential states" of spontaneous emission in the relativistic theory of electron-photon interactions.
Sucher (1987)	QED and relativistic many-electron Hamiltonians.
Au (1988)	Multipole, nonadiabatic and finite-nuclear-mass corrections for two-Coulomb-photon exchange.
Barut (1988)	Relativistic QM discussed.
Barut et al. (1988)	Self-field QED: g-2.
Barut and Salamin (1988)	Relativistic theory of spontaneus emission.
Bottcher and Strayer (1988)	"DF equations for the vacuum". Pair production in high-energy collision.

Table 3.1. (continued).

Braun (1988)	Decay law of unstable levels in QED. One- and two-photon transitions.
Grant and Quiney (1988)	Foundations of relativistic atomic and molecular theory.
Guo and Åberg (1988)	QED approach to multiphoton ionization in the high-intensity limit.
Hylton (1988)	Nuclear-size correction to the Lamb-shift in hydrogen.
Ionescu et al. (1988)	Nonlinear terms.
Ito (1988)	NR limit of the renormalized Bethe-Salpeter wave function at the origin.
Iwazaki and Kumano (1988)	Oscillations of the polarized vacuum around a large-Z nucleus. Searches neutral modes to explain the GSI positron peaks.
Leal Ferreira (1988)	A Dirac particle and its antiparticle, interacting through a ßmr linear scalar potential.
Liaw et al. (1988b)	QED-based theory for atomic energy levels and transitions.
Malenfant (1988, 1989)	The Breit equation for two equal-mass spin-½ particles. Radial equations and small-r behaviour derived.
Nakanishi (1988)	Solutions to the Bethe-Salpeter equation. Contains a 34-page bibliography, until 1987.
Zecca (1988)	Fine structure of equal-mass q-$\bar{q}$ systems.
Au (1989ab)	Transverse-photon exchange in He Rydberg states.
Barut and Dowling (1989ab)	QED without 2nd quantization. No wall effects on g-2 for a confined particle in magnetic field. The cyclotron frequency does change.
Barut and Duru (1989)	QED from classical particle trajectories.
Barut et al. (1989)	Scattering theory of relativistic composite particles.
Dietz and Hess (1989)	Derivation of "g-Hartree" equations from QED.
Kolsrud (1989)	The external field approximation of QED.
Królikowski (1989)	Analytic asymptotic solution for para (S=0) states of two equal-mass s=1/2 particles bound by the Coulomb attraction.
Lindgren (1989c, 1990)	Derives interelectronic potentials from QED. Explains the different results for Feynman and Coulomb gauges in MBPT as missing, irreducible multiphoton exchange.
Lindroth and Mårtensson-Pendrill (1989); Lindroth et al. (1989b)	Analysis of the complete Breit interaction.

Table 3.1. (continued).

Manakov et al. (1989)	Vacuum polarization by a strong Coulomb field. Analytical large-r potential given.
Mittleman (1989)	Theory for three-electron atoms from the Bethe-Salpeter equation. Includes a 3-electron term.
Pindzola et al. (1989)	Electron-impact ionization of highly charged ions in lowest-order QED.
Salomon (1989)	Monte Carlo integration of the Bethe-Salpeter equation in momentum space.
Sazdjian (1989)	N-body bound-state relativistic wave equations for spin 0 and/or ½ particles.
Scott et al. (1989)	Many-particle electrodynamics by symbolic manipulation.
Sucher (1989a)	Bound-state QED.
Sucher (1989b)	Potentials from field theory.
Veltman (1989)	Radiative corrections to polarized Compton scattering.
Barut (1990a)	The electron-positron system at short distances.
Barut (1990b)	Excited states of Zitterbewegung.
Barut and Dowling (1990a)	Self-field-based QED: Thermal radiation seen by an accelerating (a) observer ("Unruh effect"). $T_a = \hbar a/2\pi kc$.
Barut and Dowling (1990b)	Self-field QED on a two-level atom.
Barut et al. (1990)	The classical relativistic two-body problem with spin and self-interactions.
Barut and Ünal (1990)	Analytic evaluation of vacuum polarization in a Coulomb field.
Baur (1990)	Electron-positron pair production in relativistic heavy-ion collisions.
Blunden (1990)	Effect of the Dirac sea on a finite system.
Dykshoorn et al. (1990); Dykshoorn and Koniuk (1990)	Two-particle bound states in QED. Massive and massless cases. Ultra relativistic bound states.
Fainshtein et al. (1990)	Vacuum polarization by a Coulomb field. Analytical approximation of the polarization potential.
Feldman and Fulton (1990)	Log terms for leading radiative corrections to DF.
Leal Ferreira and Galeao (1990)	Two-body Dirac equation with nine different angle- and r-dependent potentials.
Shabaev (1990b)	QED theory for multiply charged ions.
L.-X. Xiao et al. (1990)	Bound-state equations for two spin-0 particles from QED. [KG] Coulomb limit derived.
Barut (1991)	The covariant many-body problem in QED.
Barut and Salamin (1991a)	2s-1s transition probability of hydrogen-like atoms, Z=1-92, from self-energy-based QED. Standard result obtained.

Table 3.1. (continued).

Barut and Salamin (1991b)	Einstein A-coefficients of spontaneous emission.
Bawin and Cugnon (1991)	"Partially screened solutions" for the Dirac equation in $Z>Z_c$ Coulomb fields.
Berseth and Darewych (1991)	Relativistic two fermion one anti-fermion wave equations.
Bialynicki-Birula et al. (1991)	Phase-space structure of the Dirac vacuum.
Blundell and Snyderman (1991)	Basis-set approach to the radiative self-energy in high-Z hydrogenic ions.
De Sanctis and Prosperi (1991)	A two-body equation for nucleons (pion exchange).
Dehnen and Shahin (1991)	Magnetically bound positronium states?
Eby (1991)	Production of low-energy electron-positron pairs by heavy ions.
Elkhovskii and Mil'stein (1991)	Vacuum polarization, induced by nuclear M1 and E2 multipole moments. Dirac-Coulomb Green function used.
Franosch and Soff (1991)	Influence of muonic vacuum polarization of strongly bound electrons.
Graf et al. (1991)	QED in strong fields: a review.
Guo and Åberg (1991)	Orthogonality and completeness of QED Volkov solutions.
Hagelstein (1991)	Partial-wave method for self-energy for non-hydrogenic electrons.
Lucha et al. (1991)	Fermion-antifermion bound states.
Malenfant (1991)	Approximate positronium solutions to the Breit-Coulomb equation through order $O(\alpha^4)$.
Moshinsky and López Laurrabaquio (1991)	Relativistic generalization of the Breit-Wigner two-particle formula, starting from two free KG or Dirac particles.
Pachucki (1991)	Time evolution in QED.
Pindzola et al. (1991)	Lowest-order QED theory using distorted wave states for inelastic electron scattering by highly charged ions.
Shabaev (1991b)	QED theory for the natural spectral line shape of resonance photon scattering on few-electron atoms.
Shvartsman (1991)	Lagrangian of a relativistic spinning particle in QED.
Tesevich (1991)	Vacuum polarisation potential for a finite nucleus near origin.
Thakur (1991)	Spin-0 - spin-(½) and spin(½)-spin(½) two-particle systems.
Thayyullathil (1991)	Fully covariant equation for the bound state problem in field theory. Positronium, compared with Dirac theory.
Zhdanov (1991)	Classical two-body problem including retardation.

Table 3.1. (continued).

Best et al. (1992)	Multiplicity distribution of electron-positron pairs created by strong external fields.
Blundell (1992)	Screened QED calculations on high-Z ions.
Capri and Roy (1992)	A vacuum for a Dirac particle in an external EM field.
Crater et al. (1992)	Nonperturbative solution of two-body Dirac equations in QED. (Applications on meson spectra.)
Darewych and Berseth (1992)	Two- and three-fermion systems in the Hamiltonian QED.
Elkhovskii et al. (1992)	Logarithmic corrections in the two-body problem in QED.
Engel et al. (1992)	Gradient expansion of Green functions of noninteraction particles.
Feinberg and Sucher (1992)	Spin-dependent two-photon exchange forces between a spin-0 particle and a charged spin-½ particle.
Feldman et al. (1992)	Leading radiative corrections to the DF approximation.
Galeao and Leal Ferreira (1992)	General method for reducing the two-body Dirac equation. Unequal masses.
Gorshkov et al. (1992)	QED theory of U^{90+} line shapes.
Greiner and Reinhardt (1992)	Book on QED.
Indelicato and Mohr (1992)	Coordinate-space approach to bound-electron self-energy in V(r), not necessarily Coulomb.
Kinoshita (ed.) (1992)	Book on precision tests on QED.
Klein and Dreizler (1992)	Relativistic two-body equations derived from QED. Equal-mass and Dirac particle + heavy mass limits taken.
Kluger et al. (1992)	Fermion pair production in strong, homogeneous, time-dependent electric field, E(t).
Li and Zhang (1992)	Spinor structures of the Bethe-Salpeter irreducible kernels.
Malik et al. (1992)	Relativistic terms in the reduction of the Bethe-Salpeter equation.
D. Miller et al. (1992)	Finite-element QED in 3+1 D.
Miyazawa and Tanaka (1992)	Relativistic two-body differential equation that reduces to the Dirac equation. Boundary conditions differ from Bethe-Salpeter.
Moore and Scott (1992)	Quantization of a QED Lagrangian via a 1/c series.
Pachucki (1992)	Higher-order binding corrections to the Lamb shift in H-like atoms.
Pilkuhn (1992)	Equal-time relativistic two-body equations for all combinations of spinless and Dirac particles.

Table 3.1. (continued).

Pindzola (1992)	Positron-impact ionization of highly-charged ions in lowest-order QED.
Seke (1992b)	Solution of the renormalization problem in NR QED.
Thakur (1992)	Classical mechanics of directly interacting relativistic particles.
T. Zhang et al. (1992)	Positronium FS and hfs to order α^5 from a new relativistic bound-state formalism for two fermions.

Table 3.2. Higher-order corrections: hyperfine interactions and magnetic moments.

Reference	Comments
Martynenko and Faustov (1987)	Hfs of muonium. Corrections of order $(Z\alpha)^2$ and $(m_1/m_2)\ (Z\alpha)^2$.
Milstein and Yelkhovsky (1990)	Vacuum polarisation by the nuclear quadrupole moment.
Zhang and Koniuk (1992)	Muonium hfs in a new bound-state formalism.

Table 3.3. Higher-order corrections: energy levels.

Reference	Comments
Hossein Partovi and Jabbarian-Lotfabadi (1978)	Positronium
Borie and Rinker (1982)	Muonic atoms.
Mohr (1983b)	n=1 and 2 states of H-like atoms, Z=10-40.
Borie (1984)	Vacuum polarization and fine structure in antiprotonic atoms.
Ayres (1986)	Fermion-antifermion bound states.
Indelicato (1986)	Various levels of Breit interaction and the 1s binding energy of He-, Ne-, Xe- and Rn-like ions, Z=100...170. SCF Gaunt term tested.
Mohr (1986)	Review on QED effects in many-electron and few-electron atoms.
Indelicato et al. (1987)	Radiative corrections for He-like ions.
W.C. Martin (1987)	Lamb shifts for 1sns and 1snp terms of He I. Various sources combined.
Passante and Power (1987)	Lamb shift in NR QED.
Quiney et al. (1987b)	SCF treatment of the Breit interaction advocated. He- and Be-like systems.
Adkins et al. (1988)	Three-photon contribution to positronium hyperfine interval.
Beier and Soff (1988)	The Källén-Sabry $\alpha^2(Z\alpha)$ contribution to the Lamb shift of H-like atoms, Z=1-110.
Borie and Jödicke (1988)	Energy levels of antiprotonic atoms.
Cheon (1988)	Casimir effect on the $2s_{\frac{1}{2}}$ - $2p_{\frac{1}{2}}$ Lamb shift of a hydrogen atom between two conducting plates.
Drake et al. (1988)	The Lamb shift of He^+.
Gorceix and Indelicato (1988)	Effects of the complete Breit interaction on 1s2s and 1s2p He-like systems, Z=6...92.
Mohr (1988a)	Review on QED calculations on H-like atoms.
Mohr (1988b)	H- and He-like atoms.
Sallhofer (1988, 1989a-c) 1990 ab)	Hydrogen in QED.
Silver (1988)	Precision spectroscopy on 1- and 2-electron ions of medium and high Z.
Soff and Mohr (1988)	Vacuum polarization for finite nuclei. H-like atom K- and L-shells,Z=30...170.
Adkins (1989)	Review on positronium bound states.
Grotch (1989)	Status report on the Lamb shift.
Kim (1989)	Breit correlation in Al-like ions.
Manakov et al. (1989)	Vacuum-polarisation effects on H-like energy levels.
Mohr (1989a)	QED as a perturbation in relativistic MBPT.

Table 3.3. (continued).

Mohr (1989b)	High-Z few-electron atoms.
Petelenz and Smith (1989)	Vacuum polarization in muonic molecules, ppμ, ddμ etc., using the Uehling potential. Earlier values underestimated 2-8 times.
Plunien et al. (1989)	Nuclear polarisation contribution to the Lamb shift in heavy atoms. For $1s_{\frac{1}{2}}$ of $_{92}U^{238}$, a nuclear rotator, the shift is about 1 eV. For $_{82}Pb^{208}$ a vibrator, about 0.1 eV is obtained.
Sapirstein (1989a)	Two-photon exchange graphs for He-like systems in the Furry picture.
Sapirstein (1989b)	Rewiev.
Schmidt et al. (1989)	Muonic 1s - 5g levels in atoms with Z = 30-100. Vacuum polarization to order $\alpha(Z\alpha)^n$, $n\geq3$ included.
Seely (1989)	QED contributions to the 2p-2s transition energies of Li-like ions.
Soff (1989)	Vacuum-polarization charge densities for spherically symmetric external potentials.
Soff and Mohr (1989)	Vacuum-polarization corrections for H-like U.
Yennie (1989a)	Recoil effects in H-like bound-state problems.
Yennie (1989b)	PT approach to many-electron energy levels.
Doncheski et al. (1990, 1991)	Lamb-shift in H-like atoms.
Drake and Swainson (1990)	Bethe logarithms for H, $n\leq20$. Approximations for 2-electron atoms.
Ishikawa (1990a)	Be-like ground states, Z=4...50, with SCF Breit term.
Radozycki (1990a)	The EM virtual cloud in the H atom ground state.
Radozycki (1990b)	The $2p_{3/2}$ state.
Blaive et al. (1991)	Discrete-state contribution to the Lamb shift in hydrogen atoms.
Cheng et al. (1991)	Screened Lamb-shifts for Li-like U, Na-like Pt and Cu-like Au.
Eberlein (1991)	Level shifts for a hydrogen atom between two conducting plates.
Hersbach and Ruijgrok (1991)	Quasipotential theory for H-like atoms.
Indelicato and Mohr (1991ab)	QED effects in atoms. Effect of electron interactions on the self energy.
Mohr (1991)	Lamb shift for the n=4 state of He^+.
Plunien et al. (1991)	Nuclear polarisability and the Lamb shift.
Soff (1991)	Review on few-electron atoms.
Snyderman (1991)	Electron radiative self-energy for large $Z\alpha$. H-like atoms treated, others discussed.
Barut et al. (1992)	Lamb shift in self-field QED.

Table 3.3. (continued).

Blundell (1992)	Screened QED calculations in high-Z ions.
Bukowski et al. (1992)	Bethe logarithm and Lamb shift for H_2^+ and isotopic species.
Drake and Yan (1992)	Rydberg levels of He.
Goldman and Drake (1992)	Rydberg levels of He. Long-range Casimir-Polder effects seen.
Komachiya and Fukuda (1992)	On-shell QED expansions for energy levels of H-, He- and Li-like atoms.
Mohr (1992)	Self-energy correction to n=1, 2 levels of H-like atoms, Z = 5-110.
Mohr and Kim (1992)	Self-energy of excited states (n=3-5) in a strong Coulomb field, Z =10-110.
Zhang and Koniuk (1992)	Muonium FS splitting in a new bound-state formalism.

Table 3.4. Higher-order corrections: interatomic and -molecular interactions.

Reference	Comments
Meath and Hirschfelder (1966b)	Retarded intermolecular forces.
Bernabéu and Tarrach (1976)	Interactions between two particles, at least one of them spinless and at least one neutral.
Golshan and Kobe (1986)	Retarded interactions between nonidentical two-level atoms.
Plunien et al. (1986)	Review on the Casimir effect.
Spruch (1986)	Review on the retarded, Casimir long-range potentials.
Barut and Dowling (1987)	Casimir-Polder forces from "QED without 2nd quantization".
Milonni et al. (1988)	Interpretation of the Casimir force between two parallel, conducting plates.
Mosteepanenko and Trunov (1988)	Review on the Casimir effect.
Babb et al. (1992)	Casimir shifts for He-like low-Z Rydberg ions.
Milonni and Shih (1992)	Source theory of the Casimir force.

4. MULTIELECTRON ATOMS: METHODS

Table 4.1. General methods and basic theory for multielectron atoms. See also Table 1.1. for general references and the Table 3.1 for QED aspects.

Reference	Comments
Fock (1933,1934)	The exchange energy for Dirac electrons.
Johnson Jr. and Breit (1933)	Breit interaction for one electron outside closed shells.
Breit (1937)	Approximately relativistic equations for nuclear particles.
Brown and Schaefer (1956)	Expansion in angular momenta in bound-state PT.
Malli and Saxena (1971)	Spin-spin interactions in f^4 configurations.
Braun and Parera (1985)	Bethe-Salpeter equations for two-electron atoms.
Parera López et al. (1985); Parera and Grave de Peralta (1987)	Relativistic electron-pair theory in multielectron atoms.
Braun and Parera (1986)	TP between degenerate levels in a many-electron atom.
Chang et al. (1986)	Two-component Pauli-like effective Hamiltonians in Dirac theory. Tested on H-like atoms and on rare-gases.
Feldman and Fulton (1986,1987);	Derive the DF, 1/Z and RRPA models from QED.
Fulton (1987,1989)	Fundamentals of basis-set Dirac calculations.
Grant (1986a)	Advocates self-consistent treatment of the Breit term.
Heully et al. (1986a)	Transformed 1- and 2-electron Dirac Hamiltonians for MB calculations.
Heully et al. (1986b)	Unsuitable positive-energy projection operators for 1-electron atoms introduce negative-energy states, don't remove them.
Rosenberg and Spruch (1986)	Extremum principles for relativistic bound-state energies.
Rutkowski (1986c)	New PT approach for two-electron atoms.
Sazdjian (1986)	Relativistic wave equations for systems of two (spin 0 or ½) particles.
Sebastian (1986)	Relativistic invariance of the two-photon transition amplitude of a composite system.
Sucher (1986-1989ab)	Relations of the many-electron Hamiltonian to QED.

Table 4.1. (continued).

Blundell et al. (1987b)	1st, 2nd and 3rd-order MBPT formulae for one-valence-electron atoms.
Brown (1987a)	Review on the relativistic atomic many-body problem.
W.Q. Chen and Cook (1987)	Quasirelativistic treatment of nuclear motion in atoms and molecules.
Crater and van Alstine (1987)	Two-body Dirac equations for particles interacting through world scalar and vector potentials.
Glöckle et al. (1987)	A solvable 2-fermion 1D model with δ-function interaction. Lorentz-boost operator constructed.
Goldman (1987)	Accelerated variational convergence in DF-LCAO calculations by a virial-theorem method.
Grant (1987)	Relativistic electron-electron interaction.
Lindgren (1987a)	Relativistic many-body problems: proceedings of Trieste, 1986.
Lindgren (1987b)	The NR and R coupled-cluster approaches: a review.
Lindgren and Lindroth (1987)	Review on R MBPT.
Lindroth (1987a-c)	The relativistic pair equation.
Lindroth et al. (1987)	A relativistic pair equation, projected onto positive-energy states. Permits higher-order Breit corrections.
L.D. Miller (1987)	FW reduction of the DF equations for atoms.
Olsson and Lindgren (1987)	Analyse the FS and hfs tensor operators needed in relativistic MBPT.
Sapirstein (1987)	QED of many-electron atoms: a Furry picture based on the many-electron field. MBPT. Quotes Mohr (1986), Labzovskii (1970ab).
Broyles (1988)	Relativistic propagator for a multi-electron atom consisting of n spin-½ fermions of different masses.
Coutinho et al. (1988b)	A "two-body Dirac equation" in 1D for various interaction potentials.
Datta and Devaiah (1988)	The minimax technique in relativistic HF calculations.
Drake and Goldman (1988)	Finite-basis-set-methods in atomic physics.
Grant (1988a)	Review on high-Z atoms.
Grant (1988b)	Review on relativistic atomic calculations.
Grant and Quiney (1988)	Foundations of relativistic atomic and molecular theory.
Johnson (1988)	Review on RRPA.
Johnson et al. (1988a)	B-spline Dirac basis.
Liaw et al. (1988b)	QED-based theory for atomic energies and transitions.
Lindgren (1988)	A relativistic MBPT in Feynman gauge.

Table 4.1. (continued).

Lindroth (1988)	Numerical solutions of the relativistic pair equation.
Pilkuhn (1988)	A "Kramers-type" equation for two spin-1/2 particles in an external field derived from the Breit equation.
Quiney (1988); Quiney et al. (1989c, 1990)	Relativistic MBPT.
Shabaev (1988)	Nuclear recoil effects for multicharged ions.
Bagrov and Obukhov (1989)	Separation of DF equation.
Broyles (1989)	Continuum dissolution discussed. Positive-energy states propagate forward in time, $E<-mc^2$ states backwards. Therefore no danger of continuum dissolution.
Chaix and Iracane (1989)	From QED to DF.
Chaix et al. (1989)	Variational stability of the QED vacuum in the mean-field theory.
Chang and Chung (1989)	Electron correlation due to intrashell core excitation and intershell core-valence interaction.
Darewych and Horbatsch (1989,1990)	Two-body Coulomb systems of spin 0, ½.
Datta (1989)	Relativistic equations of motion method.
Hess and Ohno (1989)	The g-Hartree method tested on Be and Ne.
Jankowski and Rutkowski (1989)	Double-PT for relativity and correlation. Applications for He, Be- and Ne-like systems ($Z\leq 80$) and for Zn^{2+}.
Jansen and Hess (1989b)	Test the 'no pair' Hamiltonian of Hess (1986) on Au.
Johnson et al. (1989b)	Relativistic, QED and PNC effects in atoms: The Santa Barbara 1988 workshop.
Lindgren (1989ab)	Reviews on relativistic MBPT.
Lindgren (1989c,1990)	Derivation of interelectronic potentials from QED. Explains the different results for Feynman and Coulomb gauges in MBPT as missing, irreducible multiphoton exchange, see next entries.
Lindroth and Mårtensson-Pendrill (1989); Lindroth et al. (1989b)	Analysis of the complete Breit interaction, cp. Gorceix and Indelicato (1988). Excitations <u>from</u> $\epsilon<0$ states are allowed, excitations <u>into</u> them not.
Mårtensson-Pendrill (1989ab)	R/NR pair-correlation theory. Numerical solution in a 2D grid. Projection operators needed. Applications discussed.
Mittleman (1989)	Theory for 3-electron atoms from the Bethe-Salpeter equation.
Nicolaides (1989)	"State-specific theory".
Oreg et al. (1989)	Configuration-average energy shift owing to CI. Both ls and lsj coupling.

Table 4.1. (continued).

Polyzou (1989)	Relativistic two-body models.
Roothaan (1989)	Discusses retardation effects and the many-electron Dirac problem.
Rosenberg (1989)	Virtual-pair effects in atomic theory.
Salomonsson and Öster (1989)	Relativistic all-order pair functions from discretized single-particle Dirac functions. N^3 operations needed for N radial lattice points. Convergence to $0.075\alpha^2(l+\frac{1}{2})^{-2}$.
Sampson et al. (1989)	A new DS program for highly charged ions.
Schwarz et al. (1989)	The radial origin of direct and indirect relativistic effects in atoms analysed.
Shadwick et al. (1989)	A method optimizing variationally the relativistic atomic potential. Equivalent to DF.
Tisenko (1989)	Dul'yan-Faustov pseudopotential equation for the He atom FS.
Bijtebier (1990ad)	Three-fermion bound states: separable equations.
Bijtebier (1990b)	Scattering from a relativistic bound state.
Bijtebier (1990c)	Two relativistic fermion bound states in a potential.
Cheung and Li (1990)	A two-body Dirac equation with phenomenological potentials. Reduced to two coupled 2nd-order equations. Klein paradox discussed.
Darewych (1990)	Three-fermion wave function with Coulomb interactions.
Kim (1990)	Relativistic and QED effects in highly-charged ions.
Migdalek (1990)	Book on model potentials for atoms.
Scott et al. (1990)	PT by symbolic computation.
Sneddon and Whittingham (1990)	Radial matrix elements involving continuum Dirac functions.
Styszynski and Karwowski (1990)	Screening constants in MCDF.
Franosch and Soff (1991)	Influence of nuclear shape and of muonic vacuum polarization for strongly bound electrons.
Gaida et al. (1991)	Changing centers-of-mass in the relativistic Lagrangean mechanics of a system of particles.
Grant (1991)	Review on relativistic basis-set calculations.
Hamacher and Hinze (1991)	"Finite-volume variational method" for the Dirac equation.
Johnson (1991, 1992)	Review on R MBPT.
Kagawa et al. (1991)	STO-basis-set CI theory.
Lindgren (1991)	Review on R MBPT.
Liu and Kelly (1991)	MBPT, based on MCDF.
Parpia and Mohanty (1991)	Theory part for the MOTECC 91 atomic program MCGDFB.

Table 4.1. (continued).

Samzow and Hess (1991)	Two-electron terms in the "no-pair" Hamiltonian.
Avgoustoglou et al. (1992)	MBPT formulae through 3rd order for 1-particle-1-hole excited states of closed-shell atoms.
Crater and Van Alstine (1992)	Two-body interactions by classical relativistic field theory.
Grant (1992)	Review on basic theory.
Hersbach (1992)	A momentum-space theory for two spin-$\frac{1}{2}$ particles. Arbitrary mass ratio. Reduces to the Breit equation.
Lister and Judd (1992)	Matrix elements of the spin-other-orbit operators in the atomic f shell.
Parpia et al. (1992b)	Nuclear-motion corrections for the GRASP2 package. Ne-Rn.
Scott et al. (1992)	Accurate (18-figure) (1D) FEM solution of the two-body Dirac equation with static Coulomb interactions.
Szász (1992)	Book on HF-(or DF-) level atomic theory.
Uylings (1992)	Second quantization for atoms in various angular-momentum couplings.

Table 4.2. Published programs for atoms. For a more detailed review of pre-1979 programs, see Grant (1979). Further non-relativistic programs with relativistic perturbation are listed there.

Reference	Comments
Rinker (1979)	Energy levels and transition intensities in muonic atoms. Dirac equation solved in finite nucleus potential + Uehling + Källen-Sabry potential.
Fraga et al. (1987)	A Breit-Pauli-level CI program. Uses numerical radial functions from Froese Fischer's program.
Joc and Bojara (1987)	A PC version of Desclaux' code.
Bieron (1988)	PC version of Grant's atomic program.
Band et al. (1989b)	The RAINE package. Includes EM transitions and nuclear processes.
Dyall et al. (1989b); Parpia and Grant (1989)	GRASP: The Oxford MCDF package.
Dzuba (1989)	The Novosibirsk atomic package.
Scott et al. (1989)	Many-particle electrodynamics by symbolic manipulation.
Shadwick et al. (1989)	A program for variational optimization of atomic potentials. Equivalent to DF.
Froese Fischer (1991a)	A MCHF package including Breit-Pauli corrections.
Froese Fischer (1991b)	A BP CI program for the MCHF package.
Froese Fischer and Godefroid (1991)	Transition probability program, LS and LSJ. EL and ML transitions.
Hibbert and Glass (1991)	A program for angular integrals of the Breit-Pauli Hamiltonian.
Mohanty et al. (1991b); Parpia and Mohanty (1991)	The MOTECC 1991 atomic GTO basis programs.
Perger and Karighattan (1991)	A continuum wave function solver for the package of Grant.
Salvat and Mayol (1991)	Accurate numerical solutions of Dirac equations for central fields.
Kagawa (1992)	Program for fractional parentage coefficients of jj-coupled states.

Table 4.3. Numerical, non-statistical four-component methods.

Reference	Comments
Rabin (1982)	Solves the lattice fermion doubling problem.
Stacey (1982)	Elimination of fermion doubling. Used for atoms by Salomonsson and Öster (1989).
Kogut (1983)	"Fermion doubling": spurious states for a discretized Dirac eqation.
Heully (1985)	Thesis on relativistic MB calculations.
Johnson et al. (1988a)	Finite B-spline basis-set for Dirac equation.
Salomonsson and Öster (1989)	Ways to remove spurious states from discretized basis functions.
Durand and Gara (1990)	Matrix methods for the numerical solution of relativistic wave equations.
Jaskólski et al. (1990)	Outward integration procedure for QR radial equations.
J. Wu et al. (1990)	Numerical methods for TD nuclear Dirac equations in 3+1 or 1+1 dimensions.
Perger et al. (1991)	Numerical treatment of continuos functions a frozen DF potential.
Cai et al. (1992)	Extension of GRASP, the Oxford MCDF code, to thousands of configurations.

Table 4.4. Four-component LCAO approaches for many-electron atoms. For one-electron atoms, see Tables 2.3. and 2.4.

Reference	Comments
Goldman and Dalgarno (1986)	A method avoiding spurius roots, variational collapse and continuum dissolution. He, Ne^{8+}; Ne^{6+}; Ne^{4+}. STO-basis.
Grant (1986ab)	Fundamental theory for basis-set work. He-like and Be-like systems, Ne. SCF vs. PT Breit.
Krause (1986)	He-like systems, Z=2-100. Screened hydrogenic basis in a variational treatment.
Y.S. Lee (1986)	An approximation, neglecting small-component Coulomb and exchange contributions. Test on I^{n+}.
Y.S. Lee and Baeck (1986)	Conditions for kinetic balance tested on U^{90+}.
Mark (1986)	GTO basis sets for H-Ne.
Hegarty and Aerts (1987)	Ne.
Matshuoka (1987)	Nuclear attraction integrals for GTOs for a homogeneously charged spherical nucleus.
Matsuoka and Huzinaga (1987)	Well-tempered (geometric series, $\alpha=\alpha_0\beta^{n-1}$, n=1-N) GTO basis calculations for He-Ar, Ag, Xe. Finite nuclei.
Mukoyama and Lin (1987ab)	STO-basis applied for the Dirac equation in a DS potential. One spurious root for kappa > 0.
Mukoyama and Lin (1987c)	Inner-shell ionization in ion-atom collisions.
Quiney (1987); Quiney et al. (1987a)	Finite-basis studies of the Dirac equation.
Quiney et al. (1987b)	SCF treatment of the Breit interaction. He- and Be-like systems.
Baeck and Lee (1988)	Open-shell DF-LCAO. Boron SO splitting.
Datta and Devaiah(1988); Datta and Madhusudana Rao (1988)	He.
Goldman (1988a)	He, Be, C and Ne sequences using a method avoiding spurious roots. Breit terms also included.
Goldman (1988b)	Variational treatment of the Breit terms.
Ishikawa and Sekino(1988)	Be, Ne with various GTO basis sets and finite nuclei.
Goldman (1989a)	Accurate polarizabilities for 1-electron atoms, Z=1...115, by a gauge-invariance method.

Table 4.4. (continued).

Grant (1989)	Assessment of basis-sets for Dirac and QED calculations.
Ishikawa et al. (1989)	Be, Ne^{6+}, Ar^{14+}, Ne. Up to 3rd-order MBPT with a GTO basis.
Y.S. Lee et al. (1989)	STO basis-set recipes for Li-F, Na-Cl, U^{82+}.
Matsuoka (1989)	Comments on "unified" and "separated" basis spinors: equivalent.
Matsuoka and Okada (1989)	Tl-Rn using a well-tempered GTO basis.
Mohanty and Clementi (1989a)	DF-GTO finite-nucleus results for He-Ar, Xe, Rn.
Mohanty and Clementi (1989b)	Reviews on GTO relativistic calculations for atoms.
Okada and Matsuoka (1989)	Well-tempered GTO basis for He-Hg.
Quiney et al. (1989a)	Ar-like systems.
Quiney et al. (1989b)	Review.
Quiney et al. (1989c)	Relativistic MBPT.
Sekino and Ishikawa (1989)	MBPT on Ne.
Baeck and Lee (1990)	Al SO.
Ishikawa (1990a)	Be-like ground states, Z=4, 10, 18 and 50, with SCF Breit term.
Ishikawa (1990b)	He-like ground states, Z=2...50. Ne, Ar. MBPT.
Ishikawa (1990c)	Summarises Ishikawa (1990ab).
Ishikawa and Sekino (1990)	Variational bounds for finite c and finite nuclei. C, Hg^{74+}, Hg.
Ishikawa et al. (1990)	Effects of GTO contraction. Ne, Ar, Ge.
Kumar et al. (1990)	K- and L-shell ionization of Au by H^{+}, He^{2+} impact.
Matsuoka (1990a)	A finite-nucleus model with constant dV/dr proposed for STO basis. $V(r)=v_0 + v_1 r$, r< R. Tests on H, Ag^{46+}, H^{79+}.
Mohanty and Clementi (1990a)	Kinetically balanced geometric (well-tempered) GTO basis sets for Z=2-86. Single-configuration DF results compared to numerical ones.
Okada et al. (1990)	Well-tempered GTO basis for He-Hg. DF + Breit at SCF level.
Quiney (1990ab, 1991)	Reviews on relativistic finite-basis calculations.
Sekino and Bartlett (1990)	Coupled-cluster E for Be-like systems, Z=4...50. No essential contributions beyond MBPT(4).
Grant (1991)	Review on basis-set atomic calculations. Hg with SCF versus PT Breit.
Ishikawa (1991a)	Kr. Up to 3rd-order MBPT with GTO basis.
Ishikawa (1991b)	Review on basis-set DF and MBPT calculations.

Table 4.4. (continued).

Ishikawa (1991c)	Effects of GTO basis-set contraction on relativistic and Breit energies. Be...Sr.
Ishikawa and Binning (1991)	Ar.
Ishikawa et al. (1991)	DFB GTO solutions for He-Xe, Be-Sr.
Kagawa et al. (1991)	STO-basis-set CI theory. Applications on Ne-like ions, Z=18...54.
Mohanty et al. (1991b)	Review on atomic basis-set calculations. Description of the MOTECC 1991 program REATOM.
Mukoyama and Lin (1991)	Virtual orbitals used to describe continuum states in ionization during ion-atom collisions.
Visser et al. (1991)	An open-shell GTO DF program tested on C and Sn atoms.
Wilson (1991)	Review on relativistic MBPT. Gives details on Ar ground-state E.
Datta (1992)	Minimax techniques for two-electron atoms.
Goldman (1992)	Fundamentals of basis-set approach tested on the Dirac-Coulomb case.
Ilyabaev and Kaldor (1992)	E of He-Xe and Be. CC using a no-pair Hamiltonian. GTO basis.
Ishikawa (1992a)	E of Xe. MBPT with well-tempered GTO.
Ishikawa (1992b)	Xe pair correlation energy.
Ishikawa et al. (1992b)	DF-Breit on Yb, Hg, Pb, Rn.
Matsuoka (1992)	I, Au. Contractions tested.
Malli et al. (1992)	He...Xe using a "universal" (18s, 12p, 11d) basis.
Parpia and Mohanty (1992)	Finite-nucleus calculations with a Fermi-distribution for He-like ions, Z=10...160. Hg.
Parpia et al. (1992)	DF and DF-Breit E of $(ns)^2$ and $(np)^6$ systems, He...No; H^-, F^- - At^-.

Table 4.5. Various four-component local-density methods.

Reference	Comments
Liberman (1968)	An exchange potential tested on Ar and Hg.
Euwema and Stukel (1971)	Several density functionals tested on E of He-Xe.
Ramana and Rajagopal (1981c)	Theory of spin polarised inhomogeneous relativistic electron gas.
Datta (1987)	Relativistic extension of the Hohenberg-Kohn theorem.
Dreizler et al. (1987)	Relativistic density functional theory.
Baltin and March (1988)	Relativistic electron gas in a weak local potential.
Y.-F.Guo and Whitehead (1988, 1989ab)	Several LSD potentials implemented at QR (Cowan-Griffin) level.
Glushkov (1989)	LDF model including BP terms.
Sampson et al. (1989)	An accurate DS program for highly-ionized atoms. Big mesh, 2nd-order Dirac equation used. QR option.
Sen et al. (1989b)	A "Z-transition state" concept for energy differences of isoelectronic atoms and molecules. QR. $Z^* = (Z_A + Z_B)/2$.
Dietz and Hess (1990)	Inhomogeneous many-electron systems and the "g-Hartree" method.
Dreizler and Gross (1990)	Book on density functional theory.
Glushkov (1990)	An expression for the electron-electron repulsion potential.
Dietz and Hess (1991)	HF-type equations from QED with non-linear gauge fixing.
Guo and Whitehead (1992)	Ne-Rn treated at NR/QR/R Ξ level.

Table 4.6. Thomas-Fermi calculations

Reference	Comments
Malzacher and Dreizler (1986)	Discuss the non-integrable density of relativistic TF models.
March (1986)	Applies relativistic TF theory on bond lengths of CH_4-PbH_4.
Engel and Dreizler (1987); Engel et al. (1987)	Relativistic density-functional theory including gradient corrections ("TFDW"). Derivation from field theory.
S.H.Hill et al. (1987)	Statistical inclusion of h_d and H_B in RTF theory. Results compared with DF ones for Cu-like systems, Z=29...58 and neutral atoms, Z=20...120.
Engel and Dreizler (1988, 1989)	Solution of the RTFDW model for atoms and positive ions.
Englert (1988)	Semiclassical theory of atoms. Book.
March (1988)	Approximate R electron densities from NR TF theory.
Membrado et al. (1988)	Relativistic TF potential outside a surface.
Leung and Pei (1989)	High-density expansions of the relativistic TF equation.
March (1989)	Relativistic TF theory: a review.
H.Müller et al. (1989)	Extension of the relativistic TFDW model to arbitrary external fields.
Yonei (1989)	Relativistic TF models of compressed atoms: Fe and Au. Significant R/NR differences at high compression, even for light atoms.
Centelles et al. (1990)	Relativistic TF with $\hbar^2$ corrections for nuclei.
Pohlner and Dreizler (1991)	Fourth-order gradient corrections to the relativistic Thomas-Fermi-Weizsäcker model.
Stroucken and Dreizler (1991)	Relativistic TF theory at finite temperatures.
Cinal and Englert (1992)	The Scott (1952) nuclear singularity correction in momentum space. Hg.
Von-Eiff and Weigel (1992)	Nuclear RTF model with quantum corrections.
Von-Eiff et al. (1992)	Relativistic TF model for nucleons in a vector and scalar potential.

Table 4.7. Independent-particle models. See also Table 2.4.

Reference	Comments
Bohr and Coster (1923)	Introduce a screening parameter, δ, for the Sommerfeld relativistic term $E = -[(Z-\delta)/n]^4[n/k-3/4]/2c^2$.
Parker (1986)	Inner-shell energy levels with $V = -Z_{eff}/r$ for every shell, plus corrections.
Zapryagaev et al. (1986)	Relations between the quantum defects, phases and the Green function.
Ivanov and Safronova (1987a)	Screening parameters and relativistic corrections.
Johnson (1987)	Parity violation using several model potentials (Tietz, Green, Norcross).
Lombardi (1987)	Na valence levels. Determines quantum defects and core polarizabilities.
Salvat et al. (1987a)	A 5-parameter MP consisting of three Yukawa potentials for Z=1-92, fit to DS.
Churilov et al. (1988)	n=4, _n=4 transitions of Ni- and Zn-like ions, Z=30 - 50.
Glushkov (1988)	A model for multielectron atoms, based on screened Coulomb functions.
L.N. Ivanov et al. (1988)	Review on multicharged ions.
Johnson et al. (1988a)	B-spline basis used with a Tietz potential for Cs and Tl.
Laughlin and Victor (1988)	Review on model-potential methods.
Malinovskaya (1988)	Cl-, Ar- and K-like ions, Z=19-36.
Rogers et al. (1988)	A parametric potential of Yukawa terms plus long range Coulomb tails, fit to QR calculations. Both neutral and highly ionized atoms considered.
Zapryagaev etal. (1988)	Polarizabilities of Li- and Na-like ions using a quantum defect method.
Bao et al. (1989)	Quantum defects for s, p, d, f and g states of ions with $2 \leq Z \leq 95$.
Martin (1990); Martin and Karwowski (1991)	Quantum-defect orbitals for valence, Rydberg and continuum atomic states.
Qiu and Li (1990)	Energy levels for a Dirac electron in a spherical TF potential, confined to radius R_w. Fe as example.
Glushkov (1991b)	Ga-like systems, Z = 31-36.
Glushkov (1992ac);Malinovskaya and Glushkov (1992)	K-, Rb- and Cs-like systems.
Glushkov (1992b)	Kr, Xe. Claims to find positive EA.
Loginov (1992)	$5d^9 6p$ levels of Tl IV-Br VI.
Misra et al. (1992)	Parametrized formula for x-ray spin doublets.

Table 4.8. Definitions, reviews and background for effective potential calculations.

Reference	Comments
Marketos (1989)	Discusses theoretical justifications for atomic, Phillips-Kleinmann-type calculations.
Migdalek (1990)	Book on model potential methods for atoms.
Walzer (1990, 1991ab)	Radial and energetic atomic parameters derived from the PP of Bachelet et al. (1982) for classifying binary intermetallic compounds.

Table 4.9. Effective-potential methods. For a comprehensive summary of work on molecules, see Table 7.7. Other tests on atoms are also given in references there and in ch. 5.

Reference	Comments
Taksar et al. (1971)	A simple PP for Na valence transitions.
Durand (1986a)	Core-valence correlation in PP metods: a review.
Grave de Peralta and Boada (1986)	Discuss pseudopotentials for one- valence-electron atoms.
Syromyatnikov and Savicius (1986)	Semiempirical, relativistic method for atomic energy levels.
Durand and Malrieu (1987)	A review on effective-Hamiltonian theory.
Hurley and Christiansen (1987)	PP QMC, applied on Li and K EA.
Mohan and Hibbert (1987)	A 2-electron MP for 6s-6p transitions of Hg.
Silberbach (1987)	Semiempirical PP for Ba, Au, Hg, Tl and Pb fit to three lowest s, d and f states.
Ermler et al. (1988a)	Review.
Fuentealba et al. (1988)	Correlation energy differences between N- and (N-1)-electron systems from a polarization potential.
Gropen (1988)	Review.
Laughlin and Victor (1988)	Review on model potentials for 1- and 2-valence-electron atoms.
Dolg (1989)	Energy-adjusted QR PP for Ln. 4f in core.
Hamann (1989)	Generalized norm-conserving pseudopotentials for arbitrary electron energies. Tested on bulk BaSe. Avoids problems with f-resonances for Ba in a plane-wave expansion and with multiple reference states for various l.
Hibbert (1989)	Reviews model potentials in oscillator -strength calculations.
Bylander and Kleinmann (1990)	4f resonances of Ba using a norm-conserving PP.
Masovic (1990)	A SO PP for band-structure calculations.
Milman et al. (1990)	Relativistic PP for transition-metal atoms. Four-component DFT. M, M^+, M=Sc-Cu, Y-Ag, Lu-Au.
Sellers and Ove (1990)	Anisotropic PP for modelling partially filled d shells.
Mitás et al. (1991)	Nonlocal PP in QMC. Si, Sc and Cu IP and EA.
Fernandez Pacios (1992)	Ar-core PP for Sc-Cu, improved valence excitation energies.

Table 4.9. (continued).

Flad et al. (1992)	Cartesian Gaussian projection operators for quantum Monte Carlo.
Leininger et al. (1992)	K-Cs, Ca-Ba and Fe-Os valence levels as tests of the Barthelat-Durand, Christiansen, Hay-Wadt and Stoll-Preuss PP.
Seijo et al. (1992)	Correct valence orbital nodal structure required for valence E_{corr} of X^-, X, X^+; X = F-I.

Table 4.10. Available relativistic effective potentials. QR = quasirelativistic (one-component), DF = Dirac-Fock, LD = local density, SO: spin-orbit perturbation potential given.

Reference	Comments
Greenside and Schlüter (1983)	$_{21}$Sc-$_{29}$Cu. LSD. SO.
Hurley et al. (1986)	$_{19}$K-$_{36}$Kr. V_{SO} included. Both Ne- and Ar-like cores included for Sc-Kr.
Dolg et al. (1987a)	Sc-Zn with a Ne-like core.
G.Durand et al. (1987)	Hg.
La John et al. (1987)	$_{37}$Rb-$_{54}$Xe, including V_{SO}.
Sakai et al. (1987a)	The nd-transition metals $_{21}$Sc...$_{80}$Hg. Only the valence s and d electrons in valence space.
Sakai et al. (1987b)	Ditto. The semicore p-shell also in valence space.
Schwerdtfeger (1987)	Tl.
Wadt (1987)	Pu.
Igel-Mann et al. (1988a)	Main-group elements in groups 13-17, n=2-5 ($_5$B to $_{53}$I).
Jasien and Stevens (1988)	$_{24}$Cr.
Dolg (1989)	Ln, 4f in core.
Dolg et al. (1989a)	Ln, Ce-Yb. Valence space from $4s^2$ up. SO potential given.
Dolg et al. (1989c)	Ln, La-Lu. Valence space from $5s^2$ up.
Schwerdtfeger et al. (1989b)	R/NR 19-e PP for Au.
Schwerdtfeger et al. (1989c)	R/NR Pb. SO.
Strömberg et al. (1989)	R/NR Cd and Hg.
Andrae et al. (1990)	QR and SO potentials for 4d and 5d metals ($_{39}$Y-$_{48}$Cd,$_{72}$Hf-$_{80}$Hg).
Cristiansen (1990)	Al. SO included. Core polarisation tested.
Kaupp et al. (1990a)	Zn 2-el. PP.
Musolino et al. (1990)	Sb. DFT.
Ross et al. (1990)	$_{55}$Cs-$_{57}$La, $_{72}$Hf-$_{86}$Rn. V_{SO} included.
Sellers (1990a)	Nb.
Sellers and Ove (1990)	Anisotropic PP for modelling partially filled d shells. Co.
Dolg et al. (1991)	$_{58}$Ce (12-el. PP).
Ermler et al. (1991)	$_{87}$Fr-$_{94}$Pu. 6s6p6d5f5g in valence space.
Fernandez Pacios and Botella Olcina (1991a)	Improved Ar-core PP for $_{21}$Sc-$_{29}$Cu.
Kaupp et al. (1991a)	Ca, Sr, Ba. 10-electron PP.
Küchle et al. (1991)	$_{80}$Hg-$_{86}$Rn. Both QR and NR basis sets given. A parametrized core-nucleus repulsion correction.
Wallace et al. (1991)	$_3$Li-$_{18}$Ar basis sets.
Allouche et al. (1992)	Ba. CP and SO potentials.
Barandiarán and Seijo (1992)	$_3$Li-$_{57}$La.
Stevens et al. (1992)	$_{19}$K-$_{57}$La, $_{72}$Hf-$_{86}$Rn.

Table 4.11. One-component and perturbation calculations.

Reference	Comments
Fraga et al. (1986)	Matrix elements of the Breit Hamiltonian in various coupling schemes.
Menendez et al. (1988)	BP terms as tests of the quality of STO atomic wave functions.
Uylings (1988,1989)	Angular formulae for two-electron BP terms.
Vijayakumar et al. (1989)	A LDF method with 1-component, SO-split one-electron functions. IP and EA.

Table 4.12 (1/Z)- and other similar expansions for many-electron atoms. For 1-electron atoms, see table 2.3.

Reference	Comments
Mohr and Safronova (1986)	Perturbation expansions for energies of 2-electron systems.
Safronova (1986a)	1/Z PT for $1s^2 2l2l'$-$1s^2 2l2l''$ TP. BP terms included.
Shestakov (1986)	3rd-order 1/Z PT on $3d^9 4s^2\ ^2D$ FS of Cu-like systems, Z=28-80.
Ivanov and Safronova (1987b)	An αZ expansion for $1s^{n1} 2s^{n2} 2p^{n3}$ systems.
Sakibaev and Safronova (1988)	Comparison of PT in αZ and 1/Z with MCDF for 2 $^3S_1$-^3P_J energies.
Ivanov and Safronova (1989a)	An αZ expansion for $1s^{n1}...3d^{n6}$ systems. Satellite spectra of 2p-1s and 3p-1s type.
Kim (1989)	Breit correlation for Al-like ions is Z^2 and Z^3. for $3p_{1/2}$ and $3p_{3/2}$, respectively.
Anno (1990)	Regularities of relativistic effects on total energies in 1/Z theory.
Pal'chikov and Safronova (1990)	1/Z analysis of DF theory.
Safronova et al. (1990)	New terms in 1/Z and αZ estimated for Be-like systems (Z = 18, 26, 42) by comparing MCDF and PT.
Shabaev (1990)	PT for relativistic atoms.
Karwowski et al. (1991)	DF + Breit energies expanded in a double series in 1/Z and $(\alpha Z)^2$. Main correlation-relativity crossterm from H_{Br}. He-, Be-, and Ne-like series.
Kagawa and Safronova (1992)	1/Z and αZ expansions for He-like systems. Z = 10-100.

Table 4.13. Relativistic nuclear calculations.

Reference	Comments
L.D.Miller (1974,1975ab)	Local approximations to the exchange potential in nuclear DF theory.
L.D.Miller (1976)	Elastic electron scattering formalism for relativistic nuclear models.
Brockmann (1978)	Nuclear relativistic Hartree-Fock theory: formulation, implementation, results for ^{16}O and ^{40}Ca.
Brockmann and Weise (1981)	SO coupling in nuclei.
Eisenberg (1981)	A relativistic nucleon in scalar and vector potentials.
L.D.Miller (1983ab)	Nucleon-nucleus scattering in a Dirac formalism.
Brown (1986)	Review.
Glöckle et al. (1986)	Relativistic 3-body effects reduce bound-state E by about 3 %, if R and NR 2-body E is held constant.
Gross (1986)	Relativistic equations for nuclear systems.
Kurasawa and Suzuki (1986)	Coulomb sum rule for electron scattering by nuclear matter. RRPA.
Boussy et al. (1987)	Relativistic HF for nuclei. NR limits discussed.
Brown (1987b)	Review.
Brown et al. (1987)	Review.
De Sanctis and Prosperi (1987)	One- and two-photon matrix elements of weakly bound systems.
Glöckle et al. (1987)	A solvable 2-body, 1D model with δ-function interaction. Lorentz-boost operator constructed.
Kurasawa and Suzuki (1989ab)	Coulomb sum rules for electron scattering by nuclear matter: Dirac sea and sigma-omega effects.
Lev (1988)	Relativistic corrections to binding energy for ≥4 nucleons.
Malfliet (1988)	Relativistic nuclear MBPT.
Thies (1988)	Disputes relativistic effects in nuclear physics.
Bijtebier (1989ab,1990a-d)	Few-fermion bound-state and scattering formalism.
De Sanctis (1989)	Relativistic corrections to photon-scattering polarizabilities.
Mc Neil et al. (1989)	Use of B splines (Johnson et al., 1988 a) in Dirac SCF and RPA nuclear models. ^{16}O, ^{40}Ca.
Plunien et al. (1989,1991)	Nuclear polarizability contributions to electronic Lamb shift.
Reinhard (1989)	Relativistic mean-field description of nuclei and nuclear dynamics, a review.
Brockmann and Machleidt (1990)	Relativistic nuclear structure. Includes review.

Table 4.13. (continued.

Centelles et al. (1990)	Relativistic TF with h^2 corrections for nuclei. Tested on a harmonic-oscillator model.
Dawson and Furnstahl (1990)	Relativistic spectral RPA in finite nuclei.
Mishustin (1990)	Instability of the Dirac nucleon sea in relativistic nuclear collissions.
J. Wu et al. (1990)	Numerical methods for time-dependent, 3+1 or 1+1 dimensional nuclear Dirac equations.
De Sanctis and Prosperi (1991)	Two-body interactions for nucleons. Pion exchange.
Keister and Polyzou (1991)	Review on relativistic Hamiltonian dynamics in nuclear and particle physics.
Toyama et al. (1991)	Relation between bound-state radius and scattering length.
Wasson (1991)	Nuclear Dirac-Hartree methodology.
Weigel et al. (1991)	Semiclassical expansions in nuclear DF theory.
Zhang and Onley (1991)	Retardation effects in finite nuclei. Retardation of the pion exchange may change the total binding energy by up to 5%.
Berghammer et al. (1992)	A 1D model for Coulomb dissociation.
Brockmann and Toki (1992)	Relativistic density-dependent Hartree approach for finite nuclei.
Cruz Barrios and Nemes (1992)	Field theoretical Lagrangians for mean-field approximations.
Jin et al. (1992)	Electron Coulomb effects in quasi-relativistic (e, e'p) reactions.
Marcos et al. (1992)	R/NR nuclear HF models.
Nikolaus et al. (1992)	R HF point coupling model for nuclear ground states.
Price et al. (1992)	R RPA for nuclear ground states. Contributions from the negative energy sea at one-loop level included.
van Dijk (1992)	Relativistic effect on the radius of a model deuteron.
Von-Eiff and Weigel (1992)	Relativistic TF model for finite nuclei including quantum corrections.
Von-Eiff et al. (1992)	Relativistic TF model for nucleons in a vector and scalar potential.
Zamick et al. (1992)	Interplay of relativity and core polarization in SO splitting.
X.-Q. Zhu et al. (1992)	One-time relativistic equation for nucleon-nucleon scattering derived from the Bethe-Salpeter equation.

5. MULTIELECTRON ATOMS. RESULTS

'Dielectronic recombination' by an ion means the absorption of one electron, from an electron beam or another atomic or molecular system, and the simultaneous excitation of an existing electron to a higher state. We include papers on it in Table 5.12.

Table 5.1. Tabulations of atomic ground-state properties.

Reference	Comments
Band and Trzhaskovskaya (1986)	Wave function expansions near origin from DS and DF functions.
Chen and Crasemann (1990)	Auger and Coster-Kronig radial matrix elements for Z=6-92.

Table 5.2. Data on atomic energy levels. The ground-state energy is denoted by E. FS = fine structure.

Reference	Comments
Fricke and Greiner (1969)	Ground-state DS configurations searched for Z=160-170. E164 a $7d^{10}(8p_{\frac{1}{2}})^2$ noble gas. Next noble gas is $E170, 7d^{10}8p^6 9s^2$.
Safronova et al. (1971)	S XI and S XII, including BP terms.
Safronova and Labzovskii (1971)	BP terms for 1s2s and 1s2p 2-electron systems.
Dehmer (1973)	Atomic SO splitting arises in the K-shell region. Z-dependence analysed.
Beck and Nicolaides (1976)	Alkali atom nd ^2D FS.
Cole and Harmon (1981)	Orbital eigenvalues and E for 4f atoms in various LDF schemes.
Beck and Nicolaides (1984)	Fine structure of Be^- bound states.
Bruch et al. (1984)	B III 1s2pnp ^2P and 1s2pnd ^2D states at BP level.
Dyall and Grant (1984)	Ar K_β x-ray spectrum. MCDF-EAL.
Baluja (1986)	$2s2p^3\ ^5S$ - $2s^2 2p^2\ ^3P$ TP in the C-sequence, O III - Fe XXI.
Band et al. (1986)	X-ray transitions.
Bauche et al. (1986)	D_1 and D_2 lines of Fr. Isotope shifts for $p_{1/2}$ and $s_{1/2}$ electrons.
Biémont (1986)	Sulfur sequence 3s-3p, 3p-3d and 3p-4s, up to Ti VII.
Biémont and Hansen (1986b)	Forbidden transitions in $3p^4$ and $4p^4$ configurations.
Cogordan and Lunell (1986)	$2p^{-1}3s$, 3p and 3d levels of Ne-like ions, Z=20-54.
Das and Grant (1986)	3s3p FS levels of Mg-like systems.
Fawcett (1986)	Fe XV 3-3 and 3-4 transitions.
Froese Fischer (1986)	$2p^{-1}3s3p$, 3s3d and 3s4s quartet states of Na I and Mg II.
Froese Fischer and Godefroid (1986)	P-like $3p^3$ ^4S, ^2D, ^2P terms, Z = 16...42.
Frost et al. (1986)	Pb II SO splitting.
Gogava et al. (1986)	Nuclear and QED effects for Li-like ions, Z = 20...92.
Gurchumeliya et al. (1986)	Zn-like series.
Hagelstein (1986a)	Ni-like Gd.
Hagelstein (1986b)	F-like Se.
He et al. (1986)	Positronium anion ground-state energy.
Indelicato (1986)	The 1s binding energies of He-, Ne-, Xe-, and Rn-like ions, Z=100...170.
Indelicato et al. (1986a)	He-like Kr.
Ivanova et al. (1986)	Mg-like systems, Z=25-84.
Johnson and Sapirstein (1986)	Ground-state energies of He-like systems, Z=1-100, using the B-spline MBPT.
Karim and Bhalla (1986)	He-like Cr.

Table 5.2. (continued).

Kotochigova and Tupitsyn (1986a)	MCDF for low-lying levels of Ba.
Maurer and Watson (1986)	Multiple K+L-shell vacancy states, Z=9-18.
Migdalek and Baylis (1986a)	Cd-like series, $5s^2$-5s5p transitions. Limited intravalence CI + polarisability core-valence correlation term.
Migdalek and Baylis (1986b)	$6s^2$-6s6p of Yb.
Mu and Crasemann (1986,1988)	Two-photon transitions in inner shells of Mo, Ag, Xe. DS.
Parera and Lopez Boada (1986)	Valence levels of alkaline earths.
Parker (1986)	Inner-shell energy levels with a $-Z_{eff}/r$ potential for every shell.
Riisager and Rosén (1986)	M x-ray shifts for Dy as function of atomic charge states.
Ross et al. (1986)	SO splitting of B-Tl, F-At. PP.
Rutkowski (1986c)	E of He-like atoms, Z=2-36 using a new PT approach.
Shestakov (1986)	The $3d^9 4s^2\ ^2D$ FS of Cu-like systems, Z=28-80. 1/Z PT.
Syromyatnikov and Savicius (1986)	Semiempirical, relativistic method for atomic energy levels.
Zhao et al. (1986)	X-ray energies of Ac-U. DS.
Babb and Spruch (1987,1988)	Retardation effects on Rydberg states of He.
Beck et al. (1987)	No bound states for Sc^-, several for Cu^-.
Bhattacharya et al. (1987)	M-shell vacancy effects on L-x-ray spectra using screened hydrogenic functions.
Biémont and Hansen (1987a)	2p-3s, 2p-3d, 2s-3p and 3p-3d transition energies for Ne-like ions, K X-Se XXV.
Biémont and Hansen (1987b)	M1 and E2 transitions within $3p^N$ and $4p^N$. Ga I - Xe XXIV.
Carroll et al. (1987)	Sulfur 1s IP.
Chen and Crasemann (1987c)	$1s2s^22p$, $1s2s2p^2$ and $1s2p^3$ configurations of Be-like ions, Z=6...26.
Cheng and Wagner (1987)	4s-4p transitions in Cu-like, $4s^2$-4s4p transitions in Zn-like ions, Z=50...92. No significant deviation from experiment.
Combet Farnoux (1987)	A review on giant resonances in heavy elements.
Crasemann et al. (1987)	A bibliography on theoretical atomic-electron binding energies.
Curtis (1987)	Lowest P-term fine structure for the Cu, Zn, Ga and Br series, Z≤92.
Drake (1987)	1s nd levels of He.
Dzuba et al. (1987a)	Au, Tl.

Table 5.2. (continued).

Fawcett (1987a)	C-like series, Z=9-28. Allowed 2-2 and 2-3 transitions.
Fawcett (1987b)	C I, N II, O III.
Francisco and Pueyo (1987)	Fine-structure levels of 3d metals M^{n+}, n=0,2,3,M=Sc-Zn.
Froese Fischer (1987)	2p-3s transitions of O I.
Glushkov et al. (1987)	Al-like systems,Z=23-32, from a model potential.
Gorceix et al. (1987)	Coulomb and magnetic correlation energies for $1s^2$ and 1s2p states of He-like ions, Z=10...60. Magnetic exceeds Coulomb around Z=50 for $1s^2$.
Hagelstein (1987)	Ne-like Se.
Hsuan et al. (1987)	He-, Li- and Be-like Ni.
Indelicato (1987)	Li-like ions. MCDF.
Indelicato et al. (1987ab)	He-like ions at MCDF level. A new treatment of radiative corrections.
Johnson et al. (1987)	Li-Cs valence levels.
Kelleher and Saloman (1987)	Rydberg states with anisotropic core states: Stark effect on $5d_{3/2}8l$ autoionizing states of Ba.
Kim and Greene (1987)	Two-electron excitations in Ca.
Kim and Weiss (1987)	$2s^2$-2s2p energies of Be-like ions.
Kotochigova and Tupizin (1987)	MCDF energy levels of neutral Ba, Ce, Sm, Eu, Yb. R/NR comparisons. The 4f collapse occurs between Ba and Ce.
Kulagin (1987)	Order of occupation of nf and (n+1)p levels in Ln^{q+}, An^{q+}.
Lisini and Decleva (1987a)	ns^{-1} and np^{-1} PES of the alkali atoms.
Lisini and Decleva (1987b)	The 6s to 7s shake-up satellite in Cs $5s^{-1}$ PES.
Lombardi(1987)	Na FS. Model-potential fits.
Migdalek and Baylis (1987a)	$6s^2$-6snp, n=6-20 for Hg.
Migdalek and Baylis (1987b)	$6s^2$-6s6p of Yb-like ions, Z=71-73. Influence of the 5d orbital collapse on 5d6p mixture to 6s6p studied.
Migdalek and Baylis (1987c)	$6s^2$-6s6p of Ba.
Migdalek and Baylis (1987d)	$5s^2$-5s5p of Sr I and Y II.
Migdalek and Bojara (1987, 1988)	Comparison of CI and MC for ns^2 - nsnp transitions of Cd and Hg.
Migdalek and Wyrozumska (1987)	Cs sequence. Collapse of f and d orbitals.
Mohan and Hibbert (1987)	Hg $6s^2$-6s6p using a MP.
Perger and Das (1987b)	Be sequence 2s2p FS.
Radojevic (1987)	Pb $6s^26p^2$ and $6s6p^3$ levels.
Shi et al. (1987)	X-ray energies for Y, Zr, Nb, Mo, Tc, Ru. HFS with relativistic corrections.
Steiger (1987)	Li-like ions, Z=26...94. States up to $5f_{7/2}$.
Veseth (1987a)	Isotope-shifts in C II and N II FS.

Tabel 5.2. (continued).

Wadt (1987)	Pu^{2+} excited states as tests of PP.
Zilitis (1987)	Valence levels of K-like species, Z=19...92. DF.
Band et al. (1988)	Atomic mechanisms for mixed-valence states in Ln, An.
Beck (1988)	Three bound states of Zn^-: $4s4p^2$ ^4P, $4p^3$ ^4S and $3d^94s4p^3$ ^6D.
Beck and Cai (1988)	Bound states of Mn^-.
Biémont (1988)	n = 3-4 and 4-4 transitions of Cu-like ions (Z = 38-60).
Bieron and Migdalek (1988)	Ge-like sequence.
Blomberg and Wahlgren (1988)	Pd $4d^{10}$-$4d^95s^1$ distance influenced by 4s and 4p orbital relaxation in relativistic, 1st-order PT.
Blundell et al. (1988)	Up to 3rd-order MBPT for 6s, $6p_{\frac{1}{2}}$ and 7s of Cs.
Carlsson (1988)	Cu I. Odd levels. MCHF+BP. Applied on Cu-vapor laser.
Chang and Bryan (1988)	Al II, f-level FS perturbed by 3p3d ^3F.
Chen and Crasemann (1988a)	$1s^{-1}$ states of B-like ions, Z=6...54.
Cowan et al. (1988)	Hg $5d^96s^26p_j$ levels.
Churilov et al. (1988)	n=4, $\Delta n=0$ transitions of Ni- and Zn-like ions, Z = 30 - 50.
Curtis et al. (1988)	3s, 3p and 3d levels of Ne-like systems, Z=16-18.
Drake (1988a)	Ground states of H^-, He; 1s2s of He.
Drake (1988b)	n=1, 2 states of He-like ions, Z≤100.
Drake and Makowski (1988)	1s2p states of He.
Froese Fischer (1988)	Li I 2^3S-2^3P, MI ns-np, M=Li, Na, K.
Gogava et al. (1988)	$2s^{-1}$ and $2p^{-1}$ levels of Ne-like systems, Z=18...42.
Gorceix and Indelicato (1988)	Effects of the complete Breit interaction on two-electron ion 1s2s and 1s2p energy levels, Z=6...92.
Iglesias et al. (1988)	Mo III. $4d^4$, $4d^35s$, $4d^35p$ levels.
L.N. Ivanov et al. (1988)	Review on multicharged ions, especially He-, Li- and Ne-like ones.
Indelicato (1988)	He-like systems, Z=10-92.
Johnson et al. (1988b)	Li-like n=2 levels, Z=3-92.
Johnson et al. (1988c)	Na-like n=3 levels, Z=11-92.
Y.-K. Kim et al. (1988a)	2s3p levels of Be-like ions.
Y.-K. Kim et al. (1988b)	QED contributions to ground-state FS of Al-like ions.
Klobukowski and Fraga (1988)	Accurate ground-state E for He-like systems, Z=2-4.
Liaw et al. (1988a)	Na-Cs and Ne-Xe ground and excited-state energy contributions.
Lindroth (1988)	E for $1s^2$ systems, Z=2...50, from a numerical solution of the relativistic pair equation.
Liu and Li (1988)	Fr exited states. DS.
Malinovskaya (1988)	Cl-, Ar- and K-like ions, Z=19-36. A model-potential fit.

Table 5.2. (continued).

Ohtsuki and Hijikata (1988)	He-like system 2 $^{1,3}P$ FS, $Z \leq 10$.
Rashid et al. (1988)	E of U I to U XCII. DF.
Reed (1988)	The 36 n=3 states of Ne-like Ba.
Reed et al. (1988)	n=2 states of O-like Se.
Rutkowski et al. (1988)	E of closed-shell atoms, He...Xe, using a new PT approach.
Sakibaev and Safronova (1988)	2 $^3S_1$-^3P_J energies. Comparison of MCDF and PT in αZ and 1/Z.
Sapirstein (1988)	n=2 state IP of Li-like ions.
Silver (1988)	Precision spectroscopy on 1- and 2-electron ions of medium and high Z.
Styszynski and Karwowski (1988)	E of $1s^2$ atoms, Z=2-20. MCDF with radiative corrections and relativity-correlation cross terms. Final error estimated < 0.001 a.u.
Sugar et al. (1988)	Al-like ions, Z=29-42.
Theodosiou and Curtis (1988)	IP of Na-like systems, Z=30...92.
Vainshtein and Safronova (1988)	Ne-like ions.
Veseth (1988)	FS of B-F, Al-Cl. MBPT.
Walker et al. (1988)	Excitation energies of Sc...Co as tests of PP.
Zhao and Pan (1988a)	$2p^5 3s$, 3p and 3d levels of Ne-like Kr. MCDF.
Zhao and Pan (1988b)	Fe XVII.
Zhao and Wang (1988)	Pb I $6p^2$-6p7s. MCDF.
Zhao et al. (1988)	X-ray energies of Sc-Ni. About 1% accuracy with TS DS.
Anno and Teruya (1989)	Relativistic contributions to E, Z=2-20.
Au (1989ab)	He Rydberg states: QED corrections beyond Breit.
Babb and Spruch (1989)	Retardation effects for a Rydberg electron outside a multielectron core.
Baker et al. (1989)	He energy levels.
Bauche and Bauche-Arnoult (1989)	Mixing of many transition arrays: 30 configurations of Xe^{27+}: 110 000 lines in 80 arrays.
Beck (1989)	The ^4P to ^4S transition of Mg^-.
Biémont (1989)	n=4-4 transitions in zinc-like ions.
Biémont and Hansen (1989)	3d and $3d^9$ systems.
Biémont et al. (1989)	Zn-like ions.
Blanke et al. (1989)	3d-4f and 3d-5f transitions of doubly-excited three-electron ions, N V...Mg X.
Blundell et al. (1989a)	2s,2p and 3s levels of Li and Be^+. All-order MBPT gives 0.01% accuracy.
Blundell et al. (1989b)	Ground-state energy of He from all-order MBPT. Briand et al. (1989) H-like and He-like Xe. $1s2p\ ^{1,3}P_1$.
Cai and Beck (1989)	Bound excited states of Cr^-, Fe^-, Co^- and Ni^-.

Table 5.2. (continued).

Chang (1989)	1s4f states of He.
Chung (1989a)	$1s2s2p^2$-$1s2p^3$ ^5S of Be-like systems, Z=4-10.
Crasemann (1989)	A review on relativistic phenomena in atomic physics.
Drake (1989)	Review on He.
Dzuba et al. (1989a)	Tl 6p.
Fraga et al. (1989)	Test the approach of Fraga et al. (1986, 1987) on He ^1S levels and one ^3P level.
Froese Fischer (1989)	M, M^-, M=Mg-Ba. Sc, Sc^+.
Froese Fischer and Chen (1989)	nsnp ^3P states of Rb and Cs. The latter is bound. Thumm and Norcross (1991) later find it unbound.
Glebov et al. (1989)	Ku (E104) ground state a J=2 with mainly $6d7s^27p$. The $6d^27s^2$ lies 0.5eV higher.
Indelicato (1989)	He- and Li-like ions: a review.
Ivanov and Safronova (1989b)	2l4l' states of 2-electron systems.
Jansen and Hess (1989b)	Au ^2D and ^2P levels using the 'no pair' approach.
Johnson (1989)	Li-like atoms. MBPT. The obtained $2p_{\frac{1}{2}}$-2s difference compared to Lamb-shift calculations.
Johnson et al. (1989a)	Negative ions of Pd, Ca-Ba.
Kim (1989)	3p FS of Al-like ions, Z=13-60. The Breit correlation varies as Z^2 and Z^3 for $3p_{\frac{1}{2}}$ and $3p_{3/2}$, respectively.
Lagowski and Vosko (1989)	J-independent relativistic contributions to s-d interconfiguration energies for M and M^+, M=Ca-Cu. LDF.
Migdalek and Stanek (1989)	$4s^2$-4s4p transitions in the Zn sequence.
Mukoyama (1989a)	M-shell x-rays of Dy. DF.
Nicolaides et al.(1989)	Bound exited states of atomic negative ions. New results for A^-, A=Al, Fe, Mn, Cu.
Nilsen (1989)	Dielectronic satellite spectra for Ne-like ions.
Ostrovskii and Sheinerman (1989)	Hg^+ 7p-7s, 6s and nd-ns energies. R/NR HF.
O'Sullivan (1989)	Rb IV - Rb IX. 4p-5s, 4p-4d. DF.
O'Sullivan and Kane (1989)	Ru XII and Rh XIII $4s^24p^3$ and $4s^24p^25s$ levels.
Pacheco and Sañudo (1989)	Observation of "strange matter" in nuclei through change of nuclear radius. 1s-2p levels calculated for Z=80-104.
Polasik (1989ab)	$K\alpha L^n$ lines of Mo, Pd, La, Ho. MCDF + QED.
Polasik (1989c)	$K\alpha L^oM^r$ lines of Mo, Pd, Ho.

Table 5.2. (continued).

Qian et al. (1989)	$2s^2$-2s2p for Ne^{6+}...U^{88+}. MCDF.
Raghavachari and Trucks (1989a)	The $d^n s^2$-$d^{n+1}s$ energies of Sc-Cu.
Rashid et al. (1989)	E of Be-like systems, Z=4-20. MCDF.
Rudzikas and Ryabtsev (1989)	Identification of the spectra of multielectron ions.
Saloman and Kim (1989)	Ground-state terms of S-like ions, Z=16-92. MCDF with Breit and Lamb-shift corrections.
Salomonson and Öster (1989)	E of He using all-order pair functions.
Sampson et al.(1989)	Resonance transitions of Ne- and Ni-like ions, as test of a new DS program.
Sapirstein (1989a)	E of He-like systems.
Schmidt et al. (1989)	Muonic 1s-5g levels in atoms with Z=30-100.
Seely (1989)	2s-2p transitions of Li-like ions, Z=24-54. QED included.
Seely et al. (1989)	Cu-like systems, Z=44-92. All n=4,5 levels. Values corrected semiempirically.
Tisenko (1989)	He atom FS formulated a Dul'yan-Faustov pseudopotential equation.
Tragin et al (1989)	$d^{10}nl$-$d^{10}nl'$ and d^{10}-d^9nf transitions near ionization limit for Cu- and Ni-like ions, respectively. Z=42...83, 35...92, respectively.
Aashamar and Luke (1990)	Cr II sextet-quartet mixing.
Anisimova and Semenov (1990a)	Fine structure of $np^5n's$ configurations.
Anisimova and Semenov (1990b)	Fine structure $nd^9n's$ configurations.
Anisimova and Semenov (1990c)	Fine structure of ps configurations.
Anno (1990)	E from 1/Z theory.
Au and Mesa (1990)	He Rydberg levels: corrections beyond Breit.
Biémont (1990)	Forbidden lines in the K sequence, Cd^{29+}-Ce^{39+}.
Biémont and Quinet (1990)	Ga-like ions, Br V-In XIX.
Blundell et al. (1990a)	n=2 states of Li-like U. Higher-order Breit, mass-polarization and QED included.
Blundell et al. (1990b)	3rd-order MBPT ground-state energies of Cs and Tl.
Bylander and Kleinman (1990)	4f resonances in Ba using a norm-conserving PP.
Chen and Huang (1990)	Anomalous fine-structure splittings in the DF model corrected by proper NR limits. 3p hole states of Ar-Sr as example.
Chung (1990a)	$1s^{-1}$ four-electron resonances of C.
Chung (1990b)	$1s^{-1}2l2l'2l''$ states of O.

Table 5.2. (continued).

Connerade and Karnatak (1990)	Centrifugal-barrier double-well atomic potentials and valence changes. Sm as example.
B.P. Das et al. (1990)	FS intervals for $1s^2 2p$ levels of Li-like ions, Z=5-28.
Drake (1990)	Rydberg states of He.
Greene (1990)	M^-, M = Rb-Fr. See Thumm and Norcross (1991).
Hansen (1990)	Atomic spectra for astrophysics and fusion. Proceedings of Amsterdam 1989.
Indelicato (1990)	K_α-transitions in few-electron systems.
Indelicato and Desclaux (1990)	Li-like ions, Z=15-92.
W.R. Johnson et al. (1990)	Cu like n=4 levels, Z=29-92.
Y.-K. Kim (1990)	Relativistic and QED effects in highly-charged ions.
Koc and Migdalek (1990)	nl-levels of Ag and Au. Inverted FS of Au 5f reproduced.
Lindroth and Salomonsson (1990)	Ar^{16+} 2^3S_1-1^1S_0 energy calculated as 114.072(7) au. R PF.
Marketos and Lambropoulos (1990)	The J=1/2 even spectrum of Sr II.
Mazzoni and Joshi (1990)	As I $3d^9 4p^4$ and $3d^9 4p^3 np$ levels.
Migdalek and Baylis (1990)	Ba $6s^2$-6s5d transitions.
Migdalek and Stanek (1990)	Comparison of 'optimal level' and 'average level' MCDF for ns^2-nsnp transitions of Zn I, Rb VIII, Hg I, and Rn VII. For neutrals, OL clearly better.
Nielsen et al. (1990)	2l4l' states as function of Z.
Ohanessian et al. (1990)	ΔE between $5d^n$, $6s^1 5d^{n-1}$ and $6s^2 5d^{n-2}$ for Ba^+, La^+, Hf^+-Hg^+, as tests of the QR PP.
Parera López (1990)	E of He-like atoms at DF levels using a scaled hydrogenic basis. Includes Breit.
Pararpia and Grant (1990)	Accurate ground-state E for He-like atoms.
Polasik (1990)	$K\alpha L^1 M^r$ x-ray lines of Pd.
Quinet and Biemont (1990)	Resonance transitions in Ni-like ions, Ge V - La XXX.
Safronova et al. (1990)	Be-like ions, Z=18,26,42. Radiation and correlation corrections appended to MCDF. New terms in 1/Z and αZ estimated.
Seely and Wagner (1990)	3s-3p transitions of Na-like ions, Z=39-92. QED included.
Sugar et al. (1990)	Si-like ions, Z=29-42.
Viar and Safronova (1990)	$2s^2 2p^5 3l$ and $2s2p^6 3l$ levels of Ne-like systems, Z=18...92.
Wycech et al. (1990)	FS in the antiprotonic $\bar{p}$-^{174}Yb atom.
X.Y. Xu et al. (1990)	Ru $4d^7 ns$ (n=28-50) and nd (n=24-56) Rydberg levels. DS.

Table 5.2. (continued).

Zhuikov et al. (1990)	E104 energy levels. Ground state s^2pd. MCDF.
Zilitis (1990)	Rydberg s and p levels of K-like ions.
Zou et al. (1990)	XUV spectra of C-like Co.
Aggarwal et al. (1991)	Lowest 20 levels of Ca XV.
Au et al. (1991)	Recoil corrections to Rydberg levels of He.
Band et al. (1991)	4d-nf excitations of Ba^{2+}.
Bauche et al. (1991)	Break-down of jj-coupling. $3d^{10}$-$3d^9nf$ transitions of Ta^{45+}.
Biémont (1991)	Allowed transitions in Al V-Al VII.
Blundell et al. (1991a)	All-order MBPT energies of Cs.
Cai (1991); Cai et al. (1991)	Hg $6p^2$ resonance states.
Cheng et al. (1991)	n=2 states of Li-like U, n=3 of Na-like Pt and n=4 of Cu-like Au. MBPT + QED.
Chou et al. (1991)	Pb-like $^3P_{0-1}$ transitions, Z=82-98,
Chung (1991b)	$1s^{-2}$ four-electron systems: $2s^22p^2$ $^3P>>2s2p^3$ ^5S, Z=3-10.
Couch and Scott (1991)	Kα x-ray satellites for Z=19-32. R/NR comparisons made.
Davidson et al. (1991)	Ground-state correlation energies for 2- to 10-electron ions, Z ≤ 20.
Dzuba et al. (1991a)	np-state FS for M^-, M=Ca-Ra. For Ra^-, only $7p_{1/2}$ is bound.
Dzuba et al. (1991b)	M $6p^2$ and np(n+1)s levels, M=Sn, Pb, 114. Bi $6p^3$.
Feldman et al. (1991)	$3d^4$ ^5D levels of Ti-like ions, Z=42...92.
Glushkov (1991b)	$4p^1$ and $4d^1$ levels of Ga-like systems, Z = 31-36.
Greene and Aymar (1991)	Sr-Ra excited states.
Hsu et al. (1991)	1s2s2p ^4P levels for Li-like ions.
Indelicato and Mohr (1991)	Li-like U $2s$-$2p_{1/2}$.
Ivanova and Gulov (1991)	Ne-like $2p^{-1}3l$, 4l and $2s^{-1}3l$, 4l levels, Z=27-92. Revised results for Na- and F-like ions.
Kagawa et al. (1991)	$2s^{-1}$ and $2p^{-1}$ levels of Ne-like ions, Z=18...54. Finite-basis CI.
Karwowski et al. (1991)	E of He-, Be- and Ne-like series as a double series in 1/Z and $(\alpha Z)^2$.
Y.-K. Kim et al. (1991)	ns-np transitions in Li-, Na- and Cu-like ions, Z≤92.
Litzén and Zeng (1991)	4s-4p transitions in Ga-like ions, Z=44-49.
Liu and Kelly (1991)	E of Be from MCDF-based MBPT.
Mårtensson-Pendrill et al. (1991)	E of Be, now agrees with experiment.
Martin et al. (1991)	Quantum defect orbital study of 3s-3p and 3p-3d in the Na-like sequence, Z=11...99.

Table 5.2. (continued).

McKenzie and Drake (1991)	E of Li -7.478 060 326(10) au, exp. -7.478 060 34(20). also QED corrections for $1s^2 2s$ and $1s^2 2p$ states, Z=7...36.
Migdalek and Baylis (1991a)	Yb $6s^2$, 6s6p and 5d6s levels.
Migdalek and Baylis (1991b)	La II $5d^2$, 5d6s and 5d6p levels.
Perger et al. (1991)	$6p^2$ resonances of Hg.
Quinet and Biemont (1991)	X-ray spectra of Ni-like ions, Ag XX -Pb LV.
Quinet et al. (1991)	Allowed and forbidden transitions in Ne-like ions Ni XIX - U LXXXIII.
Samzow and Hess (1991)	FS of Br as test of the "no-pair" Hamiltonian.
Tayal (1991)	Ga II 4s4p, $4p^2$ and 4s4d level energies. BP PT.
Thumm and Norcross (1991)	The 6s6p $^3P^o_J$ states of Cs^- are unbound, narrow resonances.
Vukajlovic et al. (1991)	E difference of $3d^{n-1}4s^1$ and $3d^{n-2}4s^2$ of Ca-Cu. DFT.
Zilitis (1991)	Rydberg d and f levels of K-like ions. DF.
Ali (1992)	FS of K-like (Z=22-54) and Rb-like (Z = 40-60) ions. MCDF.
Ali and Kim (1992)	K ground-state FS.
Andersson and Roos (1992)	Ni atom d^8s^2,d^9s and d^{10} states. NR correlation at CASPT2 level, $\langle h_m+h_d \rangle$ from Martin and Hay (1981).
K. Ando et al. (1992ab)	$1s^2 2lnl'$ (n=2, 3, 4) levels of Na VIII - S XIII. Comparison of MCDF and 1/Z.
Anno and Teruya (1992)	Comments on E(Z) for He-like systems.
Avgoustoglou et al. (1992)	$2p^{-1}3s$ - $2p^6$ energy of Ne-like Xe.
Babb et al. (1992)	Casimir shifts for He-like Rydberg ions, Z = 2...20.
Band and Trzhaskovskaya (1992)	5d-5f energies of gaseous and metallic U and Th. Single-configuration DF.
Biémont et al. (1992)	Intra $3d^2$, $3d^2$-3d4s and $3d^2$ - 3d4d transitions for Z = 22-47. MCDF, HFR and "SST" compared.
Blundell (1992)	$2s-2p_{1/2}$ of Li-like U, $3s-3p_{3/2}$ of Na-like Pt, $4s-4p_{1/2}$ of Cu-like Bi. Accurate screened QED used.
Bruch et al. (1992)	Ne^{q+} K-shell binding energies, q=4-6. MCDF, 1/Z and a saddle-point method used.
Cai et al. (1992)	Pr^{3+} levels using large-scale MCDF.
Cheng and Huang (1992)	4s-4p transitions of Zn-like ions, Z=31...92. MC RPA.
Chou and Huang (1992a)	6s-6p transitions in Hg-like systems, Z=80-93. MC RPA.
Chou and Huang (1992b)	5s-5p of Cd-like systems, Z = 48-65.

Table 5.2. (continued).

Chung (1992)	E of He- and Li-like systems, Z=11-20.
Connerade and Sarpal (1992)	$3p^{-1}$ levels of Ca I. MCDF.
Deutsch and Kizler (1992)	$1s^{-1}$ levels of Xe.
Dolg et al. (1992a)	Yb^{n+} (n=0-2) energy levels, as test of PP.
Drake and Yan (1992)	Very high precision Rydberg levels for He, $n \leq 10$, $L \leq 7$.
Eissner and Tully (1992)	Two-electron, $2p^2$-2s3p and $2p^2$-2s2p transitions of Be-like systems Z = 6...26.
Goldman and Drake (1992)	He Rydberg levels.
Hessels (1992)	Higher-order relativistic polarisation corrections to He Rydberg states, n = 10.
Ilyabaev and Kaldor (1992)	Ne excited levels. CCSD.
Indelicato and Lindroth (1992)	K_α ($1s^{-1}$ - $2p^{-1}$) energies for Z = 31-100. MCDF+QED. Uncertainty of finite-nucleus corrections is the bottleneck.
Johnson and Sapirstein (1992)	n = 2 triplet states of He-like ions, Z = 10-36.
Koc and Migdalek (1992)	Yb II and Lu III $4f^{14}nl$ levels, especially FS.
Kuplyauskene and Zhukauskas (1992)	Decay of $2p^{-1}3l3l'$ states of Na-like Cl and Ar.
Lao and Christiansen (1992)	Ne ground-state valence E_{corr} from PP Monte Carlo.
Leininger et al. (1992)	Valence levels of K-Cs, Ca-Ba and Fe-Os as test of four different PP.
Lindroth and Hvarfner (1992)	2 ^1S-2 $^{1,3}P_1$ transitions of Be-like Fe and Mo. Theoretical uncertainty dominated by radiative effects.
Lindroth et al. (1992)	E of Be. "Experimental NR energy" -14.667 353(2) a.u.
Loginov (1992)	$5d^9 6p$ levels of Tl IV - Bi VI.
Malinovskaya and Glushkov (1992)	K-like ions.
Mäntykenttä et al. (1992)	Satellites in 4d, 5s and 5p PES of Cs and Ba. MCDF.
Marian et al. (1992)	Cu valence levels, especially ^2D FS.
Mei and Davenport (1992)	IP and s-d excitation energies of Ca-Cu. DF and various DFT compared.
Miecznik et al. (1992)	High-spin states of B-like systems: $1s2s2p^3$ $^6S^o$ -to- $1s2s2p^2 3s$ $^6P^e$ and $1s2s2p^2 3d$ $^6P^e$, Z = 4...13.
Misra et al. (1992)	Parametrized formula for x-ray spin doublets.
Mooney et al. (1992)	K, L and M x-ray of Xe.
Parpia and Mohanty (1992)	E for He-like ions, Z = 10...160 and for Hg. A finite nucleus with Fermi-distribution.

Table 5.2. (continued).

Rashid and Ahmad (1992)	Predicted wavelengths for K-like ions with ± 1/3 , ±2/3 additional (quark) charges.
Seijo et al. (1992)	Valence E_{corr} for I^-, I, I^+.
Safronova and Wyart (1992)	$2s^{-1}$ 31 levels of Ne-like ions, Z = 30...92.
Scofield and MacGowan (1992)	4d-4p laser lines of Ni-like Ta-U.
Sugar et al. (1992)	Rb-like $4p^6 4d$ - $4p^5 4d^2$ transitions, Z = 47-60.
Theodosiou et al. (1992)	2s-2p energies of Li-like systems, Z = 3-92.
Vidolova-Angelova (1992)	Rydberg states of Lu.
W.-J. Wang (1992)	N-like ions, Z = 19-22. MCDF.
Z.-W. Wang et al. (1992a)	$1s^2nd$ and $1s^2nf$ levels of Li-like systems, Z = 3-10.
Z.-W. Wang et al. (1992b)	$1s^2ns$ (n=3-5) states of Li-like systems, Z = 3-10.
Wijesundera et al. (1992a)	Hg^- $6s^2 6p_{1/2,\ 3/2}$ resonances calculated to lie at +0.19, +0.21 eV (exp. +0.63(3)).
Yamamoto et al. (1992)	Energy-levels of Hf.
Yang and Li (1992)	FS of 4f and 3d levels in K-like ions, Z=26, 31, 36.
Y. Zhang et al. (1992a)	Na-like ions, n≤ 15, l ≤ 6, Z = 38-45.
Q.-R. Zhu et al. (1992)	Li-like ions, Z = 20-25.

Table 5.3. Auger and autoionization processes. For dielectronic recombination processes, see Table 5.12.

Reference	Comments
Nicolaides (1983)	Radiative autoionization (RA) and short-wavelength lasers. Li 1s2s2p ^4P undergoes relativistic RA.
Aksela et al. (1986a)	$N_{4,5}OO$ resonance Auger spectra of Xe.
Aksela et al. (1986b)	$M_{4,5}NN$ Auger of Kr.
Aspromallis and Nicolaides 1986)	Relativistic and Coulomb autoionization in $2p^43s$ ^2S and $2p^43d$ ^2P states of F.
Aspromallis et al. (1986)	Relativistic autoionization of $2s2p^2$ ^4P state of Be^-.
Beck and Nicolaides (1986)	Alkaline earth Auger energies.
Cavell and Sodhi (1986)	Auger parameters of phosphorus compounds.
Karim and Bhalla (1986)	2lnl' autoionizing states of He-like Cr.
Kotochigova (1986)	Autoionization treated at MCDF level. 5dnp, n=9, 10 for Ba (J=1).
Levin et al. (1986)	Kr L-MM Auger spectra.
Mannervik and Cederquist (1986)	Relativistic autoionization of Li ^4P_J levels: comments on Nicolaides and Aspromallis (1986).
Nicolaides and Aspromallis (1986)	Relativistic autoionization of Li ^4P_J.
H. Aksela and S. Aksela (1987)	Review on free-atom Auger spectroscopy.
Aksela et al. (1987)	$L_{2,3}MM$ Auger of Ni.
Armen et al. (1987)	Post-collision interactions in inner-shell photoionization. Ar, Xe.
Bruneau (1987)	A relativistic close-coupling approach to the Auger process. Application on the Ne K-LL.
Chen and Crasemann (1987a)	1s2p3d $^4F_{9/2}$ metastable states of Li-like ions, Z=6...42. Breit-induced Auger transitions important.
Chen and Crasemann (1987b)	Auger-decay of $1s^{-1}$ states of Be like ions, Z=6...26.
Chen and Crasemann (1987c)	Auger-decay of $1s^{-1}$ states for B-like systems, Z=6...54.
Radojevic (1987)	Low-energy $6s6p^3$ autoionizing states in Pb.
Tulkki et al. (1987)	Post-collision interactions (Auger and Coster-Kronig) in inner-shell photoionization. Ar, Xe.
Aksela et al. (1988a)	Auger of Ar.
Aksela et al (1988b)	Resonance Auger of Rb.
Chen and Crasemann (1988a)	Auger energies and rates of $1s^{-1}$ states of B-like ions, Z=6...54.
Chen and Crasemann (1988b)	L-shell transitions of Be-like ions, Z= 30-54. Autoionizing resonances.

Table 5.3. (continued).

Cowan et al. (1988)	Hg $5d^9 6s^2 6p_j$ autoionization lifetimes.
Karazija and Rudzikaite (1988)	Mean energy and spin doublets of Auger lines.
Lefebvre-Brion et al. (1988)	SO effects in autoionization of HCl.
Nicolaides and Aspromallis 1988)	Autoionizing states of 2- and 3- electron model atoms with Z=2.05.
Sampson et al. (1988)	Rates of populating excited n=4 levels of a 28-electron, Ni-like ion when a core-excited 29-electron, Cu-like ion decays.
Aksela (1989)	Auger spectra of free atoms: a review.
Aksela et al. (1989a)	Auger of $3d^{-1}np$ states of Kr.
Aksela et al. (1989b)	Auger of $1s^{-1}$ states of Ne.
Campbell and Wang (1989)	L-subshell x-ray emission rates including overlap and exchange effects. Interpolated DF.
Chen (1989a)	Auger and radiative decays of $2p^{-1}3l3l'$ and $2s^{-1}3l3l'$ states of Na-like ions, Z=18...92. Effects of CI and Breit Hamiltonian studied.
Chen (1989b)	L-shell fluorescence yields from Ne- and Na-like low-lying autoionizing states.
Chen (1989c)	Relativistic effects on x-ray and Auger transitions of highly charged ions.
Chen et al. (1989)	The 2p-3p4s Auger spectrum of free Ca atoms: strong correlation effects due to collapse of d AOs.
Chung (1989b); Davis and Chung (1989)	Spin-induced autoionization of Li-like systems. 1s2s2p ^4P, Z=3-18.
Dyubo and Safronova (1989)	Nonradiative decays of Be-like ions.
Froese Fischer and Idrees (1989)	Autoionization of core-exited ^5P states Na^-.
M. Meyer et al. (1989)	Autoionization of the Ca $2p^5 3d$ core resonances.
Safronova (1989)	Autoionization states of atomic systems.
Aksela et al. (1990a)	2p-excited Auger of Cl, applied on HCl.
Aksela et al. (1990b)	Coster-Kronig width of Rb.
Aksela et al. (1990c)	$M_{4,5}NO$ and $M_{4,5}NN$ Auger of Rb.
Aksela et al. (1990d)	Auger decay of Rydberg-excited Ne 1s, Ar 2p, Kr 3d and Xe 4 d.
Chen (1990b)	X-ray and Auger transitions in atoms and ions.
Chen et al. (1990a)	Auger- and Coster-Kronig radial matrix elements for Z=6-92.
Chung (1990c)	Auger-spectra of Be and B.
Ford et al. (1990)	Autoionization and Auger Spectra of Mn and Sm vapours. HFR.
Ivanov et al. (1990)	Autoionization states of 2-electron systems.

Table 5.3. (continued).

Radojevic and Talman (1990)	Beutler-Fano autoionizing resonances in Ne.
Chen (1991b)	Auger rates and fluorescence yields for a double-K-hole state.
Chi et al. (1991)	Autoionizing levels of Be.
Cowan and Wilson (1991a)	Cd $4d^9 5s^2 5p$ autoionization lifetimes.
Crater (1991)	Singlet-positronium decay.
Fritzsche and Zschornak (1991)	L-MM Auger spectra of Kr.
Fritzsche et al. (1991)	MCDF K-LL Auger rates for Ne-like systems, Z=10...92.
Greene and Aymar (1991)	Autoionization of Sr-Ra.
Hayaishi et al. (1991)	Kr 3d and Xe 4d conjugate shake-up satellites in treshold-electron spectra.
Hwang et al. (1991)	Autoionizing levels of Zn. MC-RRPA.
Ivanov and Safronova (1991)	Autoionization 1s2l4l' states.
Vidolova-Angelova and Ivanov (1991)	Autoionizing Rydberg levels of Tm.
Vijayakumar and Gopinathan (1991)	Auger energies from LDF. Ne-Xe, Cr...Cu, Ge.
Whitfield et al. (1991)	Shake-modified resonant autoionization of Mg.
Zimmerer et al. (1991)	Relativistic Auger rates for two-electron ions. Breit effects.
Aksela et al. (1992a)	Resonantly excited $2p^{-1}ns$, md states of Ar, $3d^{-1}np$ of Kr.
Aksela et al. (1992b)	Kr $3d^{-1}$ np, n = 5,6 Auger.
Aksela et al. (1992c)	Decay of $2p^{-1}$ in HCl.
Batkin et al. (1992)	K-shell autoionization in beta decay.
M.H. Chen (1992)	Effect of intermediate coupling on angular distribution of Auger electrons. $M_{4,5}$-NN of Kr, $M_{4,5}$-NN and $N_{4,5}$-OO of Xe. MCDF.
Fritsche et al. (1992)	Zn, L_1 level width and Coster-Kronig yields.
Fritzsche and Fricke (1992)	2p Auger spectra of Mg-like ions, Z = 13-36. MCDF.
Hayaishi et al. (1992)	Ar 2p shake-up structures.
Kuplyauskene and Zhukauskas (1992)	Autoionization of Na-like Cl and Ar.
Leväsalmi et al. (1992)	KLL spectrum of Ne.
Lohmann (1992)	Angular distribution and spin polarisation of Auger electrons from Hg.
Szunyogh et al. (1992)	Relativistic theory of Ti or Pd core-core-valence Auger spectra.
Tulkki et al. (1992b)	Ne KLL and Ar LMM Auger rates.
Yamamoto et al. (1992)	X-ray and Auger energies of Hf.

Table 5.4. Ionization potentials and electron affinities. (For a recent summary of the experimental EA for the elements 1-85, see H. Hotop and W.C. Lineberger, J. Phys. Chem. Ref. Data 14 (1985) 731-750).

Reference	Comments
Beck and Nicolaides (1979)	One-electron binding energies: a review of the contributions.
Hess (1986)	Relativistic increase of Ag IP, EA 0.47 and 0.15 eV, respectively. Br ground state. No-pair formalism used at MRD-CI level.
Beck et al (1987)	No bound states found for Sc^-, several for Cu^-.
Dzuba et al. (1987a)	Au, Tl IP.
Hurley and Christiansen (1987)	Li and K EA from PP MC calculations.
Ohno (1987a)	IP of Ca by g-Hartree method.
Ohno (1987b)	IP of He, Be, Ne, Mg, Ar.
Radojevic et al. (1987)	EA of F-I.
Zhao and Pan (1987)	DS IP of K-Cs, Cu, Ag.
Y.-F.Guo and Whitehead (1988)	IP and EA at QR-LSD level for Z= 37...80.
Ohno (1988)	IP of Be-like systems, Z=4-10.
Ortiz (1988)	EA of K-Cs. PP, up to 4th-order MBPT.
Rashid et al. (1988)	IP_n of U.
Dzuba et al. (1989a)	Tl 6p IP.
Froese Fischer (1989)	Sc IP. Ca, Sr, and Ba EA: 0.062 (exp. 0.043(7)), 0.106 and 0.148 eV, respectively. Relativistic EA decrease almost 0.1 eV for Ba.
Froese Fischer and Chen (1989)	Cs 6s6p ^3P predicted to have a positive EA, Rb 5s5p not. See Thumm and Norcross (1991, 1992).
Fuentealba et al. (1989)	EA of Ca, Sr, Ba. Five different density functionals tested.
Y.-F.Guo and Whitehead (1989)	EA of Mg-Ra and An (Ac-Lr) at LSD level.
Y.-F.Guo et al. (1989)	EA of rare gases (He-Rn) and some An (Pu-Es) at LSD level.
Jansen and Hess (1989b)	Au EA and IP using the 'no pair Hamiltonian.
Johnson et al. (1989b)	EA/eV: Pd 0.525, exp. 0.558(8) Ca 0.056 0.043(7) Sr 0.093 Ba 0.192
Raghavachari and Trucks (1989b)	IP of Sc-Cu. Corrections of Martin and Hay (1981) used.
Rubio et al. (1989)	Spherical DS models for the IP_n of Cu_N, Ag_N clusters, N≤25.

Table 5.4. (continued).

K.D.Sen et al. (1989a)	Electronegativities, $\chi = -[\partial E/\partial N]_Z$ (E total energy, N number of electrons) calculated for non-integral (n/3) nuclear charges, Z, near halides. LSD.
Vosko et al. (1989)	EA of Sr, Ba and Ra. from DFT. p^1, d^1 and d^1 configurations predicted, respectively.
Fuentealba et al. (1990)	EA of Ca-Ba. None for Be, Mg.
Illas et al. (1990)	Rh IP and EA.
E.Johnson et al. (1990)	IP_n of Ti-Hf and E104.
Koc and Migdalek (1990)	IP of Ag and Au.
Marian (1990b)	Cu EA increased by 0.02 eV by relativity.
Sundholm and Olsen (1990a)	QR EA of B.
Zhuikov et al. (1990)	E104 (Ku) IP_1-IP_4. MCDF.
Chung (1991a)	IP of Li-like $1s^2 2s$ systems, Z= 3-10.
Cowan and Wilson (1991b)	EA for Be, C-Pb, Mg-Ra and Zn-Hg calculated at HFR level.
Küchle et al. (1991)	EA and IP of Hg-Rn, as tests of new PP. QR/NR.
Mitás et al. (1991)	Si, Sc and Cu IP and EA from QMC.
Nicolaides and Aspromallis (1991)	No EA for He or Xe. Levinson's theorem and MCHF used, respectively.
Nogueira and Guenzburger (1991)	Valence-orbital ionization potentials (VOIP) for 5d elements, Hf-Hg, from DFT. R/NR.
Tupitsyn (1991)	U IP. MCDF.
Vosko et al. (1991a)	Yb EA predicted to be 0.054(27) eV for the $6s^2 6p_{\frac{1}{2}}$ state. The $6p_{3/2}$ is unbound. DFT.
Vosko et al.(1991b)	La and Ac EA from DFT.
Chung (1992)	IP of Li-like systems, Z = 11-20.
Glushkov (1992b)	Obtains positive EA for Kr and Xe in a model potential method.
Ionova et al. (1992)	IP_n of V-105, 103-105. MCDF.
Leininger et al. (1992)	EA and IP of K-Cs, Ca - Ba and Fe -Os using four different PP.
Miecznik et al. (1992)	EA of Be in a $1s2s2p^2$ ^5P state.
Samzow et al. (1992a)	IP and EA fo Ag and Au as tests of a 'no-pair' method.
Vijayakumar and Gopinathan (1992)	IP_1-IP_3 of He - Zn using the relativistic, correlated Ξ method.
Yamamoto et al. (1992)	IP of Hf.

Table 5.5 Supercritical (Z>137) systems. For a more thorough compilation, see the treatises of Greiner et al. (1985) and Greiner (1987). Several further calculations on many-electron systems are covered in Ch. 7.

Reference	Comments
Pomeranchuk and Smorodinsky (1945)	Dependence of the critical radius for Z>137 on nuclear radius.
Voronkov and Kolesnikov (1960)	ns-states for finite nuclei with Z>137.
Klein and Rafelski (1975)	Bose condensation in supercritical external fields: KG particles and $Z \geq 10^3$.
Bosch (1986)	A review on superheavy atoms.
Herath Banda et al. (1986)	δ-electron emission from superheavy collision systems with Z_{tot}=110-171.
Soff et al. (1986,1987)	Exotic phenomena in collisions of very heavy ions.
C.-Y. Wong (1986,1987)	Suggested origin of the positron peaks.
Greiner (1987)	Physics of strong fields. Book.
Rumrich et al. (1987)	Influence of strong **B** (10^{15} G) on positron production in heavy-ion collisions.
B.Müller (1987)	The many facets of the Dirac vacuum.
Bottcher and Strayer (1988)	Pair production in heavy-ion collisions. A one-dimensional TD model solved numerically.
Butler et al (1988)	Positron interactions with element 164: knock-out and positronium formation.
Ionescu et al. (1988)	Nonlinear terms ?
Seba (1988)	Absorption of Dirac eigenvalues by the continuum. 1D and 3D.
B.Müller et al. (1989)	Attempts to explain the GSI positron lines.
Rhoades-Brown et al. (1989)	Pair production associated with electron capture in heavy-ion collisions.
Rumrich et al. (1989)	Continuum states.
Mishustin (1990)	Instability of the Dirac nucleon sea in relativistic nuclear collisions.
Rosenberg (1990)	Dynamics of neutral vacuum decay.
Strayer et al. (1990)	Muon pair production and subsequent μ^- capture into a 1s state. Numerical 3D solution for Au+Au.
Bawin and Cugnon (1991)	"Partially screened solutions" for the Dirac equation in $Z>Z_c$ Coulomb fields.
Graf et al. (1991)	Review on QED in strong Coulomb fields.
Momberger et al. (1991)	Electron-positron pair production in relativistic heavy-ion collisions.
Horbatsch (1992)	Search for narrow resonances due to spin-spin interactions.

Table 5.5. (continued).

Thiel et al. (1992)	Electron-positron pair creation in U^{92+} - U^{91+} collisions.
Wells et al. (1992)	Lepton-pair production in relativistic heavy-ion collisions. Au + Au at 2-100 GeV/nucleon 3 + 1D FEM solution in a Cartesian lattice.

Table 5.6. Electromagnetic transition probabilities.

Reference	Comments
Drake and Dalgarno (1968); Drake et al. (1969)	Two-photon decay of 2 $^3S_1$ He-like systems attributed to singlet-triplet mixing in the intermediate P state.
Taksar et al. (1971)	Na 3p, 3d TP from a simple PP.
Nicolaides (1972)	C I $2s2p^3$ and O I $2p^3 3s$ $^5S_2$ state lifetimes. SO allowed E1 dominates, $^3P_2$ mixed to upper state.
Lin and Feinberg (1974)	Radiative corrections to M1 of H-like ions.
Barbieri and Sucher (1987)	Radiative corrections to one-photon decay rates.
Borisoglebskii and Yakimovich (1985)	Nuclear E2-induced, $\Delta L=\Delta j=\pm 3$ electronic transitions.
Band et al. (1986)	X-ray transitions.
Biémont (1986)	Sulfur sequence 3s-3p, 3p-3d and 3p-4s TP, up to Ti VII.
Biémont and Hansen (1986a)	M1 and E2 TP in Ge and As sequences.
Biémont and Hansen (1986b)	M1 and E2 TP within $3p^4$ and $4p^4$ configurations.
Braun and Parera (1986)	TP between degenerate levels of the relativistic many-electron atom.
Fawcett (1986)	Fe XV 3-3 and 3-4 transitions.
Froese Fischer (1986)	$2p^{-1}$ 3s3p, 3d and 4s quartet level lifetimes.
Froese Fischer and Godefroid (1986)	E2 and M1 TP for P-like, $3p^3$ systems, Z=16...42.
Fulton and Johnson (1986)	2s-np, 2p-3d TP for Li at DF level using "effective current" approach derived from QED. Length and velocity forms equal.
Karim and Bhalla (1986)	E1 TP for 2l3l' and 2l4l' states of He-like Cr.
Kotochigova and Tupitsyn (1986b)	MCDF calculations of TP of Ba.
Krause (1986)	2-1 TP of He-like systems, Z=2-100, in a screened hydrogenic basis.
Migdalek and Baylis (1986a)	Cd sequence $5s^2$-5s5p TP.
Migdalek and Baylis (1986b)	Yb $6s^2$-6s6p TP.
Mu and Crasemann (1986, 1988)	Two-photon transitions in inner shells of Mo, Ag, Xe, DS.
Safronova (1986a)	$1s^2 2l2l'$ - $1s^2 2l3l''$ TP from 1/Z PT.
Sebastian (1986)	Relativistic invariance of the two-photon transition amplitude of a composite system.
Vidolova-Angelova et al. (1986)	Tm $4f^{13}6s$ $(n_R l_R)$ Rydberg states, n_R=10-50, l_R=0,1.
Biémont and Hansen (1987a)	2p-3s, 2p-3d, 2s-3p and 3p-3d TP for Ne-like ions, K X - Se XXV.

Table 5.6. (continued).

Biémont and Hansen (1987b)	M1 and E2 TP within $3p^N$ and $4p^N$. Ga I - Xe XXIV.
Brage and Litzén (1987)	Ni-like 4s-4p transitions, Zr XIII - Mo XV. MCDF.
Chen and Crasemann (1987a)	1s2p3d $^4F_{9/2}$ metastable states of Li-like ions, Z=6...42. E1, E2 and M2 processes.
Chen and Crasemann (1987b)	Radiative decay of $1s^{-1}$ states in B-like ions, Z=6...54.
Dzuba et al. (1987a)	Au, Tl E1 TP.
Fawcett (1987a)	Allowed 2-2 and 2-3 TP for the C-like ions, Z=9-28.
Fawcett (1987b)	C I, N II, O III.
Fechner et al. (1987)	Eu I $4f^7 6s6p$ TP.
Froese Fischer (1987)	2p-3s TP of O I.
Glushkov et al. (1987)	Al-like systems, Z=23-32. E1 TP. Model potential.
Johnson et al. (1987)	Li-Cs ns-np TP.
Migdalek and Baylis (1987a)	Hg $6s^2$-6snp TP, n=6-20.
Migdalek and Baylis (1987b)	$6s^2$-6s6p TP, Lu II - Ta IV.
Migdalek and Baylis (1987c)	Ba $6s^2$-6s6p TP.
Migdalek and Baylis (1987d)	$5s^2$-5s5p TP, Sr I, Y II.
Migdalek and Bojara (1987, 1988)	ns^2-nsnp TP of Cd and Hg.
Migdalek and Wyrozumska (1987)	Cs sequence. Collapse of f and d orbitals seen in TP.
Mohan and Hibbert (1987)	$6s^2$-6s6p TP of Hg using a MP.
Steiger (1987)	E1, E2, M1 and M2 TP for Li-like ions, up to $5f_{7/2}$ levels. MCDF + Breit + QED. Z=26...94.
Su and Eberly (1987)	"Essential states" in the theory of electron-photon interactions.
Verhey et al. (1987)	M1 $^2P_{1/2}$ - $^2P_{3/2}$ TP for the B-like sequence. 1st-order Breit and QED included.
Ali and Kim (1988)	E2 and M1 TP for the K isoelectronic series. (4s above 3d for Sc^{2+}- Cr^{5+}).
Barut and Salamin (1988)	Relativistic theory of spontaneous emission. Applied on 2p-1s and 2s-1s of hydrogen and muonium.
Biémont (1988)	n = 3-4 and 4-4 TP for Cu-like ions, Z = 38-60.
Bouchiat and Piketty (1988)	M1- and E2-hfs-induced 6s-7s TP for Cs.
Brage (1988)	Thesis on TP calculations.
Carson (1988)	Bound-bound multipole TP for H-like atoms.
Curtis et al. (1988)	3s, 3p and 3d level TP for Ne-like systems, Z=16-18.

Table 5.6. (continued).

Fawcett and Cowan (1988)	Fe I. HFR.
Froese Fischer (1988)	MCHF TP of 2^3S - 2^3P Li II. Also the ns-np TP of Li I, Na I, K I.
Luo et al. (1988)	Si II resonance lines.
Mohanty and Sampson (1988)	E1 TP for H-like ions as test of various QR approximations.
Saloman and Kim (1988, 1989)	M1 and E2 TP between ground-state terms of S-like systems, Z=15-92. For heaviest atoms $3p^4$ mixes significantly with p^2d^2 for $^3P_1$, $^1D_2$ and $^1S_0$ states.
Theodosiou and Curtis (1988)	Na-sequence TP, Z=11-54...92. 3p, 3d.
Zhao and Pan (1988a)	$2p^53s$, 3p and 3d TP of Ne-like Kr. MCDF.
Zhao and Pan (1988b)	Fe XVII.
Zhao and Wang (1988)	Pd I 6p7s TP. MCDF.
Becker et al. (1989)	M1 and E2 TP for N-like, $2p^3$ levels, Z=9-26.
Biémont (1989)	n=4-4 TP in zinc-like ions.
Biémont and Hansen (1989)	TP in 3d and $3d^9$ configurations.
Biémont et al. (1989)	Zn-like ions.
Blundell et al. (1989a)	All-order E1 TP for 2s, 2p and 3s states of Li and Be^+. Agreement with experiment 0.1 %.
Chen and Crasemann (1989c)	n=2 and 3 E1 TP for O-like ions.
Curtis (1989)	M1 TP for nsnp states in the Be, Mg and Zn series.
Curtis and Theodosius (1989)	4p and 4d TP for Cu-like systems, Z=29-92.
Davis and Chung (1989)	Li-like 1s2s2p ^4P_J TP, Z=3-18.
Drake and van Wijngaarden (1989)	Radiative transitions in one- and two-electron ions.
Dzuba et al. (1989b)	Cs 6p, 7p E1 TP.
Goldman (1989b)	Two-photon TP for 2s H-like systems, Z=1...100.
Gulov and Ivanova (1989ab)	Ne-like ions.
Hibbert (1989)	Reviews model potentials in oscillator-strength calculations. Al II, Zn, Cd-like and Hg ns-np E1 TP.
Ivanova et al. (1989)	Forbidden 2-3 radiative transitions in Ne-like ions.
Jankowski and Polasik (1989)	$K\beta/K\alpha$ x-ray intensity ratios for Ti...Ge. Influence of Breit and QED terms considered.
Migdalek and Stanek (1989)	Zn sequence $4s^2$-4s4p TP.
Mukoyama (1989a)	M-shell x-ray TP of Dy. DF.
Mukoyama and Adachi (1989)	K-shell x-ray TP in superheavy elements.
Ostrovskii and Sheinerman (1989)	Hg^+ E1 TP for 7p-7s, 6s and E2 TP for nd-ns. R/NR HF.

Table 5.6. (continued).

Sampson et al. (1989)	E1 TP for Ne- and Ni-like ions as test of a new DS program.
Sen and Puri (1989a)	E1 TP for ns-np of Be-Ra. LSD. Isoelectronic cations (q=+1 to +3) included.
Sen and Puri (1989b)	E1 TP for ns-np of alkali metal-like systems.
Theodosiou (1989)	TP of Ca^+. ns, np, nd, 4f.
Tong and Li (1989); Tong et al. (1990)	Two-photon decay rates in atomic inner shells. Mo, Ag, Xe. Relativistic decrease analysed.
Tulkki and Åberg (1989)	Photoabsorption of positive heavy ions. Oscillator strength concentrates to nl ->n (l+1) transitions. Origin a phase-shift of π between the wave functions in a Coulomb field.
Vidolova-Angelova et al. (1989)	Tm Rydberg states.
Zilitis (1989)	TP of K-like systems, Z=19...92.
Beck and Cai (1990)	Tl^+ $6s^2$ - 6s6p E1 TP.
Biémont (1990a)	Forbidden lines in the K sequence, Cd^{29+} - Ce^{39+}.
Biémont (1990b)	Review on heavy-element TP.
Biémont et al. (1990)	n=4-4 TP for Ge-like ions Rb VI - Ag XVI.
Biémont and Quinet (1990)	Ga-like systems, Br V - In XIX.
Curtis (1990)	Semiempirical formulations of line strengths using singlet-triplet mixing angles.
B.P. Das and Idrees (1990)	nsnp $^3P_1$ $^1S_0$ TP for B^+ - Tl^+.
B.P. Das et al. (1990)	M1 FS TP between $1s^22p$ levels of Li-like systems, Z=5-28.
Davis and Chung (1990)	Li-like $2p^2np$ $^{4,2}S$ and 1s2pmp $^{4,2}P$ states.
Greene (1990)	nsnp ^3P lifetimes of M^-, M=Rb-Fr.
Guet et al. (1990)	3s-3p TP of Na-like ions. Z = 11-29.
Hansen (1990)	Oscillator strengths for astrophysics and fusion. Proceedings of Amsterdam 1989.
Hartley and Mårtensson-Pendrill (1990)	E1 transitions of Cs and Tl.
Lindroth and Salomonsson (1990)	Ar^{16+} 2 $^3S_1$ - 1 $^1S_0$ transition dominated by M1. Calculated lifetime 209.4(4) ns.
Migdalek and Baylis (1990)	$6s^2$-6s5d E2 TP for Ba.
Migdalek and Stanek (1990)	ns^2-nsnp TP for Zn I, Rb VIII, Hg I and Rn VII. Various approximations compared.
Mohan and LeDourneuf (1990)	E2 and M1 for the J = 3/2 - J = 1/2 FS transition of Si^{5+} $2p^5$.
Nefiodov (1990)	Spectral line shape in non-resonant laser field.
Pal'chikov (1990)	Two-photon transitions.

Table 5.6. (continued).

Sampson et al. (1990)	TP of Na-like ions, Z=22-92.
Tiwary et al. (1990)	Rb I, Sr II, CS I, Ba II ns-np TP at BP level.
M. Wilson (1990)	Radiative decay rates in Hg^+.
Zhu and Pan (1990)	MCDF methodology for E1 TP.
Baik et al. (1991)	E1, E2 and M1 TP for Na-like ions, $56 \leq Z \leq 92$.
Band et al. (1991)	4d-nf TP of Ba^{2+}.
Biémont (1991)	Allowed transitions in Al V - Al VII.
Bieron et al. (1991)	np^2-np(n+1)s TP for Ge I...Bi II.
Blundell et al. (1991a)	All-order TP for Cs.
Chou et al. (1991)	Pb-like $^3P_{0-1}$ M1 TP. Z=82-98.
Dzuba et al. (1991b)	Bi $6p^3$ M1 TP.
Eissner (1991)	Breit-Pauli calculations of E1 and M1 TP. He-like systems.
Fawcett (1991)	Review on oscillator strengths.
Fawcett and Wilson (1991)	Yb II.
Feldman et al. (1991)	M1 TP between $3d^4$ ^5D levels of Ti-like ions, Z=42...92.
Froese Fischer and Godefroid (1991)	MCHF BP program for E1, E2,... and M1, M2... TP.
Glushkov (1991)	E1 TP of Fr-like ions using a MP method.
Guet and Johnson (1991)	ns-np, ns-(n-1)d and np-(n-1)d TP for Ca^+-Ba^+. E1, E2.
Ivanova and Gulov (1991)	E1-E3 and M1-M3 TP for $2s^{-1}nl$ and $2p^{-1}nl$, n=3, 4, levels of Ne-like systems, Z=27-92.
Kagawa et al (1991)	E1 TP for $2s^{-1}$ and $2p^{-1}$ levels of Ne-like systems, Z=18...54. STO-CI.
Karwowski and Martin (1991)	E1 TP for the ns-np transitions in the Li-, Na- and Cu-like sequences using "relativistic quantum defect orbitals".
Martin et al. (1991)	3s-3p and 3p-3d TP for the Na-like series, Z=11...99. QDO.
Migdalek and Baylis (1991a)	Yb $6s^2$-6s6p and -5d6s E1, E2, M1 and M2 TP.
Migdalek and Baylis (1991b)	La II 5d6p lifetime.
Perger et al. (1991)	$6p^2$ resonance width for Hg.
Quinet and Biemont (1991)	X-ray TP of Ni-like ions,Ag XX-Pb LV.
Quinet et al. (1991)	Allowed and forbidden transitions in Ne-like ions, Ni XIX - U LXXXIII.
Reiche and Zschornak (1991)	X-ray emission rates i ncluding electron-exchange corrections. MCDF.
Sampson et al. (1991)	TP of F-like ions, Z= 22-92.
Shabaev (1991b)	QED theory of resonance line shapes in few-electron atoms.
Tayal (1991)	Ga II 4s4p, $4p^2$ and 4s4d-level TP.
Y. Zhang et al. (1991)	Na-like Fe.
Zhu et al. (1991)	n=3 to n=2,3 TP in F-like Se.
Biémont et al. (1992)	Intra-$3d^2$, $3d^2$-3d4s and $3d^2$-3d4d TP (M1, E2) for Z = 22-47. MCDF, HFR and "SST" compared.

Table 5.6. (continued).

Bieron and Migdalek (1992)	As I, Sb I, Bi I $np^2(n+1)s$ TP. MCDF.
Chou and Huang (1992a)	6s-6p E1 TP of Hg-like systems, Z=80-93.
Chou and Huang (1992b)	5s-5p TP of Cd-like systems, Z = 48-65.
Eissner and Tully (1992)	Be-like systems, Z = 6...26. $2p^2$-2s2p and two-electron $2p^2$-2s3p TP.
Glushkov (1992ac)	s-p and p-d TP for K-, Rb- and Cs-like systems.
Gorshkov et al. (1992)	QED theory of U^{90+} line profiles.
Grotch et al. (1992)	Relativistic wave-function corrections to E1 TP of bound $b\bar{b}$ systems.
Grozdanov et al. (1992)	Photoexcitation of H-like Rydberg states in microwave fields.
Hibbert et al. (1992)	$2p^5 3l$ lifetimes of S VII-Ar IX.
Kuplyauskene and Zhukauskas (1992)	Decay of $2p^{-1}3l3l'$ states of Na-like Cl and Ar.
Lamoreaux and Fortson (1992)	Electric-field (Stark effect) changes of Hg $6s6p(^3P)$-$6s^2$ TP.
Lavín et al. (1992)	Na-like systems, 3s-np (n=4-6), Z=18...42. Quantum defect theory.
Liaw (1992)	Transition amplitudes in DF theory. B-splines. Li-, B-, Na- and Al-like systems.
Loginov (1992)	$5d^6 6p$ lifetimes of Tl IV - Bi VI.
Martin et al. (1992)	Excited-state p-d and np-6s TP for Cu-like ions, Z = 33...70.
Miecznik et al. (1992)	High-spin ^6P-^6S TP of B-like systems, Z = 5...13.
Pinnington and Baylis (1992)	Hg-like systems, Z = 80, 82, 83.
Safronova and Wyart (1992)	Ne-like systems, Z = 30...92. $2S^{-1}3l$-state TP.
Seke (1992c)	Non-exponential $2p_{\frac{1}{2}}$-1s decay of Dirac hydrogen.
Theodosiou et al. (1992)	2p lifetimes in the Li sequence, Z = 3-92.
Vidolova-Angelova (1992)	Rydberg-state lifetimes of Lu.
Zhang and Sampson (1992)	$\Delta n=0$ transitions of Be-like systems, Z = 8-92.
Y. Zhang et al. (1992a)	Radiative TP for Na-like ions, $n \leq 15$, $l = \leq 6$, Z = 38-45.
Q.-R. Zhu et al. (1992)	Li-like ions, Z = 20-25.
Zilitis (1992)	Principal series of K-like ions, Z = 22...92.

Table 5.7. Polarizabilities and screening constants. α_L and χ_L stand for electric and magnetic polarizabilities and γ_L and σ_L for electric and magnetic screening constants, respectively.

Reference	Comments
Dzuba et al. (1986b)	Shielding of external electric fields in atoms. Radial dependence for Tl^+.
Lombardi (1987)	Determines core dipole and quadrupole polarizabilities for Na from model-potential fits.
Silberbach (1987)	Polarizabilities of Ba, Au, Hg, Tl and Pb as test of a semiempirical PP.
Gray et al. (1988)	Experimental dipole and quadrupole polarizabilities for Na^+ from Rydberg states.
Zapryagaev et al. (1988)	Polarizabilities of Li- and Na-like ions from the quantum defect method.
Goldman (1989a)	Accurate dipole polarizabilities for H-like systems, Z=1...115.
Pal'chikov and Tkachev (1989)	Electric polarizability and hyperpolarizability of He-like systems.
Zhou and Norcross (1989)	Scalar and tensor polarizabilities α_0 and α_2 for Cs $6p_{3/2}$. Also α_0 for 6s, 7s, $6p_{1/2}$. Model potential.
De Sanctis (1991)	Polarizabilities of exotic atoms. All EL evaluated. E1 relativistic α^2 correction.
Sadlej (1991)	Au α_1. QR/NR.
Sadlej et al. (1991)	Polarizabilities of Ca-Ba. Relativistic decrease analysed.
Kutzner et al. (1992)	Frequency-dependent polarizabilities of H^-, F^- - I^-.

Table 5.8. Electric and magnetic hyperfine properties.
E0: Isotope and Moessbauer isomer shifts, E2: Nuclear electric quadrupole interactions, E4: Nuclear electric hexadecapole interactions, M1: Magnetic dipole and M3: Magnetic octupole hyperfine effects.
For Sternheimer factors see Table 5.7.

Reference	Comments
Schüler and Schmidt (1936)	Angular parts and relativistic corrections for E2 hfs of p electrons.
Desclaux (1971)	M1 and E2 hfs of Sc, Cu, Ga, Br and Li-Fr at DF level.
Huang and Hughes (1979)	M1 hfs of muonic He, $\alpha\mu^-e^-$. Relativistic, recoil and radiative corrections included.
Mårtensson-Pendrill and Salomonsson (1984)	M1 and E2 hfs of Ca^+ 4s, 4p and 3d states.
Band et al. (1985)	M1 hfs in highly excited H-like, Li-like and Na-like atoms, $Z \leq 28$.
Bauche et al. (1986)	Cs and Fr isotope shifts.
Baumann and Braun (1986)	Yb 6s6d state E2, M1. Exp.,DF.
Bouazza et al. (1986)	Pb II.
Childs et al. (1986)	$4f^{11}5d6s^2$ of Er I. M1 and E2 hfs. MCDF.
Nielsen and Pfeufer (1986)	E0 hfs of Er I, $4f^{11}5d6s^2$. MCDF.
Swainson and Drake (1986)	M1 and E2 hfs of muonic Li, Be and B.
Vainshtein et al. (1986)	Hfs parameters for Li-like systems.
Blundell et al. (1987a)	Field isotope shifts in atoms. New theoretical formulation. Z=19-95 tabulated.
Druzbick and Williams (1987)	M1 hfs of ^3He 1s2s and $^3He^+$, 1s and 2s.
Dzuba et al. (1987a)	Au, Tl.
Johnson et al. (1987)	Li-Cs valence states. M1.
Martynenko and Faustov (1987)	M1 hfs of muonium.
Nielsen et al. (1987)	M1 and E2 hfs of Er I + II + III MCDF.
Olsson and Lindgren (1987)	Analyse the hfs tensor operators needed in relativistic MBPT. Sandars and Beck (1965) OK.
Wendt et al. (1987)	E0, E2 and M1 hfs of Ra I and Ra II.
M. Wilson (1987)	QR calculations of charge densities at nucleus for Re as function of configuration.
Yelkhovsky (1987)	Comments on the nuclear M1-induced hydrogen-atom 1s (F=3/2) E2. See also Pilkuhn (1987).
Zimmermann (1987)	Effect of s-electron normalization on M1 hfs.
Amus'ya et al. (1988bc)	M1 hfs in the He^{++}-μ-e atoms.
Bouazza and Bauche (1988)	Pt II, Au II, Bi II M1 data interpreted at DF level.
Childs and Nielsen (1988)	La I $(5d+6s)^3$ M1, E2 hfs. MCDF.

Table 5.8. (continued).

Grexa et al. (1988)	Tl np state A, n=6-8.
Kutzelnigg (1988)	Origin and meaning of the "Fermi contact" (s-AO M1 hfs) interaction.
Millack (1988)	M1 hfs for a single valence electron, Li-Cs, Cu-Au, B-Tl. The g-Hartree method used.
Trusov and Eglais (1988)	E0 of Fe.
Young et al. (1988)	Sc II hfs. MCDF.
Aaen Andersen et al (1989)	M1 and E2 hfs of $4f^{12}5d$ levels of Er II. MCDF with core exitations and CI.
Blundell et al. (1989a)	M1 and E2 for Li and Be^+ from all-order MBPT.
Dzuba et al. (1989b)	Cs ns, np (n=6, 7) M1 hfs.
Kuten' and Rapoport (1989)	An atomic octupole (M3) moment is induced in the F=3/2 $1s_{1/2}$ and $2p_{1/2}$ states of H-like atoms by the M1 hfs.
Mansour et al. (1989)	Sc II. E2 well predicted by MCDF, M1 hfs less well.
Millack (1989)	M1 hfs of Li and B using "2nd-order g-Hartree" approach.
Panigrahy et al. (1989)	M1 hfs in Be^+-Ne^{7+}, Bi^{80+}. Radiative corrections included.
M.-K.Chen (1990)	M1 hfs of muonic He.
Hartley and Mårtensson-Pendrill (1990)	Hfs of Cs and Tl.
Milstein and Yelkhovsky (1990)	Vacuum-polarization "dressing" of nuclear Q.
Neugart et al. (1990)	M1 hfs of Ra isotopes.
Sen et al. (1990)	Eu $4f^75d$ and $4f^76p$ field isotope shifts, E0.
Shabaev et al. (1990)	Nuclear-size effects, based on nuclear $\langle r^2\rangle$ and $\langle r^4\rangle$ estimated for multiply charged ions, Z≤100. Precision ≤ 0.2%.
Sundholm and Olsen (1990b)	QR corrections to E2 hfs of S^- ($^2P_{3/2}$).
Beck and Datta (1991)	M1 hfs of the $5s^1$ Ag I series, Ag I-Sb V.
Blundell et al. (1991a)	All-order MBPT M1 hfs for Cs.
Elkhovskii and Mil'stein 1991)	Vacuum polarization, induced by nuclear M1 and E2 multipole moments.
Hartley and Mårtensson-Pendrill (1991)	Volume and mass isotope shifts of Cs and Tl.
Panigrahy et al. (1991a)	M1 hfs of $^{213}Ra^+$.
Panigrahy et al. (1991b)	M1 hfs of M^+, M=Zn-Hg.
Andriessen et al. (1992)	Ra II 7s and 7p M1 and E2 hfs. MCDF versus MBPT.
Beck (1992)	Y II $4d^2$ M1 hfs. MCDF + CI using H-like orbitals.
M.-K. Chen (1992)	M_1 hfs of $(1s)_e$ $(2s)_\mu$ muonic helium. NR Hylleraas + 1st-order R and QED corrections.
Indelicato et al. (1992)	Decay of He-like Gd 2 $^3P_0$ to $1\,^1S_0$ due to M1 hyperfine mixing with 2 $^3P_1$.

Table 5.8. (continued)

Mårtensson-Pendrill and Ynnerman (1992)	E0, M1 and E2 hfs of Ba^{+} (6s, 6p).
Mårtensson-Pendrill et al. (1992)	Isotope shifts of Ca.
Pindzola et al. (1992)	Dielectronic recombination between ground-state hyperfine levels of Bi^{82+}.
Shabaeva and Shabaev (1992)	M1 hfs of Li-like Fe^{23+}.
Villemoes et al. (1992)	Sc II 3d4s, $3d^2$ and 3d4p-level M1 and E2 hfs. MCDF.

Table 5.9. Average radii $\langle r^n \rangle$ and magnetic g-factors.

Reference	Comments
Karaziya (1981)	Excited-electron orbit collapse and atomic spectra. The d shells collapse from outer to inner well around Z=20, 38, 56, 88 and 120, f shells around 57, 90 and 122, g at 124. Effective potentials sketched.
Amus'ya (1987)	Quadrupole moments of atoms with $J=\frac{1}{2}$.
Veseth (1987b)	g_J for Al-Cl.
S. B. Zhang et al. (1987)	"Nodal radii" (radius to last node) calculated for s, p and d orbitals of Li-La, Hf-Rn. Relativistic effects up to 10% for s, show no "gold maximum".
Cortona (1989)	$\langle r^n \rangle$ for Gd^{3+} in a spin-polarized LD model.
Raspini (1989)	Relativistic Zeeman effect in positronium, n=2.
Sai Sunder and Sen (1989)	Ionic radii (r_m) of Be^--Ba^- and some metastable atoms. QR LDF.
Sen and Politzer (1989)	Radii r_m for 3d, 4d and 5d metal anions. LSD.
E. Johnson et al. (1990)	Hf and E104 r_m.
Zhuikov et al. (1990)	Atomic and ionic radii of E104.
Cortona (1991)	Spin-polarized Ce^{3+} $\langle r^n \rangle$.
Demkov and Rebane (1991)	Propose a direct atomic or molecular experiment for g-2.
Dzuba et al. (1991b)	Pb $6p^2$, Bi $6p^3$ level g-factors.
Fawcett and Wilson (1991)	Yb II g-factors.
E. Johnson and Fricke (1991)	r_m for M^{n+}, M = Ti-E104, n=1-4. Used for estimating thermodynamic properties.
Kohout et al. (1991)	Search for shell structure in plots of density Laplacian or local kinetic-energy density. Be...Pb.
Aktas et al. (1992)	SO-corrections to g_J of Li.
Sundholm and Olsen (1992a)	Atomic quadrupole moment of Ca 3d4s ^1D. QR.

Table 5.10. Compton profiles, momentum distributions and spin densities. For basic theory of the Compton effect, see also Table 5.14.

Reference	Comments
Dutta et al. (1986)	Compton profiles for Kr-Rn. Screened hydrogenic functions used.
Frost et al. (1986)	Pb 6s and 6p momentum distribution. MCDF.
Glass (1987a)	Spin magnetic form factor for V. Atomic correlation and SO included.
Glass (1987b)	Ditto for Co and Ni.
Cortona (1989)	Spin densities for Gd^{3+} in a spin-polarized LD model.
Cortona (1991)	Spin-polarized Ce^{3+} spin densities.
H.-S. Li et al. (1991)	Intra-atomic exchange integrals between 4f, 5d and 6s in Ln^{3+}. Magnetic properties of rare-earth intermetallics.

Table 5.11. X-ray scattering factors.

Reference	Comments
Kane et al. (1986)	Review on elastic scattering of gamma- and x-rays by atoms.
M. S. Wang (1986)	Relativistic dispersion relation to order $\alpha^2 Z^2$ for x-ray anomalous scattering factors.
Smith (1987)	Anomalous x-ray scattering. Rayleigh scattering reduced for bound electrons from the free-electron value by relativistic effects (mainly h_m). Higher multipoles and retardation must be included for heavier elements.
Saloman et al. (1988)	Total x-ray absorption cross-sections for E = 0.1-100 keV and Z=1-92. DS.
Ehlotzky (1989)	Scattering of x-rays by relativistic electrons in a strong laser field.
Fox et al. (1989)	X-ray scattering factors for atoms, Z=2-98.
Kahane et al. (1989)	Gamma-ray Rayleigh scattering from U, E = 0.4-3 MeV.
Sasaki (1989)	Tables of anomalous scattering factors.
Wang and Chia (1989)	X-ray atomic anomalous scattering factors for Zr, Nb, Mo.
Kissel and Pratt (1990)	Z-dependent, energy-independent corrections to anomalous scattering factors. Higher multipoles important. Z=1-100.
Namikawa et al. (1990)	X-ray magnetic scattering from atomic inner-shell electrons.
Kefi et al. (1992)	X-ray anomalous scattering factors of Pd...Xe. R correction to the dispersion term.

Table 5.12 Electron and positron scattering.

Reference	Comments
Rosen (1963)	Relativistic Coulomb scattering.
Rotenberg (1966)	Small relativistic effects in a model potential study of slow-electron scattering by Na and Cs.
Spruch (1966)	Discusses R/NR comparisons for slow-electron scattering.
Meister and Weiss (1968)	Scattering of E<200 eV electrons from Ar, Xe, Hg.
Scofield (1978)	K- and L-shell ionization by relativistic electrons, Z=18-92, E=50 keV -1 GeV. DS.
Kemper et al. (1985)	Elastic scattering of slow electrons from Ar-Xe. Two-channel approach.
Bartschat and Burke (1986)	Relativistic effects on low-energy electron scattering from Hg.
Chen (1986a)	Dielectronic recombination of He-like systems, Z=6...42.
Chen (1986b)	Dielectronic recombination of Ne-like systems, Z=18...54.
Chen (1986c)	Dielectronic recombination of F- and Ne-like Se.
Eichler (1986)	Relativistic "eikonal" theory of electron capture.
Huberland and Fritsche (1986,1987)	Low-energy elastic electron scattering from Hg-Bi using a Kohn-Sham approach. Spin-polarization emphasized.
Hasenburg et al. (1986)	Relativistic effects in elastic electron scattering from heavy atoms.
Jaskolski and Karwowski (1986)	QR approach to low-energy electron scattering from closed-shell atoms.
L.H. Kim et al. (1986)	Ratio of positron to electron bremsstrahlung energy loss.
McEachran and Stauffer (1986)	Spin polarization of electrons, elastically scattered from Xe.
Rosenberg (1986)	Relativistic scattering in a slowly time-dependent electric field.
Eichler (1987)	Relativistic charge exchange with Coulomb boundary conditions.
Jaskólski et al. (1987)	Low-energy electron scattering from Xe.
Kim and Pratt (1987)	Electron bremsstrahlung from Coulomb and DS potentials, Z=13...79, E= 1 eV-0.5 MeV.
Kobus and Jaskólski (1987)	Low-energy positron scattering from Hg as test for the QR approach.
Mc Carroll (1987)	Review on relativistic effects in electron capture.
McEachran and Stauffer (1987a)	Elastic and inelastic electron scattering from Xe.

Table 5.12. (continued).

McEachran and Stauffer (1987b)	Elastic electron scattering from Hg.
Norrington and Grant (1987)	Low-energy electron scattering by Fe XXIII and Fe VII using the Dirac R-matrix method.
Salvat et al. (1987b)	Elastic electron scattering of NR electrons from a MP fit to DS.
Sienkiewicz and Baylis (1987)	Elastic electron scattering from Ar.
Sud et al. (1987)	L-shell ionization by relativistic electrons.
Zygelman and Dalgarno (1987)	Electron-impact excitation of H-like n=2 FS levels.
Butler et al. (1988)	Positron interactions with Th, (164). Knock-out and positronium formation discussed.
Chen (1988a)	Dielectronic recombination for F-like ions, Z=26...63.
Chen (1988b)	Dielectronic recombination of H-like ions, Z=8...54. 1s+e -> nln'l' -> 1s n"l" + h .
Chen (1988c)	Effect of Koster-Kronig transition on dielectric recombination of He-like ions.
Chen and Crasemann (1988c)	Dielectronic recombination for $1s^2 2l2l'$ configurations of Be-like ions, Z=30...54.
Ehlotzky (1988)	Scattering of (spinless) electrons from a potential in a strong laser field. Sum rule.
Pindzola and Buie (1988); Pindzola et al. (1988)	Electron-impact ionization of h eavy atomic ions.
Reed (1988)	Electron-collision strengths for the 36 n=3 states of Ne-like Ba.
Reed et al. (1988)	Autoionizing resonances in electron-impact excitation of O-like Se. MCDF.
Ross and Fink (1988)	Spin-polarized atomic scattering factors for electrons. DF. E = 40 keV and Au as examples.
Stauffer (1988)	Relativistic effects in electron-atom scattering: a review.
Chen and Crasemann (1989a)	Contribution of autoionizing resonances to the n=2-2 electron- collisional excitation rates for Be-like ions.
Chen and Reed (1989)	Electron-impact excitation of n=2 and 3 transitions in Ne like ions, Z=15...54.
Fox et al. (1989)	Electron scattering factors for atoms, Z=2-98.
Jaskolski (1989)	QR (1-component but SO split) approach to many-channel electron scattering from atoms. Ca^+, Ba^+.

Table 5.12. (continued).

Pindzola and Buie (1989)	Electron-impact ionization of U^{16+} and U^{82+}. A HF/HFR/DF comparison.
Pindzola et al. (1989)	Electron-impact ionization of highly-charged ions in lowest-order QED.
Qian et al. (1989)	Electron-impact $2s^2$-2s2p excitations of Be-like systems, Ne^{6+}...U^{88+}.
Rhoades-Brown et al. (1989)	Electron capture associated with pair production in heavy-ion collisions.
Ritchie (1989)	Relativistic theory for electron-ion scattering. One continuum electron + Dirac-Coulomb.
Talwar and Wright (1989)	The radiation tail in electron scattering from finite nuclei.
Zhang and Sampson (1989)	Collision strengths for excitation to the n=3 and 4 levels of Ne-like ions, Z = 22-92.
Zhang et al. (1989)	Fully relativistic and QR distorted-wave methods for collision strengths of highly charged ions. He-, Li, Ne, Na and Ni-like ions.
Bartschat (1990)	Spin-orbit and interference asymmetries in elastic electron scattering from heavy one-electron ions.
Chen (1990a)	Resonant excitation in Ca^{q+} collisions with H_2 and He targets.
Chen and Reed (1990)	Effect of autoionizing resonances on n=3-3 electron-impact excitation rates in Ne like Se.
Chen et al. (1990b)	Contribution of resonant excitation double autoionization to electron-impact ionization ot Fe^{15+}.
Czyzewski et al. (1990)	Electron elastic scattering cross sections, $20eV \leq \epsilon \leq 20keV$, $Z \leq 94$.
Dasgupta and Whitney (1990)	Dielectronic recombination data in F-like ions, Z=18-34. HFR.
Pindzola and Badnell (1990)	Dielectronic capture processes in $U^{89,90+}$, colliding with H_2.
Reed et al. (1990a)	Excitation-autoionization processes in electron-impact ionization of Au^{68+}.
Reed et al. (1990b)	Xe^{43+}. Relativistic distorted-wave calculation of the cross section for n=2 -> 3,4.
Rumrich et al. (1990)	Basis-set truncation violates gauge invariance in the coupled-channel representation.
Sienkiewicz (1990)	Low-energy electron scattering from Hg.
Yuan and Zhang (1990)	Low-energy (E = 0.01-5 eV) electron scattering with Ca-Ra. QR.
Zhang and Sampson (1990)	Ionization cross sections for highly charged ions. H, He, Li, Ne and Na-like cases.

Table 5.12. (continued).

Zhang et al. (1990a)	Collision strengths and oscillator strengths for Ni-like ions with Z=60-92.
Zhang et al. (1990b)	Li-like ions, Z=8-92.
Zhang et al. (1990c)	Cu-like ions, Z=60-92.
Badnell and Pindzola (1991)	Dielectronic recombination of Bi^{80+} and Bi^{82+}.
Bartschat (1991)	Spin-dependent effects in elastic and inelastic low-energy electron scattering from Na.
Chen (1991a)	U^{q+} collisions with light targets.
Chen (1991c)	Dielectronic recombination of Li-like systems, Z=6...54.
Chen and Crasemann (1991)	Resonance enhancement of electron-impact excitation rates for Ar-like ions.
Decker and Eichler (1991a)	Exact 2nd-order Born calculations for relativistic electron capture.
Decker and Eichler (1991b)	Electron capture in $U^{92+} + U^{91+}$ collisions.
Dzuba et al. (1991c)	Scattering of very slow electrons by Ba and Ra. Resonance enhancement.
Hussein et al. (1991)	Symmetrical representation of incoming and outgoing wave functions.
Kato and Safronova (1991)	$2s^2$-2s2p-$2p^2$ electron excitation cross sections of Be-like systems, Z=8...42.
Kessler (1991)	Review on electron-polarization phenomena in electron-atom collisions.
P. Li and Q.-Q. Gou (1991)	Elastic scattering of slow electrons by Hg. R/NR.
Mian (1991)	Low-energy electron scattering from Hg.
Nahar (1991)	Cross sections and spin polarizations for $e^{\pm}$ scattering from Cd.
Nahar and Wadehra (1991)	Ditto for Ar.
Pindzola et al. (1991)	Electron scattering theory for highly charged ions: ionization, excitation and dielectronic recombination.
Reed et al. (1991)	Electron excitation-autoionization in Na-like ions, Z=26-92.
Rosenberg (1991)	Relativistic multiphoton bremsstrahlung.
Salvat (1991)	Elastic scattering of fast electrons and positrons from atoms. V(r) sum of Yukawa terms. Al, Ag, Au.
Sienkiewicz and Baylis (1991a)	Elastic electron scattering from Xe.
Sienkiewicz and Baylis (1991b)	Elastic positron scattering on Hg. Negative-energy DF treatment.
Sienkiewicz and Baylis (1991c)	Kr.
Szmytkowski (1991)	Relativistic polarized-orbital theory for elastic electron and positron scattering from closed-shell atoms.

Table 5.12. (continued).

Thumm and Norcross (1991)	The 6 $^3P^o_J$ states of Cs^- are unbound, narrow resonances. Model potential.
Wijesundera et al. (1991a)	Electron scattering by Ne-like Se using the Dirac R-matrix method.
Wijesundera et al. (1991b)	O-like Kr.
Yuan and Zhang (1991a)	Low-energy electron scattering from Xe. QR. E= 0.01-20 eV.
Yuan and Zhang (1991b)	Mg, Zn and Cd.
Zhang et al. (1991)	Electron collision strengths and oscillator strengths for Ni-like ions, Z=60-92.
Zuo et al. (1991)	Electron-impact excitation of Xe.
Badnell and Pindzola (1992)	Dielectronic and radiative-recombination cross sections for U^{90+} near KLL resonances.
Bartschat et al. (1992)	Polarization of 0-2.7 eV light, emitted by electron impact on Cs. Dirac R-matrix framework; BP not sufficient.
Chen and Reed (1992)	Electron-impact ionization of highly-charged Li-like ions, Z = 18...54.
Fritsche et al. (1992)	Consistent theory of electron scattering by atoms.
Hsu et al. (1992)	Positron-impact ionization of H.
Jakubassa-Amundsen (1992)	Relativistic (e, 2e)collisions. K-shell ionization of Cu-Au, E=300, 500 keV.
Kao et al. (1992)	Electron-impact ionization of H-like atoms, Z=1...47. R/NR.
Karasiov et al. (1992)	Electron recombination with H-like U. Resonance effects with doubly excited, $2s^2$ or $(2p^*)^2$ states.
Kheifets and Amusia (1992)	Xe 5s (e, 2e) process.
McEachran and Stauffer (1992)	Spin polarization of electrons elastically scattered from Cd and Zn. DF.
Mikhailov and Porsev (1992)	Double ionization of the atomic K shell in positron annihilation with a K electron.
Moiseiwitsch (1992)	α-expansions for electron capture.
Moores and Pindzola (1992)	Electron impact ionization of highly charged hydrogenic ions. Fully relativistic disorted-wave approximation, including Mφller interaction.
Pindzola (1992)	Positron-impact ionization of highly-charged ions in lowest-order QED.
Pindzola et al. (1992)	Dielectronic recombination between ground-state hyperfine levels of Bi^{82+}.
Reed and Chen (1992)	Electron-impact ionization of Li-like ions, Z = 6-9.
Safronova et al. (1992a)	Electron-impact $2s^2$-2s2p-$2p^2$ transitions of Be-like O, Si, Fe and Mo.
Spies et al. (1992)	Dielectronic and radiative recombination of Li-like Au.

Table 5.12. (continued).

Srivastava et al. (1992a)	Electron impact 5s-5p excitation of Cd.
Srivastava et al. (1992b)	Ditto for Hg.
Srivastava et al. (1992c)	Electron-impact excitation of Ca and Ba D states.
Srivastava et al. (1992d)	Electron-impact excitation of P states of Ca-Ba.
Thumm and Norcross (1992)	Electron scattering from Cs. Very narrow ^3P_J resonances found.
Weigold (1992)	A review on (e, 2e) electron momentum spectroscopy of atoms, molecules and solids. Relativistic effects seen for Xe and Pb valence shells.
Wijesundera et al.(1992a)	$6s^26p$ and $6s6p^2$ resonances in electron scattering by neutral Hg.
Wijesundera et al. (1992b)	Electron scattering from Pb. The $6s^26p^3$ states claimed to be resonances, despite of known Pb EA.
H.-Y. Yang et al. (1992)	Dielectronic recombination of F-like and Ne-like Ge.
Yuan and Zhang (1992a)	Spin polarization of electrons elastically scattered from Ba.
Yuan and Zhang (1992b)	Ditto, Hg.
Zuo et al. (1992)	Electron-excitation of Ar-Xe.

Table 5.13. Particle-atom collisions.
For processes involving hydrogen-like atoms, see also Table 2.3.

Reference	Comments
Au (1986)	Two-photon exchange in electron-atom scattering.
Becker et al. (1986)	U^{92+}-U^{91+} collisions.
Chen and Crasemann (1986)	N-shell ionization of Bi and U by protons.
Hagelstein (1986a)	Electron inelastic scattering from Ni-like Gd.
Hagelstein (1986b)	Electron inelastic scattering from F-like Se.
Leung et al. (1986)	Relativistic α^2 corrections to the Bethe sum rule.
Moiseiwitsch (1986,1987)	Relativistic eikonal approximation for electron capture.
Mukoyama (1986)	Excitation cross sections of H-like ions by heavy charged particles.
Hagelstein (1987)	Dielectronic capture into excited levels of Ne-like Se.
Hagelstein and Jung (1987)	Electron-collision cross sections for Ne-like ions.
Hino and Watanabe (1987,1989)	Radiative electron capture from target atom (Be) to relativistic, naked nucleus (Xe^{54+}, U^{92+}).
Kim and Desclaux (1987)	Relativistic effects in electron-atom collisions. Li-like ions.
Mukoyama and Lin (1987c)	Inner-shell ionization in ion-atom collisions using an analytic atomic basis.
Pacher et al. (1987)	Retardation effects in radiative electron capture. Xe^{54+}+e, H^+ + H(1s).
Pindzola (1987)	Giant resonances in elecron-impact double ionization of Fr^+.
Zygelman and Dalgarno (1987)	Proton-impact excitation of H-like n=2 FS levels.
Bar-Shalom et al. (1988)	Electron collision excitations of heavy ions in a "distorted-wave approximation". He-like Al XII, Ni-like Gd XXXVII.
Kim and Desclaux (1988)	Energy-dependence of electron-ion collision cross sections. Fe^{22+} $2s^2$-2s2p excitations.
Mehler (1988); Mehler et al. (1989)	Inner-shell ionization in ion-atom collisions.
Moiseiwitsch (1988)	Second-order OBK approximation for electron capture.
Momberger et al. (1988)	Angular distributions of electrons emitted from 1s and 2s states in heavy-ion collisions. Z+Au, Z+U.

Table 5.13. (continued).

Mukoyama and Sarkadi (1988)	Dirac-Coulomb continuum function at zero kinetic energy in ion-atom collisions.
Rustgi et al. (1988b)	Ionization of K-shell electrons by highly relativistic protons.
Struensee and Cohen (1988)	n=2 FS transitions in H+p collisions.
Bell (1989)	Double and triple differential cross sections for K-shell ionization by relativistic electrons.
Chen and Crasemann (1989b)	K-, L- and M-shell cross-sections for ionization by protons, Z=22...92. DS.
El-Ashry et al. (1989)	K-shell ionization.
Jakubassa-Amundsen (1989)	K-shell ionization by fast electrons. Ag and Ta targets.
Leung (1989)	Bethe stopping theory for heavy target atoms (Al...Au).
Mukoyama (1989b)	K-shell ionization by protons: screened Dirac-Coulomb and DS wave functions compared.
Grant (1990)	Electron-atom collisions: a review.
Jakubassa-Amundsen (1990)	Relativistic 2nd-order Born theory for electron capture.
Kumar et al. (1990)	K- and L-shell ionization cross-sections of Au by proton or alpha-particle impact. DF-LCAO.
Mayol and Salvat (1990)	Cross-sections for K-shell ionization by electron impact.
Mohan and LeDourneuf (1990)	Electron-impact collision strength for the FS excitation of Si^{5+} $2p^5\ ^2P$.
Moiseiwitsch (1990)	Electron capture at relativistic energies.
Moores and Pindzola (1990a,1991)	Electron-impact ionization of highly-charged hydrogenic ions.
Moores and Pindzola (1990b)	Electron-impact ionization of highly-charged ions. MCDF + Breit. Se^{24+}, Xe^{44+}, $U^{85,86+}$.
Mukoyama et al. (1990)	K-shell ionization by mesons.
Aggarwal et al.(1991)	Electron impact excitation of Ca XV. Lowest 20 levels.
Decker (1991)	Electron-positron pair production in relativistic heavy-ion collisions (p-U, U-U).
Eby (1991)	Production of low-energy electron-positron pairs by relativistic heavy ions.
Kürpick et al. (1991ab)	S^{16+} collisions on Ar.
Legrand et al. (1991)	L-shell ionization in p+Sm collisions, E=1 MeV. Dirac-Coulomb. Semiclassical.
Lindhard (1991)	Radiation from ultrarelativistic electrons, moving parallel to a crystal axis. Discusses the Dirac equation background.

Table 5.13. (continued).

Miller and Manson (1991)	Secondary electron energy-spectra in electron-impact ionization. He, E ≤ 5 MeV.
Moores (1991)	Electron-impact ionization cross-sections of highly-charged ions.
Mukoyama et al. (1991)	Relativistic effect on the ionization probability in the geometrical model.
Mukoyama and Lin (1991)	Inner-shell ionization cross sections in ion-atom collisions using discretized states with E>0 for the continuum.
Smit (1991, 1992)	Semiclassical approach to K-shell ionisation using H-like wave functions.
Sud and Moattar (1991)	K-shell ionization by relativistic protons.
Yudin (1991)	Unitary semiclassical theory of Coulomb excitation of atoms. Dirac equation for target electrons.
Amusia (1992)	A new "polarizational" Bremsstrahlung, due to dipole polarization of a colliding atom.
Glass et al. (1992)	The 'distorted wave model' of charge exchange must have correct spinor structure. Otherwise spurious spin effects result at NR limit.
Hofstetter et al. (1992)	Ionization of hydrogen by a relativistic heavy projectile.
Khriplovich and Pospelov (1992)	High-frequency asymptotics of optical activity and energy difference of chiral molecules.
Moiseiwitsch (1992b)	Electron capture from H-like ions by ultrarelativistic charged particle.

Table 5.14. Photon scattering and photoionization.

Reference	Comments
Waller (1929, 1930ab, 1934)	Photon scattering by bound and free Dirac electrons.
Seiler (1936)	X-ray dispersion and absorption in Dirac theory.
Pratt et al. (1964a)	K-shell photoionization cross sections, E=200 keV-2MeV. Dirac-Coulomb functions.
Pratt et al. (1964b)	Spin-polarized photoelectrons.
Mikhailov (1969)	K-shell photoionization near threshold.
Nicolaides and Beck (1978)	MB theory of photoabsorption in atoms and molecules.
Bartschat et al. (1986)	Photoionization of Ba. 5d states of Ba^+ more populated than 6s or 6p.
Deshmukh and Manson (1986)	RRPA 4f, 5s and 5p photoionization parameters of Yb.
Deshmukh et al. (1986a)	Cooper minima in Rn. RRPA.
Deshmukh et al. (1986b)	Multiple minima in the 7s photoionization of Ra.
Deshmukh et al. (1986c)	Review on Cooper minima.
Fink and Johnson (1986)	Low-energy photoionization of Li-Cs. RRPA.
Schmitt and Arenhoevel (1986)	Integrated photoabsorption cross section for a Dirac particle.
Silfvast et al. (1986)	Multielectron photoionization from $3p^6$ Ar to $3p^4 4p$ Ar^+.
Svensson et al. (1986)	Yb 4f and 6s photoionization ß parameter. RRPA.
Doolen and Liberman (1987)	Photoionization and photoabsorption, H-Lr, h < 1keV.
Goldberg and Pratt (1987b)	Photoionization of the 6d state of Cs. A deep minimum found near threshold. DS.
W.T. Hill et al. (1987)	Photoabsorption of Ba^{2+}, $5p^6$ to $5p^5nl$.
Kim and Greene (1987)	Photoionization of Ca.
Manakov et al. (1987)	Photon scattering by a bound electron using the Dirac-Coulomb Green function.
Radojevic et al. (1987)	Photodetachment cross sections of X^-, X=F-I.
Sacchetti (1987)	Relativistic effects on x-ray scattering. Solid-state applications.
Svensson et al. (1987)	Cross sections for Ar in the $3s3p^6np$ ^1P region.
Tulkki et al. (1987)	Post-collision interactions in inner-shell photoionization. Ar, Xe.
Yin et al. (1987)	High-energy relativistic photoionization cross sections from ns, $np_{1/2}$ and $np_{3/2}$ shells. A power-series, screened potential used.

Table 5.14. (continued).

Yin and Pratt (1987a)	Survey of relativistic Cooper minima.
Yin and Pratt (1987b)	Ionic and point-Coulomb relativistic Cooper minima.
Bagrov et al. (1988)	Polarization mechanism of photoelectrons.
Deshmukh et al. (1988)	Photoionization of Al^+. RRPA.
Guo and Åberg (1988)	QED approach to multiphoton ionization in the high-intensity limit.
Holm (1988)	Compton scattering from bound, relativistic atoms.
L. Liu et al. (1988)	Photoionization of excited Fe atoms.
Shanthi et al. (1988a)	Near-threshold photoionization of Kr 3p.
Shanthi et al. (1988b)	Photoionization cross section, angular distribution and spin polarization of Kr 3p and 3d.
Zilitis (1988)	Photoionization cross sections for K-like ions, Z=19-74. DF.
Aymar and Lecomte (1989)	Photoionization from Rydberg states of Sr.
Bechler and Pratt (1989)	Higher retardation and multipole corrections to the dipole angular distribution of 1s photoelectrons.
Dong et al. (1989)	Photoionization, Ne, Ar, Fe, U.
Nasreen et al. (1989)	Photoionization of inner shells in the Mg^{q+} and Ar^{q+} sequences. RRPA.
Radojevic et al. (1989)	4d photoionization of Ba.
Scofield (1989,1990)	Angular distribution of photoelectrons from polarized x-rays.
Shanthi and Deshmukh (1989)	Xenon 4p photoionization near the 4d Cooper minimum. RRPA.
Tulkki (1989)	Multiple excitation at Xe 5s photoionization threshold. Multichannel MCDF.
Veltman (1989)	Radiative corrections to polarized Compton scattering.
Wague (1989)	n=2 resonant photoionization of He-like ions.
Aymar (1990)	Odd-parity spectrum of Ba.
Band et al. (1990b)	K-shell photoionization cross sections.
Cuéllar et al. (1990)	SO effects on Cs ns (n=8-12) photoelectron angular distribution.
Fink and Johnson (1990)	Two-photon ionization of closed-shell atoms. TD DF. He, Ne-Xe.
Florescu et al. (1990)	Low-frequency Rayleigh scattering including spin flip for H-like atoms.
Glotov et al. (1990)	5p and 4f photoabsorption of Yb using LDF methods.
Greene (1990)	Photoabsorption of M^-, M=Rb-Fr.
Greene and Theodosiou (1990)	Photoionization of Ba 6s6p $^1P_1$.
Kelly (1990)	Review on photoionization.

Table 5.14. (continued).

Kutzner et al. (1990)	4d photoionization of Ba.
Mikhailov (1990)	K-shell photoionization near threshold: analytic solution for a screened nuclear field.
Reiss (1990)	Relativistic strong-field photoionization (photon field stronger than atomic one).
Rozsnyai (1990)	Inner-shell photoionization of Ba^{n+}, n=0-2, Xe, Kr.
Schäfers et al. (1990)	Hg 5d and 6s photoionization. RRPA.
Shanthi and Deshmukh (1990)	Photoionization of Pd.
Tulkki et al. (1990)	Photoelectron recapture in post-collision interactions. Ar.
Zhou et al. (1990)	Anomalous photon scattering factors for Ne^{q+}, q= 0...7. Photoionization cross sections. DS.
Chi and Huang (1991)	Photoionization of Be.
Connerade (1991)	Photoionization: a review.
Greene and Aymar (1991)	Photoabsorption of Sr-Ra.
Grochmalicki et al. (1991)	Relativistic effects may inhibit stabilization of atoms against ionization in intense laser fields.
Klimenko and Klimenko (1991)	Elastic scattering amplitude for an electron in a plane wave EM field.
Liu and Li (1991)	High-energy photoionization of atomic ions.
Rosenberg and Zhou (1991)	Soft-photon approximation for bound-state Compton scattering.
Suric et al. (1991)	Compton scattering of photons by 1s shell electrons. Al, Ho, Pb.
Zapryagaev and Nefedov (1991)	Photoionization of H-like ions. E1, M1, E2 approximations. Z = 10-150.
Altun and Radojevic (1992)	3d photoionization of Kr and Br^-. R RPA.
Bergstrom et al. (1992)	Whole atom Compton scattering of unpolarized photons.
Choe et al. (1992)	Photoionization cross sections for the $6s^2$ and 6s6p levels of Yb using DFT.
Connerade (1992)	Review on "giant resonances".
Deshmukh et al. (1992)	Outer-shell photoionization of Rn and Ra. RRPA.
Johnson and Cheng (1992)	4d photoionization of Xe.
Kheifets and Amusia (1992)	5s photoionization of Xe.
Kim et al. (1992)	ns photoionization of U, E = 1 eV-100 keV. DS field.
Krainov and Roshupkin (1992)	Spin effects on angular distribution of electron emission by strong EM fields.
Radojevic and Kelly (1992)	Photodetachment of I^-.

Table 5.14. (continued).

Reiss (1992)	Interaction of atomic electrons with strong EM fields (up to 10^6eV interactions with 1 eV photons).
Scherdin et al. (1992)	Delbrück scattering (photon scattering by nuclear Coulomb potential) for large Z.
Tulkki et al. (1992)	Kr 4p, 4s and 3d photoionisation, E <260eV.
C.-M. Wu et al. (1992)	Sr photoelectron angular distribution. Double-excitation effects. MC-RRPA.
Zhou and Pratt (1992)	Spurious structures in photoionisation calculations in the independent-particle approximation.
Zhou et al. (1992)	Anomalous scattering factors for Rayleigh scattering from Ar.

Table 5.15. Atom-atom collisions and interatomic potentials. See also Table 7.10.

Reference	Comments
Knipp (1938)	Angular parts for the R^{-5} atomic quadrupole-quadrupole forces for light-heavy (large SO) and heavy-heavy combinations.
Merzbacher (1985)	Fundamental interactions in atomic collisions.
Anholt (1986)	Relativistic atomic collisions.
Anholt and Gould (1986)	Relativistic heavy-ion-atom collisions.
Anholt and Meyerhof (1986)	Relativistic heavy-ion collisions with solid targets.
Anholt et al. (1986)	Radiative processes in relativistic heavy-ion collisions with atoms.
Amus'ya et al. (1987a)	Polarizational Bremsstrahlung.
Amus'ya et al. (1987b, 1988a)	Atom-atom Bremsstrahlung.
Anholt and Becker (1987)	Ultrarelativistic heavy-ion collisions. Electron capture and 1s-ionization.
Anholt et al. (1987)	Uranium ion charge-state studies.
Deco and Rivarola (1987abc)	Charge transfer at relativistic ion-atom collisions.
Denisenko and Mrówczynski (1987)	Interaction of various relativistic elementary (H-like) atoms with matter (C-Pb).
Hino and Watanabe (1987, 1989)	Radiative electron capture for relativistic bare-nucleus atom collision, Xe^{54+} or U^{92+} on Be.
Mrówczynski (1987)	Interaction of relativistic elementary atoms with matter.
Lin (1988)	Heavy-atom collisions: a review.
Toshima and Eichler (1988ab)	Xe^{54}-Ag, -Au and U^{92+}-U^{91+} collisions: electronic excitations and charge transfer.
Aquilanti and Vecchiocattivi (1989)	Fine-structure effects on collision integrals of O and F atoms with He and Xe.
Deco and Grün (1989)	Ionization of a bound relativistic electron by impact of a bare, relativistic ion.
Deco and Rivarola (1989a)	Pair production with electron capture in relativistic heavy-ion collisions.
Deco and Rivarola (1989b)	Two-center effects in relativistic radiative electron capture.
Hutton et al. (1989)	Double and single electron capture in slow collisions of $Ar^{8+,\ 9+}$ with He.
Toshima and Eichler (1989)	Inclusion of "pseudostates" to describe the continuum.
Amus'ya (1990)	Atomic Bremsstrahlung.

Table 5.15. (continued)

Amus'ya and Solov'ev (1990)	Frequency-angle distribution of radiation in relativistic atomic collisions.
Decker (1990)	Electron capture in C^{6+}-Au and Ar^{18+}-Ag collisions. Negative-energy intermediate states included.
Nakatsuji and Ehara (1990)	CsXe. Collision-induced 6s-5d transitions in a quasistatic approximation.
Toshima and Eichler (1990a)	Distorted-wave approximations for relativistic atomic collisions.
Toshima and Eichler (1990b)	Necessity of Coulomb boundary conditions in coupled-channel calculations. U^{92}+U^{91}.
Decker and Eichler (1991a)	Exact 2nd-order Born calculations for relativistic electron capture.
Decker and Eichler (1991b)	Electron capture in U^{92+}-U^{91+} collisions.
Yudin (1991b)	Stopping power of fast multicharged ions.
Bransden and McDowell (1992)	Charge exchange in ion-atom collisions. Book.
Kürpick et al. (1992)	K-vacancy transfer in collisions of S^{15+} on Ar.
Legrand et al. (1992)	L-shell ionization in ion-atom collisions. He+Pt, Ne+Pt, Ne+Yb, S+Au.

Table 5.16. Nuclear processes involving electronic wave functions.

Reference	Comments
Green and Rose (1951)	Nuclear-structure effects in internal conversion.
Rose and Holmes (1951)	Effect of finite nuclear size in beta-decay.
Band and Trzhaskovskaya (1986)	Wave-function expansions near origin from DS and DF functions.
Band et al. (1987)	Beta-decay probabilities.
Z.-H.Chen et al. (1987)	Bound-state versus continuum beta decay of ^{187}Re.
Batkin et al. (1988)	Inner-shell ionization in beta decay.
Band et al. (1989a)	The ^{193m}Ir decay.
Trusov and Eglais (1989)	Contact charge density of Fe.
Band (1990a)	Internal conversion coefficients.
Kolomietz and Kondratjev (1990)	Nuclear gamma-transitions via the accompanying atomic excitations: nuclear M4 transitions for ^{93}Nb and ^{193}Ir. Both elastic and inelastic electronic contributions.
Band and Trzhaskovskaya (1991ab)	Internal-conversion coefficients for $_{41}$Nb ... $_{97}$Bk. DF. Various E_L, M_L.
Jakubassa-Amundsen (1991)	Transfer of electron shells during nuclear reactions.
Schober et al. (1991)	Internal-conversion coefficients for valence-electrons of Tc and U.
Batkin et al. (1992)	K-shell autoionization in beta decay.
Harston and Pyper (1992)	Exchange effects in ß decays. ^{106}Ru, ^{241}Pu. ^{14}C, ^{35}S.
Jin et al. (1992)	Electron Coulomb effects in quasielastic (e, e'p) reactions.
Németh (1992)	Comparison of DF EL, ML (L=3,4) internal conversion coefficients with experiment.

Table 5.17. Parity-violation effects in atoms and molecules. Only the time-even, parity-odd or 'TE-PO' parity violation has so far been experimentally unequivocally confirmed. Upper limits exist for the TO-PO case.

Reference	Comments
Salpeter (1958)	H-like atoms with electron dipole moment.
Gajzágó and Marx (1974)	SO required for an energy difference between mirror molecules.
Hegstrom et al. (1980)	PNC energy difference between mirror-image molecules is of order $E^{(2)} = \Sigma' \langle 0 \| V_{PNC} \| n \rangle \langle n \| h_{SO} \| 0 \rangle / (E_0 - E_n)$.
Barra et al. (1986,1988)	PNC effects on NMR chemical shifts in enantiomeric molecules estimated.
Dzuba et al. (1986a)	P and T nonconservation in rare-earth atoms.
Johnson et al. (1986)	PNC effects for monovalent atoms using DF or model potentials.
Botham et al.(1987)	PNC "equations of motion". Application on Pb.
B.P.Das (1987)	PNC TP for 6s-7s of Cs and $6p^*$-$7p^*$ of Tl.
Dzuba et al. (1987b)	PNC amplitudes of Tl.
Dzuba et al. (1987c)	Cs, Tl.
Johnson (1987)	P- and CP-violation in Rb, Cs, Au, Tl.
Kozlov (1987,1988); Kozlov et al. (1987)	PNC effects in PbF. X $^2\pi_{1/2}$.
Mårtensson-Pendrill (1987)	Cs, Tl.
Mårtensson-Pendrill and Öster (1987)	Atomic electric dipole moments. Cs, Hg, Xe ground states.
Perger and Das (1987a)	Cs, Tl.
Sandars (1987)	Review.
Bouchiat and Piketty (1988)	Cs 6s-7s PNC calibration from M1- and E2-hfs-induced TP.
Dzuba et al. (1988)	PNC in Pb and Bi.
Johnson et al. (1988d)	PNC 6s-7s transition in Cs.
Khriplovich (1988)	Book on PNC in atoms.
Kraftmakher (1988a)	PNC in Tl.
Kraftmakher (1988b)	PNC in Cs.
Parpia et al. (1988)	PNC in Cs and Tl.
Wiesenfeld (1988)	Effect of Z on PNC energy difference between enantiomers.
Blundell (1989)	MBPT calculation of PNC in Cs.
B.P.Das (1989)	Review on PNC effects in atoms.
Dzuba et al. (1989c)	Cs 6s-7s PNC E1 amplitude.
Khriplovich (1989)	T-violation in atoms.
Lindroth et al. (1989a)	Atomic (E1) dipole moments, due to an electron dipole moment. Leading terms relativistic, of order α^2. Cs, Tl.
Lindroth et al. (1989b)	Effects of H_{Br} on the Tl E1 moment.
Schäfer et al. (1989)	Proposed PNC two-photon laser experiment on U^{90+}.

Table 5.17. (continued).

Blundell et al. (1990c)	The 6s-7s PNC transition of Cs.
Boston and Sandars (1990)	The P-violating, T-invariant L=1 "anapole moment" of hydrogenic atoms.
Dzyuba et al. (1990)	PNC of Cs.
Hartley et al. (1990)	PNC and electric dipole moments of Cs and Tl.
Onishchuk (1990)	Chirality of valence electrons at nuclei in asymmetrical molecules. No effect on nuclear electron capture.
Blundell et al. (1991b)	The 6s-7s PNC transition of Cs.
Chou and Huang (1991)	MCDF theory including PNC.
Hartley and Sandars (1991)	Review on PNC effects in atoms.
Khriplovich (1991)	Book on PNC.
Flambaum (1992)	Long-range PNC interaction.
Mårtensson-Pendrill and Lindroth (1991)	P- and T-violating scalar-pseudoscalar electron-nucleon interaction. Cs, Tl.
Dmitriev et al. (1992)	P- and PT-odd terms for HgF and PbF.
Karasiev et al. (1992)	PNC effects in radiation spectra of He-like ^{235}U. MCDF.
Liu and Kelly (1992)	E1 moment of Tl.
Mårtensson-Pendrill (1992ab)	Reviews on atomic effects of nuclear PNC effects.
S. Sen and Gautam (1992)	NR aspects of SU2*U(1) PNC hamiltonians in atoms.

Table 6.1. Group theory and symmetry aspects.

Reference	Comments
Elliott (1954)	Spin-orbit coupling in band theory. Character tables.
Altmann (1986)	Rotations, quaternions and double groups.
Eschrig and Richter (1986)	Kramers' theorem. Cp. Rösch (1983a), Dongarra et al. (1984ab).
J. Meyer (1988)	Molecular basis functions for C_n, C_{nh}, S_n, C_{nv}, D_n, D_{nd}, D_{nh}, T, T_h, T_d, O and O_h. Projection operators used.
J. Meyer et al. (1989)	A program for constructing relativistic, symmetry-adapted molecular basis functions for 36 double groups.
Pitzer and Winter (1988)	A real Hamiltonian can be obtained in a $\|lm_l m_s\rangle$basis for C_{2v}, D_2, D_{2h} or higher symmetry. Applications on SO PP.
Smirnov and Evarestov (1988)	Symmetry of localised orbitals in molecules with SO interaction. Example: T_d Bi_4.

7. MOLECULAR CALCULATIONS

Table 7.1. One-electron systems. For overcritical fields, see also Table 5.5.

Reference	Comments
Klaus (1980b)	General properties of Dirac operators for several Coulomb singularities.
Becker et al. (1986)	U^{92+}-U^{91+} collisions at 1 GeV/amu. TD finite-difference solution of the Dirac equation.
Wietschorke (1986); Wietschorke et al. (1987)	Two-center continuum.
Wolniewicz and Poll (1986)	Higher ro-vibrational states of HD^+ and H_2^+
Ishikawa et al. (1987, 1988)	H_2^+ using momentum-space GTOs.
Mark and Becker (1987)	H_2^+ energy correction at R=2 a.u. using a GTO basis.
Rutkowski and Rutkowska (1987)	H_2^+ at R=2 a.u. using a new PT approach. Terms of order c^n, n=2, 4, 6 obtained.
Sundholm et al. (1987); Sundholm (1988)	Fully numerical Dirac results for H_2^+. V(R), Q_2, Q_4.
Bakalov (1988)	Mesic molecules.
Ixaru and Pantea (1988)	The two-centre Dirac equation and positron creation. A double-square-well model in 1D.
Toshima and Eichler (1988ab)	U^{92+} - U^{91+} collision system. Excitation and capture.
Tóth et al. (1988)	Two-centre Dirac equation with separable potentials.
Dietz and Roemer (1989)	Avoided level crossings and pair production in strong Coulomb fields.
Moss and Sadler (1989)	High J, low v levels of the HD^+ electronic ground state.
Petelenz and Smith (1989)	Vacuum-polarization in muonic molecules, ppμ, ddμ etc.
Rumrich et al. (1989)	Continuum states of the two-center Dirac equation. Heavy collision systems.
Aissing et al. (1990); Aissing and Monkhorst (1990)	Binding energies of muonic molecules.
Balint-Kurti et al. (1990)	Rovibrational levels of HD^+, v = 0-21, J=0,1.
Howells and Kennedy (1990)	Ground and first excited states of H_2^+ and its isotopic species.
Moss (1990ab)	H_2^+, D_2^+ rovibrational states.

Table 7.1. (continued).

Rutkowski and Schwarz (1990)	H_2^+ properties using a new PT.
Strayer et al. (1990)	Muon-pair production and negative-muon capture into the 1σ state in a superheavy collision system. Numerical, B-spline solution in 3D. Au+Au.
Toshima and Eichler (1990b)	Necessity of Coulomb boundary conditions in coupled-channel calculations. $U^{92}+U^{91}$.
Decker and Eichler (1991b)	Electron capture in $U^{92+} + U^{91+}$ collisions.
L. Yang et al. (1991)	Accurate FEM solution of the Dirac equation for H_2^+ (R=2 a.u.).
Bukowski et al. (1992)	Bethe logarithm and Lamb shift for H_2^+ and isotopic species.
Franke and Kutzelnigg (1992)	Very accurate, "direct perturbation theory" E_0, E_2, E_4, E_6 for H_2^+, HeH^{2+}.
LaJohn and Talman (1992)	Minimax variational solution of the Dirac equation for H_2^+, Th_2^{179+}.
Rutkowski et al. (1992)	H_2^+ using double PT. Effects on R, k, D_e.
Thiel et al. (1992)	Finite-difference treatment of $U^{92+} + U^{91+}$ collisions. Creation of electron-positron pairs.

Table 7.2. LCAO-DF calculations on molecules. For LCAO calculations on one- and many-electron atoms, see the Table 2.3. or 2.4. and 4.4., respectively.

Reference	Comments
Aerts (1986)	DF-LCAO methodology.
Y.S. Lee (1986)	An approximation neglecting small-component Coulomb and exchange contributions. Tested on HI.
Malli and Pyper (1986)	AuH. Both DF and CI using numerical, atomic DF basis, completed with STOs. See comments by Balasubramanian et al. (1991a) and reply by Malli et al. (1991).
Hegarty and Aerts (1987)	Kinetically balanced F_2 and GeH_4.
Lee and McLean (1987)	AgH and AuH. SCF-level STO MO energies. Effects on E_{corr} mentioned.
Baeck and Lee (1988)	Open-shell DF-LCAO. CH SO splitting.
Datta and Devaiah (1988)	H_2 using a minimax technique.
Laaksonen et al. (1988)	HCl by GTO MCDF. Energies and dipole moment given.
Ramos et al. (1988)	A four-component numerical DF basis, completed with STO:s. Bonding and dipole moments in HgH^+, TlH, PbH^+, BiH, TlI, PbTe. R/NR. (See Balasubramanian et al. 1991a, Malli et al. 1991).
Roszak and Chojnacki (1988)	Molecular calculations using a modified H-like basis.
Wilson (1988)	Review.
Baeck and Lee (1990)	Diatomic open-shell hydrides of B-F, Si, S.
Wilson (1990)	Universal basis sets and Cholesky decomposition of the two-electron integral matrix.
Mohanty and Clementi (1990b, 1991c); Mohanty et al. (1991a)	Working formulae for the authors' basis-set DF method for molecules.
Dyall et al. (1991a)	Polyatomic Gaussian-basis DF calculations reviewed. H_2O.
Dyall et al. (1991b)	CH_4 - PbH_4 at DF level. Results compared with PP and PT.
Glushkov (1991c)	Formalism for TD MCDF theory for molecules.
Visscher et al. (1991ab)	Kinetic balance and basis-set contraction tested on SiH_4, SnH_4 and atoms.
Wilson (1991)	Review on relativistic MBPT.
Baeck et al. (1992)	CO, CO^+.
Bauschlicher et al. (1992c)	KO. $^2\Sigma$ - $^2\pi$ separation at DF level.
Dyall (1992a)	XH_2, XH_4, X = Si-Pb. DF-LCAO compared with PT and PP.
Dyall (1992b)	Omission of (SS|SS) Coulomb integrals for the small component S studied on Hg^{2+}, Hg and PbO.
Fujimura and Matsuoka (1992)	Breit interaction integrals over Laguerre Gaussians.

Table 7.2. (continued).

Goldman (1992)	Spurious-root elimination tested on Dirac-Coulomb.
Ishikawa et al. (1992a)	AuH^+ ground state. First open-shell application of the Malli-Pyper method.
Malli (1992)	ThPt. Predicted SCF R_e 274 pm. R/NR. Unbound by 1.38 eV.
Matsuoka (1992b)	HX, HX^+, X=I, At.
Mohanty (1992)	Formalism for molecular Dirac-Fock-Breit. 79 references.
Visser (1992)	Thesis on group 14 MH_4 and EuO_6^{9-}.
Visser et al. (1992a)	MH_4, M = C-Pb. Effect of H_{Br} studied.
Visser et al. (1992b)	EuO_6^{9-} crystal-field levels.
Yang et al. (1992)	Numerical 2D-DS model solved for H_2, Li_2, BH with 10-figure accuracy by FEM. R/NR at $R_{exp.}$.

Table 7.3. Molecular all-electron calculations using "no-pair" or other transformed Dirac Hamiltonians.

Reference	Comments
Hess et al. (1986)	Variational use of the Pauli Hamiltonian leads to problems.
Hess (1986)	Derives the "no-pair" method. Results on Br, Ag.
Hess and Chandra (1987)	AgH X $^1\Sigma$ and A $^1\Sigma$.
Marian et al. (1988)	ThO. Bonding analysed.
Sundholm (1988)	Fully numerical solution of the DS equations (α=0.70) for H_2, LiH, Li_2, BH and CH^+. R/NR for V(R), Q_1, Q_2.
Carnell et al. (1989)	CsH. Lowest 17 states at MRD CI level using Hess' "no-pair" operator. X $^1\Sigma$ R_e contraction 3.0 and 1.4 pm at SCF and CI level, respectively. For A $^1\Sigma$ at CI level, 19.6 pm.
Jansen and Hess (1989b)	Tests on Au atom IP, EA and excitation energies.
Jansen and Hess (1989c)	AuH lowest states.
Marian et al. (1989); Marian (1990a)	NiH and NiD. Vibronic spectra using the "no-pair" Hamiltonian or PT. Includes SO.
Kellö and Sadlej (1990a)	A multiple-perturbation theory for correlation and the Cowan-Griffin QR Hamiltonian. HX, X=Cl-I. AgH.
Kellö and Sadlej (1990b)	EFG in HX, X=Cl-I. Nuclear Q for X obtained.
Knappe (1990)	GTO basis QR LDF approach.
Knappe and Rösch (1990)	The "no-pair" Hamiltonian implemented with GTOs and LDF. Tests on Ce and Pb atoms.
Marian (1990b)	The Cu atom using the "no-pair" Hamiltonian.
Kellö and Sadlej (1991)	MH, M=Cu-Au. Molecular Q.
Marian (1991ab)	CuH, CuD and other transition-metal diatomics. "No-pair" Hamiltonian.
Sadlej (1991)	Dipole moment and polarisability and Q_2 of AuH.
Sadlej and Urban (1991)	Dipole moment of AgH.
Sadlej et al. (1991)	Polarisabilities of Ca-Ba.
Samzow and Hess (1991)	FS of Br as test of two-electron terms in the "no-pair" Hamiltonian.
Bueckert et al. (1992)	2nd-order Dirac eq. used in variational Monte Carlo. E_{rel} of Li and LiH obtained from fit to various c, down to 137./10.
Hippe and Peyerimhoff (1992)	CuO ground and excited states using 'no pair'.
Häberlen and Rösch (1992)	AuH, AuCl, Au_2 using a GTO-LDF approach with a transformed QR Hamiltonian.
Häberlen et al. (1992)	$M@C_{28}$, $M@C_{28}H_4$ endohedral M(IV) compounds, M=Ti, Zr, Ce.

Table 7.3. (continued).

Ilyabaev and Kaldor (1992a)	He-Xe and Be. CC using a no-pair Hamiltonian.
Ilyabaev and Kaldor (1992b)	No-pair CCSD for excitation energies of the Ne atom.
Kellö and Sadlej (1992a)	XCN, X = F-I. QR CI.
Kellö and Sadlej (1992b)	PbH_4, BiH_3, PoH_2, AtH. Dipole moments and polarisabilities.
Marian et al. (1992)	Cu valence levels using the 'no pair' Hamiltonian. R/NR.
Rösch and Häberlen (1992)	Reply to Samzow et al. (1992b).
Sadlej (1992a)	SbH_3, H_2Te, HI. SCF-level R/NR.
Sadlej (1992b)	XX', X = F-I.
Samzow et al. (1992a)	Two-electron terms of the no-pair Hamiltonian. Ag, Au.
Samzow et al. (1992b)	Comments on Knappe and Rösch (1990). For reply, see Rösch and Häberlen (1992).
Wilkin and Salahub (1992)	SCF treatment of h_m+h_d and h_{SO} found possible using suitable (NR!) innermost contraction coefficients. Cu, Ag, Au.

Table 7.4. Molecules treated by the DS-DVM method.

Reference	Comments
Fricke and Sepp (1981)	Kr^{2+}-Kr^{2+} correlation diagram.
Ellis and Holland (1986)	Review on cluster compound calculations.
Ruscic et al. (1986)	M_2O, M=Al-Tl. PES interpreted. TlCl.
Sepp et al. (1986)	Improve numerical accuracy to obtain V(R) of diatomics. N_2, Ne_2 tests.
Thies et al. (1986)	Ne^+-Ne, Ne^+-O collision systems.
Hartung et al. (1987)	Ar-Ar^+ potential curve for laboratory energies of 15-400 keV and MO correlation diagram. The new code of Sepp et al. (1986) is used.
Hohl et al. (1987)	$M(BH_4)_4$, M=Zr, U. Bonding and PES. Results compared with QR-MS ones of Hohl and Rösch (1986).
Ryzhkov and Gubanov (1987)	EuX_6^{10-}, X=O-Se. LnS_6^{10-}, Ln=Nd, Sm, Eu, Gd. $Sm_2S_{10}^{16-}$. Bonding.
Sepp (1987); Sepp and Fricke (1987)	Positive-energy projection operators for basis-set DS calculations.
J. Guo et al. (1989)	Use DS-DVM potentials for MS calculations of the M-edge x-ray spectra of UO_2(s) cluster model and molecular UCl_4.
Rösch et al. (1989)	XAu_5^+, XAu_6^{2+}, X=nothing, C. $C(Au\ SH_2)_6^{2+}$. R/NR. Bonding analysed.
Thies et al. (1989ab)	F^{8+}-Ne and F^{6+}-Ne collision system.
DeKock et al. (1990)	CeO_2, $YbCl_2$. Both found bent, mainly due to 5d.
Goodman and Soderholm (1990)	$MBa_2Cu_3O_7$ cluster models, M=Y, Pr, Nd, Ho, Cm.
Kimura et al. (1990)	$[I(H_2O)_6]^-$ in a polarized dielectric medium. Charge Transfer To Solvent (CTTS) transitions calculated. I^- SO splitting 1.02 eV (exp. 0.88).
Ryzhkov and Gubanov (1990)	Uranyl complexes. Energy-level diagrams given.
Cheng and Ellis (1991)	Pt_n, n=2-4.
Görling et al. (1991)	$\{[(H_3P)Au]_6\ X\ \}^{m+}$, X=B, C, N. Also Au_6^{2+}, $[(H_3P)Au]_6^{2+}$. Bonding analyzed. 5d and 6s equally important. Both Au-Au, Au-X and Au-PH_3 interactions must be included.
C.-X. Guo et al. (1991)	Cluster models for Sm^{2+} in BaF_2.
Kürpick et al. (1991ab)	S^{16+} scattering from Ar.
Pierloot et al. (1991)	AnX_4, An=Th, U; X=F, Cl. PES interpreted.
Bastug et al. (1992)	Al_n (n=2-8).
Bowmaker et al. (1992)	$(RN)U(NR_2)_3$, R = H, SiH_3. Bonding and PES.

Table 7.4. (continued).

Kürpick et al. (1992)	K-vacancy transfer in S^{15+} collisions on Ar.
Nakamatsu et al. (1992)	CF_4, SF_6, UF_4, UF_6.
Onoe et al. (1992ab)	UV excited states of UF_6. XPS.
Pershina et al. (1992a)	MCl_5, M = V, Nb, Ta, E105 and Pa. Bonding analysed. E105 atomic ground state $6d^37s^2$, as for Nb.
Pershina et al. (1992b)	MBr_5, M = Nb, Ta, Pa, E105.
Pershina et al. (1992c)	$MOCl_5$, $MOBr_5$, M = V-E105, Pa.
Ryzhkov et al. (1992)	MCl_4, M = Ti-Hf, 104; Pb.

Table 7.5. Molecules treated by the DS-MS-Xα method.

Reference	Comments
Arratia-Perez and Malli (1986a)	Au_6^{2+}. S-d hybridization discussed.
Arratia-Perez and Malli (1986b)	Ag_3^{2+}, Au_3^{q+}, Au_4^{q+} (q=1, 2). S-d hybridization, g-tensors and hfs discussed.
Arratia-Perez and Malli (1986c)	Ag_5^{q+} (q=0, 2-4).
Case (1986)	SO effects in metalloporphyrins. M=Cu, Fe.
Mukoyama and Adachi (1986)	CO, UO. R/NR comparisons for orbital energies.
Zuloaga and Arratia-Pérez (1986)	<u>Cis</u>-$Pt(NH_3)_2Cl_2$. R/NR. Donation to 6p found more important than to 5d.
Arratia-Perez et al. (1987)	$Cu(CO)_3$ bonding, optical, magnetic properties.
Arratia-Perez and Malli (1987)	Ag_4^{q+} (q=1, 3) Bonding, optical and magnetic properties.
Arratia-Perez and Marynick (1987)	$Ag(CO)_3$. Bonding, optical and magnetic properties.
Ramos et al. (1987)	Au_{13} (I_h). R/NR. IP, optical spectra. SO splitting of the 5d band 2.2 eV. Relativity increases s-d hybridisation.
Arratia-Perez and Marynick (1988)	$PaCl_6^{2-}$. Energy levels, g, hfs.
Arratia-Perez et al. (1989)	Au_{13}(O_h and I_h). Bonding, g, hfs.
J. Guo et al. (1989)	M-x-ray spectra for UCl_4 and a cluster model of UO_2 using a DS-DVM potential.
W. Mueller (1989)	$Y_2Ba_2Cu_{12}O_{18}$ cluster model for solid $YBa_2Cu_3O_7$. Cu 3d state SO splitting about 0.3 eV. Bonding both ionic and covalent.
W. Müller (1989)	Cluster models for BaO/W(100): $(BaO)_nW_m$, n=1, 2, m=0...14. Also W-Os mixed clusters. Result: "a Ba salt of the O/W substrate".
Glebov et al. (1990)	U_6 octahedral and distorted clusters as models for the fcc and bcc structures. U-U bonding 40 % 6d, 30 % 6p, 20 % 5f, 3 % 7s.
Zhuikov et al. (1990)	$(104)Cl_4$ hybridization $7s^{0.34}$ $6p^{5.81}$ $7p^{0.21}$ $6d^{1.34}$ $5f^{13.98}$. Results compared with MCl_4, M=Ti-Hf.
Arratia-Perez (1991)	$Os_2Cl_8^{2-}$.
Kalinkin et al. (1991)	Cluster models for S-doped $Bi_2Sr_2CaCu_2O_8$. Sr 4p SO effects on Bi $6p_{1/2}$ levels seen.
Chermette (1992)	Review on MS Xα.

Table 7.6. Molecules treated by the quasirelativistic DS-MS Xα or "RXα" approach. See Table 2.2. of Pyykkö (1986a) for the QR 1-electron equation.

Reference	Comments
Agaskar et al. (1986)	$Os_2Cl_8^{2-}$. Evidence for a $\sigma^2\pi^4\delta^2\delta^{*2}d^5$-$d^5$ triple bond.
Andersen et al. (1986)	$Ln(cp)_2$, Ln = Sm, Eu, Yb. PES interpreted.
Hofmann and Rösch (1986); Hofmann et al. (1986)	$[(\eta^5\text{-}C_5H_5)_3Re_3(\mu^2\text{-}O)_6]^{2+}$. Expected $(1e')^2\ ^3A_2$ ground state confirmed. Also the $Re_3O_6^{5+}$ fragment.
Hohl and Rösch (1986)	$M(BH_4)_4$, M=Zr, Hf, Th, U. Bonding and PES.
Katrib et al. (1986)	$Re_2X_8^{n-}$, X=Cl, Br, n=2,4,6. Re(4f) binding energies and multiple bonding.
Kovba and Topol' (1986ab)	Low-lying states of AlO-InO.
Loder (1986); Loder et al. (1988)	TlX, X=F-I, NO_3. Tl_2O, Tl_2S. PES interpreted: 6s character in two MO:s, more in the lower.
Mattar and Ozin (1986)	Ag_3^{q+}, q=0-2. D_{3h}. Eigenvalues, spin densities, IP.
Moine et al. (1986)	$(MCl_6)^{5-}$, M=Cu, Ag, as models for impurities in LiCl. SO in PT. Geometries and excitation energies.
Axe and Marynick (1987)	$HgTe_2^{2-}$, $PbTe_2$. Relativistic reduction of 5s-$5d_{zz}$ σ_g repulsion found.
Bice (1987)	Lead (II) halide PES.
Bursten and Clark (1987)	$M_2(O_2CH)_4$, M=W. A review on multiple M-M bonds.
Bursten and Novo-Gradac (1987)	$(cp)_2M\text{-}Ru(cp)(CO)_2$, M=Zr, Th. Th metal character $s^{0.097}p^{0.036}d^{0.718}f^{0.155}$.
Bursten and Strittmatter (1987)	$(cp)_3UL$, L=CO and OC. U-C preferred to U-O.
El-Issa et al. (1987)	<u>Cis</u> and <u>trans</u> $PtCl_2(NH_3)_2$.
Goursot et al. (1987a)	$PtCl_5^{2-}$. Photoreduction of $PtCl_6^{2-}$ discussed.
Goursot et al. (1987b)	$[Ta_2Cl_6(NH_3)_4]^{q-}$, q=0,1. Electronic transitions.
Green et al. (1987)	$Ln(C_5H_5)_2$, Ln=Eu, Yb. Bonding and PES.
Kondratenko et al. (1987)	EXAFS and XANES spectra of Pt in $PtCl_n^{2-}$, n=4,6.
Makhyoun (1987)	$NpO_2Cl_4^{2-}$, $NpO_2(NO_3)_3^-$. The $5f^1$ levels studied, including SO. Effective ligand-field parameters obtained.
Makhyoun et al. (1987)	$Th(\eta^5\text{-}C_5H_5)_2\ (\mu\text{-}PH_2)_2\ Ni(CO)_2$. Evidence for a Th-Ni dσ-dσ bond.
Scioly et al. (1987)	$Ta_2Cl_4(PH_3)_4H_n$, (n=2, 4), $Ta_2Cl_4(PH_3)_4$. Free and hindered rotation of the hydride ions for n=4 and 2, respectively.
Topol' et al. (1987)	RuO_4, OsO_4 PES.

Table 7.6. (continued).

Akrivos and Aldridge (1988)	$PtCl_2(OH)_2(NH_3)_2$.
Axe and Marynick (1988)	20-electron Zintl anions $Sn_2Bi_2^{2-}$, $Pb_2Sb_2^{2-}$ ("tetrahedral"), $Tl_2Te_2^{2-}$ (boat).
Berksoy and Whitehead (1988a)	Al_2X_6, X=F-I. NQCC interpreted.
Berksoy and Whitehead (1988b)	$SnCl_2Ph_2$ monomer and dimer NQCC, IS.
Cayton (1988)	Organometallic "piano-stool" systems $(cp)ML_n$, n=3, 4. M=Mo, W, Re,..; $U_2(OH)_{10}^{2+}$, $(cp)_2U_2O_4$.
Dai and Ma (1988a)	$MoCl_2^{2+}$, $MoCl_4$.
El-Issa et al. (1988)	IrX_6^{n+}, n=1-4, x=Cl-I. IrX_n, n=1-4.
Makhyoun (1988a)	$[W(WS_4)_2]^{2-}$. Confirms W(II) and W(VI) oxidation states for middle and end atoms, respectively. W-W bond order 0.5.
Makhyoun (1988b)	$5g^1$ complexes EO_2^{2+} and EF_6 of E= element 125. NpO_2^{2+}.
Makhyoun and El-Ezaby (1988)	UOX_5^{2-}, X =F-Br. Axial compression of the <u>trans</u> U-X bond suggested. Ligand-field parameters for the $5f^1$ levels derived.
Makhyoun and Hasanein (1988)	$UO_2Cl_4^{2-}$. Dependence on U-O studied.
Bowmaker et al. (1989)	X_2^n, n=-1, 0, +1, X=Cl-I. NQCC interpreted.
Bursten et al. (1989a)	$(cp)_3An$, An=Th-Pu.
Bursten et al. (1989b)	$(cp)_3AnL$, L=H, CO, NO, OH, Cl, cp.
Bursten et al. (1989c)	$(cp)_3AnL$ versus Cl_3AnL, An=Th-Cf.
Cotton and Feng (1989)	$Ru_2(HNNNH)_4$, $Rh_2(HNCHNH)_4$. The M-M δ^* and π^* levels discussed.
Daul (1989)	Inclusion of multiplet states and SO splitting in MS_2 $X\alpha$ calculations.
El-Issa et al. (1989)	Bonding in $MoS_nO_{4-n}^{2-}$.
Goursot et al. (1989)	Pt(III) complexes containing aquo and chloro ligands: $PtCl_kO_l(OH)_m(H_2O)_n$, CN=4-6. Bonding and CT transitions.
King et al. (1989)	$[Au(H_2PCH_2PH_2)]_2^{2+}$. Bonding discussed: Origin of the Au(I)...Au(I) attraction not understood.
Makhyoun and Sawan (1989)	$Cu_3AsSe_6^{6-}$ as model for Cu_3AsSe_4.
R.M. Miller et al. (1989)	CrO_4^{2-}, CrO_3X^-, CrO_2X_2, X= F, Cl. Excited states studied.
Morin et al. (1989)	Inclusion of SO effects in MS-LSD methods by a j-dependent QR method. Results for Pt_n, n=2, 4, 5, compared with full Dirac calculations.
Pershina et al. (1989)	$HfCl_4$, $(E104)Cl_4$. Bonding analysed.
D.-S. Yang et al. (1989)	<u>Cis</u>-$PtMe_2(C_2H_4)_2$. PES.

Table 7.6. (continued).

Novo-Gradac (1990)	Bimetallic organoactinide compounds, $Cp_nMM'Cp(CO)_2$, n=1, 2, M=Zr, Ru, Th, U. Also various M_2L_6, L=CH_3, Cp. 5f contributions increase along Th, U, Pu. $U_2(OMe)_{10}$. Lack of U-U bonds discussed.
Rogemond et al. (1990)	BiO_6^{9-}, GeO_4^{4-} and GeO_6^{8-} cluster models for $Bi_4Ge_3O_{12}$.
Tahri et al. (1990)	AnX_8^{4-}, An=Th, Pa, X=Cl, Br. The f-f and f-d optical transitions interpreted, including SO.
D.-S. Yang et al. (1990a)	<u>Cis</u>-$PtMe_2(EH_3)_2$ (E=N-As), $PtMe_2(C_2H_4)_2$, $PtMe_2(CNH)_2$. NR comparison for <u>cis</u>-$PtMe_2(PH_3)_2$. Only small effects on orbital energies.
D.-S. Yang et al. (1990b)	$PtMe_3(HC(O)CH\ COH)$. PES. Extensive 5d delocalization to the ß-diketonato and methyl groups.
D.-S. Yang et al. (1990c)	Cp Pt Me_3.
D.-S. Yang et al. (1990d)	$Pt(CF_3)_2$, $Pt(CF_3)_2L_2$ (L=C_2H_4, PH_3). Significant C 2s character in the Pt-CF_3 bonds. Little interaction between d_π and C-F σ^*.
Berksoy-Bölük (1991)	$PbCl_2Ph_2$ NQCC, IS.
Cayton et al. (1991)	Dinuclear U(V) systems. U_2H_{10}, $U_2(OH)_{10}$ models for known $U_2(OR)_{10}$. Also $(cp)_2U_2O_4$. U-U bonding searched.
Chermette et al. (1991)	$[Cr(NH_3)_6]^{3+}$. SO-induced intersystem crossings studied. LSD potential chosen. Weighted average of monoatomic SO used.
Cotton and Feng (1991)	$[W_3OCl_6(O_2CH)_3]^-$ energy evels and bonding.
El-Issa et al. (1991)	ML_5, M=Sb, Bi; L=-H,-C≡CH models for $BiPh_5$. MCl_6^{2-}, M=Sn, Pb: LUMO stabilization important for colour. MS_4^{2-}, M=Mo, W: LUMO destabilization not important.
El-Issa and Zeedan (1991)	$[M'(MS_4)_2]^{2-}$, M'=Ni-Pt, M=Mo, W. Optical transitions and bonding.
Kryuchkov et al. (1991)	M_2^{n+}, M=Mo, Tc, Ru, Re, n=0-6, as models for multiply-bonded dimers.
Ren (1991)	Diruthenium and diosmium organometallics
Schneider (1991)	Symmetric and asymmetric, multiple M-M bonds, M=Mo, Ta-Re. AnX_3, An=Th-Pu, X=H, CH_3, NH_2, OH. Also UX_4.
Strittmatter (1991); Strittmatter and Bursten (1991)	$An(cp)_3$ compounds An = Th-Cf. Also $Ln(cp)_3$, Ln=Ce-Dy. PES for $Zr(cp)_3Cl$.
Subramanian et al. (1991)	MCl_4, M=Ti-Hf. PES, EA.
Chermette (1992)	Review on MS Xα.
Jolly and Marynick (1992)	Sb_7^{3-}. 5p bonding. NR/QR.

Table 7.6. (continued).

Gallego-Planas and Whitehead (1992)	Pentastanna [1.1.1.] propellane, bicyclo [1.1.1] pentastannane. QR/NR study of bonding.
Nour et al. (1992)	PaX_8^{4-}. QR + SO. Optical spectrum of ThX_4:Pa^{4+}(X = Cl, Br) assigned.
Schwerdtfeger et al. (1992b)	NQCC of AuCl, $AuCl_2^-$, AuX_4^-, X=F-I. R/NR.

Table 7.7. Molecules treated by pseudopotential methods.

Reference	Comments
Cohen and Basch (1983)	Ethene and ethyne complexes of Ag.
Low and Goddard (1984b)	Pd insertion to H-H, H-C and C-C bonds. Existence of H-Pd-H a relativistic effect.
Flad et al. (1985ab)	H adsorption on cluster models of Cu and Ag.
Flad et al. (1985c)	Comparisons between the group 1 and 11 clusters of Li-K and Cu, Ag.
Sakaki et al. (1985, 1987)	Nucleophilic attack by water on a Hg(II)-ethylene complex.
Balasubramanian (1986a)	BiH^+. Eight low-lying states. Relativistic avoided crossings found. Bi^+ SO lowers D_e.
Balasubramanian (1986b)	BiH. 10 low-lying states.
Balasubramanian (1986c)	BiF.
Balasubramanian (1986d)	PbS.
Balasubramanian (1986e)	Sn_3.
Balasubramanian (1986f)	Ga_2.
Balasubramanian (1986g)	SnH_2.
Balasubramanian et al. (1986)	Br^+-Kr collisions.
Basch et al. (1986a)	A cis-$Pt(NH_3)_2(CH_2OH)(OCH_3)$ model for ascorbic acid complexes. Pt-C bond energy higher than Pt-O one. Strong trans influence for the NH_3.
Basch et al. (1986b)	$Pt(NH_3)_3^{2+}$ complexes with guanine. adenine, cytosine and thymine.
Bauschlicher et al. (1986)	CsOH, BaOH.
Baykara et al. (1986)	Hydrogen atoms on and in PdH_n cluster models.
Bernier et al. (1986)	HgH, lowest states including SO.
Bertoncello et al. (1986)	$SnL_nL'_{4-n}$, L = CH_3, Cl, NCS. PES interpreted.
Boland (1986)	AgH, AuH at NR and QR HF level.
Caballol et al. (1986)	XH_4^+, X = Si-Sn. Geometries.
Cabot et al. (1986)	MO_2, M = Ga-Tl, superoxide.
Christiansen (1986)	A core-valence correlation potential tested for K.
Di Bella et al. (1986)	$Pt(acac)_2$ PES (acac=acetylacetonate).
Fernandez et al. (1986a)	SnH_4 VUV spectrum.
Fernandez et al. (1986b)	$SnCl_4$ and $Sn(CH_3)_4$ VUV spectrum and PES.
Gavezzotti et al. (1986)	Pt_2, PtH and PtCO.
Hay et al. (1986)	Cl_2 Th-(μ-$PH_2)_2Pt(PH_3)$: a compound with a Th-Pt bond. Mainly 5d-to-6d donation in a σ HOMO.
Hliwa et al. (1986)	Low-lying states of CuH.
Igel-Mann et al. (1986)	Alkali dimers, XY, X,Y=Li-Cs. Ground-state properties.

Table 7.7. (continued).

Illas et al. (1986)	Geometrical isomers of AgO_2: C_s 0.4 kcal/mol below C_{2v}.
Jarque et al. (1986)	PdH_2. Side-on preferred to head-on.
Koga and Morokuma (1986)	$M(CH_3)(H)(CO)(PH_3)$, M=Pd, Pt. The carbonyl insertion proceeds via methyl-group migration. TS established. Pd less endothermic, has lower $E^{\neq}$, due to weaker M-C bonds.
Low and Goddard (1986a)	MR_1R_2, M=Pd, Pt; R=H, CH_3. Models for reductive coupling on a metal surface.
Low and Goddard (1986b)	$M(CH_3)_2(PH_3)_2$, M=Pd, Pt. $Pt(CH_3)_2(Cl)_2(PH_3)_2$. $Pt(Cl)_2(PH_3)_2$. $Pt(H)(CH_3)(PH_3)_2$. Models for reductive elimination from bis(phosphine) complexes. Explains why Pd(II) favours reductive elimination but Pt(0) favours oxidative addition.
McMichael Rohlfing et al. (1986)	M, MH, M=Pd, Pt. X $^2\Sigma$ and $^2\Delta$, respectively.
Nicolas and Barthelat (1986)	$Cu-C_2H_4$. Bonding and optical spectrum.
Novaro et al. (1986)	$M-H_2$ systems, M=Li, Cu, Pd, Ag and Pt. C_{2v} only.
Pettersson and Langhoff (1986)	GeH.
Poulain et al. (1986)	$Pt-H_2$. The excited $^1A_1$ state is binding.
Rappé (1986)	TeF_6 EA. Ground-state properties of TeF_6 and TeF_6^-.
Ricart et al. (1986)	SnX_2, X=Cl-I. Ground-state properties and IP.
Ross et al. (1986)	SO splitting of group 13 and 17 atoms, B-Tl, F-At.
Ruiz et al. (1986)	CuH+H->Cu + H_2 proceeds without barrier; CuH_2 is unstable, in agreement with matrix data.
Schwerdtfeger (1986)	Thesis on relativistic pseudopotential methods. Dimers and hydrides of Br, I, Au-Pb. Ions included.
Schwerdtfeger et al. (1986)	X, HX, X_2, X=Br, I.
Selmani et al. (1986)	Ag_n + O, O_2; n=2, 4.
Silberbach et al. (1986)	M_2^+, M=Rb and Cs.
Walch et al. (1986)	Dimers and trimers of Cu, Ag, Au.
Wisner et al. (1986)	$M(CH_3)_2(PH_3)_2$, $M(PH_3)_2$, M=Pd, Pt. CH_3 bonds strongly to Pd, while PH_3 prefers Pt. See Low and Goddard (1986ab).
Zangrande et al. (1986)	<u>Trans</u>-$Pt(PH_3)_2X_2$, X=Cl-I. PES.
Alvarez et al. (1987)	Br_4, Br_4^{2-}, Br_4K_2.
Andzelm et al. (1987a)	As_2, As_4 geometry and PES.
Andzelm et al. (1987b)	MM', MM'=Si-Sn. Geometry, ground electronic state.
Balasubramanian (1987a)	ScH_2. $X^2\Sigma_g^+$.
Balasubramanian (1987b)	GaAs, $GaAs^+$. $X^3\Sigma^-$ and $X^4\Sigma^-$, respectively, predicted.
Balasubramanian (1987c)	Ge_2. 14 bound low-lying states found.

Table 7.7. (continued).

Balasubramanian (1987d)	SnS.
Balasubramanian (1987e)	Se_2.
Balasubramanian (1987f)	PtH_2. X^1A_1(H-Pt-H 85°). Pt, PtH^+ tests.
Balasubramanian (1987g)	$GaAs_2$. X^2B.
Balasubramanian (1987h)	Pt_2.
Balasubramanian et al. (1987e)	PdH.
Balasubramanian et al. (1987a)	TeH.
Balasubramanian and M.Z. Liao (1987)	Au_3
Balasubramanian et al. (1987c)	SeH, SeH^+.
Balasubramanian et al. (1987b)	$KrHe^+$.
Balasubramanian and Pitzer (1987)	Review.
Balasubramanian and Ravimohan (1987)	Te_2.
Balasubramanian et al. (1987d)	SbH.
Bernier and Millié (1987)	HgH_2 potential-energy surfaces.
Caballol et al. (1987)	$Cu(CO_2)$ geometry.
Chapman et al. (1987a)	HI. SO decreases the dipole moment by 3.6 % at R_e.
Chapman et al. (1987b)	HBr. SO decreases D_e by 0.16 eV, contracts R_e by 0.5 pm.
Czuchaj et al. (1987)	MHe, MNe, M = Mg, Cd, Hg.
Dolg et al. (1987b)	MO, M = Sc-Zn. FeH.
G. Durand et al. (1987)	Mg_2^{2+}, Hg_2^{2+}. SO added for Hg.
Fernandez et al. (1987)	SnH_4^+ geometry, SO splitting.
Flad et al. (1987)	Cluster models for silver halide surfaces.
Francisco and Pueyo (1987)	Fine-structure of M^{n+}, n = 0, 2, 3; M = Sc-Zn using Huzinaga-type NR PP.
Fuentealba and Reyes (1987)	MH^+, M = Be-Ba.
Fuentealba et al. (1987)	MH, M = Li-Cs, Be-Ba. Ground-state properties.
Hay (1987)	Classical $M(H)_2$ and non-classical M-(η^2-H_2) complexes of five-coordinate W(0), d^6. L=PH_3, CO.
Hurley and Christiansen (1987)	Li and K EA from PP MC.
Igel-Mann et al. (1987)	CaO. Ab initio and semiempirical pseudopotentials compared.
Jarque et al. (1987)	Pd-C_2H_4 as model for heterogeneous catalysis.
Kozlov et al. (1987)	PNC effects in PbF. A QR PP calculation completed with monoatomic PNC matrix elements.

Table 7.7. (continued).

Langhoff et al . (1987)	MH, M=Y-Ag. Three atomic asymptotes important in bonding: $4d^n5s^2$, $4d^{n+1}5s^1$ and $4d^{n+2}5s^0$.
Lespes et al. (1987)	CH_3SnH_3. VUV and PES.
R.L. Martin (1987)	AgH, Ag_2, AgO. Ground-state properties.
McKee (1987)	O, O_2, C_2H_4 interactions with Ag_2 and Ag_2^+: models for surface-adsorbate interactions.
Merchán et al. (1987)	CuCO, $CuCO^+$.
Nakatsuji et al. (1987)	Pd-H_2, Pd_2-H_2 models for hydrogen chemiabsorption on Pd. The latter shows catalytic activity. Bonding to 4d primary, to 5s secondary. Excited states unimportant.
Neisler (1987); Neisler and Pitzer (1987)	Hg_2^{2+}. Stabilised by relativity by 1.0 eV wrt $2Hg^+$. Cavity models for hydration.
Nizam et al. (1987)	PbX_2, X=F-I.
Radzio and Andzelm (1987)	Non-additive interactions in Xe_3.
Ross et al. (1987)	RbH. Lowest states.
Russo et al. (1987)	PdX, X=C-Sn; RhC. Ground-state properties. LSD.
Sakai and Miyoshi (1987)	MF_6^{n-}, M=Cr-W, n=0-2. EA deduced.
Sánchez Marcos et al. (1987)	$Mo(CO_2)_2(PH_3)_4$, $Mo(CO_2)_2(CNH)(PH_3)_3$. Perpendicular carbon dioxides preferred.
Savin et al. (1987)	IP of a Cs_4O cluster. Decrease by oxygen explained as 2s repulsion of a_1 HOMO.
Schilling et al. (1987a)	SrH^+-CdH^+. Bonding analysed.
Schilling et al. (1987b)	MCH_3^+, M = Sc...Zn, Y...Cd. $D(M^+-CH_3) > D(M^+-H)$ by about 6 kcal/mol on the average. Bonding similar.
Schwerdtfeger (1987)	TlH^+, TlH, TlH_3. Ground-state properties. R/NR.
Schwerdtfeger et al. (1987)	HX^n, X=Br, I; n= -1, 0, +1.
Smith and Goddard (1987)	$Re_2Cl_8^{2-}$. Re-Re quadruple bond energy 85(5) kcal/mol (exp. 97(12)). Rotational barrier 3.0 intrinsic strength of bond 6(3) kcal/mol.
Wadt (1987)	5f-5f excitations of PuF_6.
Walch (1987)	Excited states of Ag_3. Ag_3^+.
Winkler et al. (1987)	Mössbauer isomer shifts in SnX_4, X=F-I, H, Me. Atomic DF integrals grafted to QR PP.
Anslyn et al. (1988)	$Cl_3MoC_3H_3$. Metallatetrahedrane preferred to metallacyclobutadiene.
Balasubramanian (1988a)	Br_2, Br_2^+.
Balasubramanian (1988b)	PbCl.
Balasubramanian (1988c)	MH_2, M = Ge-Pb.
Balasubramanian (1988d)	Pd_2.
Balasubramanian (1988e)	SnCl.

Table 7.7. (continued).

Balasubramanian (1988f)	MH_2, M = Co. Results compared with M = Sc, Y, Pd, Pt.
Balasubramanian and Feng (1988)	Ga_3, Ga_3^+.
Balasubramanian et al. (1988a)	$Ar-Cl^+$ collision system.
Balasubramanian et al. (1988b)	Pd + H_2 potential-energy surface, PdH^+. The Pd-H bonds are weaker, more ionic than Pt-H ones.
Balasubramanian and Li (1988a)	GeH. Dipole moment 0.098 D (exp. "1.24D").
Balasubramanian and Li (1988b)	In_2. Calculated D_e 0.87 eV, larger than that of Tl_2.
Balasubramanian and D.-W. Liao (1988a)	RhH_2 potential-energy surface.
Balasubramanian and D.-W. Liao (1988b)	RhH.
Balasubramanian and M.-Z. Liao (1988a)	AuH_2.
Balasubramanian and M.-Z. Liao (1988b)	SeH_2, SeH_2^+.
Balasubramanian and M.-Z. Liao (1988c)	Ag_3, Au_3.
Balasubramanian and Ravimohan (1988)	YH_2.
Basch et al. (1988)	TeO_2. A lower, open C_{2v} and higher (2.04 eV) ring geometry found.
Cauletti et al. (1988)	Sn-S and Sn-Se bonding in $(Me_3Sn)_2X$, $(Me_2SnX)_3$, X = S, Se.
Chapman et al. (1988a)	HX^-, X = Br, I. The HI EA predicted to be > 0.
Chapman et al. (1988b)	MH, M = Ge-Pb. Spectroscopic constants and dipole moments. Significant SO differences between $X^2\pi_{1/2}$ and $^2\pi_{3/2}$.
Daniel et al. (1988)	Olefin hydrogenation by the Wilkinson catalyst $RhCl(PR_3)_3$. Comparisons with RhH, Pd and Pt systems.
de Loth et al. (1988)	The Cu(II) - V(II) exchange interaction evaluated in a model complex for CuVO $(fsa)_2$ en · CH_3OH.
Di Bella et al. (1988)	Glyoximate complex of Pt. PES.
Ermler et al. (1988a)	Review.
Ermler et al. (1988b)	Anisotropic semiconductor clusters: PbI_2, GaAs, GaAs:S.
Fernandez Pacios et al. (1988)	Core-polarization corrections to PP. Na_2, K_2, NaK.
Fernandez Pacios and Gomez Calzada (1988)	Core-valence partition discussed for 3d metals.
Francisco and Pueyo (1988)	SO splittings for 3d ions in crystals.
Gavezzotti et al. (1988)	CO + Pt_n, n = 1, 3, 4, 7.
Gropen (1988)	Review.

Table 7.7. (continued).

Igel-Mann et al. (1988b)	XH, XO, X=K, Ca,Ga-Br. Ground-state properties.
Illas et al. (1988)	H chemisorption on M_5 models for M(100), M=Cu, Ag.
Jasien and Stevens (1988)	CrO, CrO^+.
Jeung and Koutecky (1988)	ScX, X=H, C, N, O.
Koga et al. (1988)	$Rh(H)(C_2H_4)(CO)_2(PH_3)$. Berry pseudo-rotation and olefin insertion around d^8 Rh(I).
Krauss et al. (1988ab)	Binding of Pt di-and triammines to oligonucleotides. Also $[Pt(NH_3)_4^{2+}]$ models bound to H_2O or $H_2PO_4^-$.
Langhoff and Bauschlicher (1988a)	MO, MS^+, M=Y, Zr, Nb.
Langhoff et al. (1988)	YX, X=F-Br.
Lee et al. (1988)	Mo_2, Mo_2^+. LDF. Ionization shortens and strengthens the bond.
Z.-X. Ma and S.-S. Dai (1988a)	Mo_2. Ground state.
Z.-X. Ma and S.-S. Dai (1988b)	KX^-, X=Cl-I.
McAdon and Goddard (1988ab)	M_N ring models for 1D metals, M=Cu-Au, Li, Na. N=2-12. Also M_2^+, M_3^+.
McKee and Worley (1988)	$Rh(CO)_n^{q+}$, n=1, 2; q=0,1.
P.K. Miller et al. (1988)	$OTeF_5^{q-n}$, q = 0,1. $NaOTeF_5$.
Miralles-Sabater et al. (1988)	$M^+ + C_2H_2$, M=Cu, Ag. A model for metal-olefin complexes.
Miyoshi and Sakai (1988a)	$ZrCl_4$, AgH, AuH, ZrO, Mo_2.
Miyoshi and Sakai (1988b)	AuF_6^{q-}, q = 0-3.
Miyoshi et al. (1988)	MF_6^{q-}, q=0,1; M=Cr-W. The EA of WF_6 is 1.52 eV smaller than that of MoF_6.
Nakamura and Morokuma (1988)	$Pt(PH_3)_2(CH_2{=}C{=}O)$ and $Pt(PH_3)_2(CH_2)(CO)$. TS from ketene to carbene carbonyl searched. Thermolysis of the ketene complex discussed.
Nakatsuji et al. (1988)	H_2-Pt_n, n=1-3, as models for hydrogen chemisorption on Pt. Pt and Pt_3 react but Pt_2 has a high barrier. SO small for Pt-H_2 X $^1A_1$ but important at large separation, mainly due to Pt atom ^3D_j effects. Pd≠ Pt.
Ortiz (1988)	EA of K-Cs.
Pitzer and Winter (1988)	Inclusion of SO PP for molecules. A real Hamiltonian obtained for C_{2v} D_2, D_{2h}, or higher symmetry in a $\|lm_lm_s\rangle$ basis.
Planelles et al. (1988)	$CuCH_2$. X $^2B_1$ (d^{10}, $\sigma^2\pi$) ionic state with a strong Cu-C bond.
Pouchan et al. (1988)	CH_3SnH_3 vibrational spectrum. MP2.
Rasch and Tobisch (1988)	Pt, PtH, PtH_2.

Table 7.7. (continued).

Saalfrank et al. (1988)	Te_∞ chains of trigonal tellurium. Cohesive properties, including inter-chain interactions.
Sakai and Miyoshi (1988)	EX_3, E=As, Sb; X=F-I. Geometries and dipole moments.
Selmani and Salahub (1988a)	XH_3, XH_4, X=C-Sn. LSD.
Selman and Salahub (1988b)	XH_2, X=Si-Sn. Singlet-triplet splitting at LSD level.
Tadjeddine et al. (1988a)	CH_3I. IP including SO.
Tadjeddine et al. (1988b)	CH_3I^+. Molecular states related to photofragmentation.
Tanpipat (1988)	MX, M=Sc, Lu, Lr; X=H, O, F, Cl. Lr resembles Lu (cp. Pyykkö (1979c)).
Walker et al. (1988)	Excited states of Sc...Co for various core sizes.
Andreocci et al. (1989, 1990)	Alkyl acetylides of tin and lead. PES.
Bagus et al. (1989)	Halogens (F-Br) bound to Ag_n surface models (n = 4, 7, 10). Essentially ionic bond. "Image charge" important.
Balasubramanian (1989a)	Pd_3. X $^1A_2$.
Balasubramanian (1989b)	MH_2^+, M = As-Bi. AsH_2.
Balasubramanian (1989c)	Review on relativity and chemical bonding.
Balasubramanian (1989d)	GaH_n, GaH_n^+, n = 1-3.
Balasubramanian (1989e)	Review on heavy p-block diatomic hydrides, halides and chalconides.
Balasubramanian (1989f)	Review on coinage-metal clusters.
Balasubramanian and Feng (1989)	M_n, M_n^+ (M = Ag, Au; n = 1-4). IP and AE.
Balasubramanian et al. (1989)	Au_4. X^1A_1 rhombus.
Balasubramanian and Li (1989)	Sb_2. $X^1\Sigma_g^+$ has a D_e of 2.17 eV, SO increased by 0.1 eV.
Balasubramanian and D.-W. Liao (1989)	Rh_2.
Balasubramanian and M.-Z. Liao (1989)	AgH_2.
Balasubramanian and Nannegari (1989)	AsH.
Balasubramanian and Ravimohan (1989)	Nb + H_2 potential-energy surface.
Balasubramanian and Wang (1989a)	ZrH.
Balasubramanian and Wang (1989b)	YH, $X^1\Sigma$ gross populations $6s^{1.55}$ $6d^{0.45}5d^{0.69}$.
Balasubramanian and Wang (1989c)	Tc + H_2 and Ru + H_2 reactions.
Basch (1989)	X_3, X_3^-, X = Se, Te.
Bauschlicher (1989)	EA of Au_3.
Bauschlicher et al.	$LaFe^{2+}$, $LaRu^{2+}$, YRu^{2+}. Multiple d-d'

Table 7.7. (continued).

Langhoff (1989)	bonds of order 2-3.
Bauschlicher et al. (1989a)	M_2, M_3, MM',MM'M",M = Cu-Au: structures and EA.
Bauschlicher et al. (1989b)	MCH_3^{n+}, M = Y-Ag.
Bowmaker et al. (1989)	X_2^n, n = -1, 0, +1, X = Br, I. Ground-state properties, EA, IP.
Brusich (1989)	Organometallic Th chemistry. L = H, CH_3, Cl.
Burton et al. (1989)	$Pd(acac)_2$, acac = acetylacetonate, O=CH=CHCH=O. Geometry, bonding and PES.
Castillo et al. (1989)	Cu + CH_4 -> $HCuCH_3$ -> CuH + CH_3. CI.
Cave et al. (1989)	$X_2Y_2^{2-}$ Zintl ions. $Pb_2Sb_2^{2-}$ and Sb_2Bi_2 are pseudo-T_d, $Tl_2Te_2^{2-}$ butterfly-like C_{2v}. Also isoelectronic neutrals.
Chang and Pitzer (1989)	$U(COT)_2$. Green color due to 5f -> 6d excitations. Charge $U^{+0.98}$, $6d^{1.98}$ $5f^{2.50}$.
Chapman (1989)	HX, HX^-, X = Br, I. MH, M = Ge-Pb. Electric dipole and transition moments.
Chapman et al. (1989)	Ar-Cl^+ collision system.
Christiansen (1989)	PP MC reviewed.
Crépin and Millié (1989)	Hg-N_2 potential curves. A Hg(^{3}P) exciplex found.
Czuchaj et al. (1989)	CaHe, CaNe.
Daoudi et al. (1989)	MCO, M = Ru, Os.
K.K. Das and Balasubramanian (1989a)	YH_2^+, ZrH_2^+.
K.K. Das and Balasubramanian (1989b)	NbH_2^+, MoH_2^+.
Dolg and Stoll (1989)	LnH, LnO. LnF, Ln = La-Lu. The 4f AO in core. For comments on ground-states, see McDonald et al., JCP 93 (1990)7676.
Feng and Balasubramanian (1989)	In_3.
Fernandez Sanz and Márquez (1989)	H_3Sn-XH_3, X = C-Sn. Structure and vibrational spectrum.
Fernandez Sanz et al. (1989)	SnH_4 vibrational spectrum.
Fuentealba et al. (1989)	EA for Ca, Sr, Ba.
Garcia-Cuesta et al. (1989)	Pd/C_2H_2. A weakly-bonded π complex.
Igel-Mann et al. (1989)	X_2, XH, XO, XF, XS, X=In, Sn, Sb. Ground-state properties.
Illas et al. (1989)	H and O chemisorption on a Cu_5 cluster model for a Cu(100) surface.
Kim and Balasubramanian (1989)	GaH.
Kober and Hay (1989)	Transition-metal dihydrogen chemistry. $WL_5(H_2)$, L=CO, $PR_3.Cr(CO)_4(H_2)_2$.
Koga and Morokuma (1989)	Olefin hydrogenation by the Wilkinson catalyst. $H_2RhCl(PR_3)_3$. Also fragments: RhCl, H_2RhCl, etc.

Table 7.7. (continued).

Krogh-Jespersen et al. (1989)	$(NH_3)_5Ru(III)L$, $L=NH_3$, $S(CH_3)_2$.
Kudo and Nagase (1989)	PbH_4^+ Jahn-Teller distortions. Ready decomposition to $PbH_2^+ + H_2$.
Langhoff et al. (1989)	MO, MS, M=Mo, Tc.
Lee et al. (1989)	Pd_2. LDF.
Li and Balasubramanian (1989)	I_2, I_2^+, 30 and 13 electronic states, respectively, as functions of R. V_{SO} included.
Z.-X. Ma and S.-S. Dai (1989)	HgX_2, X=Cl-I.
Marino et al.(1989a)	Be_n surface models (n=19-45) for H and Cs adsorption.
Marino et al. (1989b)	Bi_6I_{18} model for BiI_3. Optical absorption spectra and geometry discussed.
Maseras et al. (1989)	$[Rh(PH_3)_4H_2]^+$: classical or non-classical?
Miralles-Sabater et al. (1989)	$Cu + H_2O^{q+}$, q=0,1.
Moullet et al. (1989)	Cs_2, Cs_2^+ using DFT. R/NR comparisons. 5d important.
Nagase (1989)	X_nH_n, X=Ge-Pb, n=4, 6, 8 (tetrahedrane, prismane, cubane).
Nizam et al. (1989); Nizam and Bouteiller (1990)	Cluster models for Pb(II) dihalides. X=F-I. Geometries of PbXX' optimized.
Novaro (1989)	Review on activation of small molecules by transition-metal atoms.
Pavolini et al. (1989)	RbCs, 30 electronic states.
Planelles et al. (1989)	$CuCH_2^+$ $X\ ^1A_1$.
Ramírez-Solís and Daudey (1989)	CuF low-lying levels.
Ramondo et al. (1989)	MXX', M=Sn, Pb; X=F-I. Structure and vibrational spectra.
Ross (1989)	Effects of SO on atoms, molecules and clusters.
Schwerdtfeger (1989)	AuX_2^-, AuX_4^-, X=F-I. Larger relative stability of Au(III) halide complexes, compared to Au(I) ones, attributed to relativity.
Schwerdtfeger et al. (1989a)	TlR_n^{m+}, n=1-4, $R=CH_3$, H, m=0, 1. TlR_2Br. TlR', $R'=C_2H_3$, C_2H. TlBr, Tl_2. Explain why organometallic chemistry uses Tl(III), inorganic Tl(I). $TlCH_3$ predicted to be stable.
Schwerdtfeger et al. (1989b)	AuL, L=H, F-I, Li, Na, S. Ions of Au_2, AuH. Largest D_e decrease (-86 kJ/mol) for AuF, largest D_e increase (+174 kJ/mol for AuLi. All contract.
Schwerdtfeger et al. (1989c)	PbH^+, PbH_n, n=1, 2, 4. Ground-state properties.

Table 7.7. (continued).

Sodupe et al. (1989a)	$Cl_4W{=}CH_2$. Conformational preferences.
Sodupe et al. (1989b)	Ground and low-lying states of FeH^+. X $^5\pi$.
Sohn et al. (1989)	Nb_2. X $^3\Sigma_g^-$. $^3\Delta_g$ slightly higher.
Spiegelmann et al. (1989)	Rb_2.
Strömberg et al. (1989)	MH^+, MCl_2, M=Cd, Hg. $Hg(OH)_2$, HgO (bad D_e). Consequences on global "mercury cycle" quoted.
Wang and Balasubramanian (1989)	TcH.
Balasubramanian (1990a)	GaAs, $GaAs^+$, $GaAs^-$.
Balasubramanian (1990b)	Review on heavy p-block dimers and trimers.
Balasubramanian (1990c)	InSb, $InSb^+$, $InSb^-$.
Balasubramanian (1990d)	$(GaAs)_2$. X^1A_g rhombus.
Balasubramanian (1990e)	InH, InH^+.
Balasubramanian (1990f)	MH, M = Y-Cd.
Balasubramanian and Dai (1990)	The Ir + H_2 and Ir^+ + H_2 potential energy surfaces. The IrH_2^+ X^3A_2 bond angle increased by 9° by SO.
Balasubramanian and Das (1990)	Reply to comments by Bauschlicher et al. (1990a) on coinage-metal tetramers.
Balasubramanian and Feng (1990a)	Pt_2 + H and Pt + H potential-energy surfaces.
Balasubramanian and Feng (1990b)	Cu_4, Ag_4.Ag-Ag 287pm, compared to Au-Au = 269 pm in Au_4.
Balasubramanian and Li (1990)	MoH, MoH^+.
Balasubramanian and Ravimohan (1990)	Zr_2.
Balasubramanian and Wang (1990)	RuH.
Ballone and Galli (1990)	LD-pseudopotential results on M_2, M_2^+, M=Cu-Au. D_e overestimated by a factor of 3, R_e underestimated by 10.
Barandiaran et al. (1990)	YO, TcO, AgO, AgH. Rel. contractions given.
Barnes et al. (1990)	Mono- and dicarbonyl ions of 3d and 4d metals. MCO^+, $M(CO)_2^+$, M = Sc-Cu, Y-Ag.
Barone et al. (1990)	X_4H_9 and X_5H_{12} cluster models for diamond-like crystals, X = C-Ge.
Bauschlicher and Langhoff (1990)	Transition-metal cations: a review on 3d- and 4d-metal Ar, $(H_2O)_n$, CO, H, CH_3,... complexes.
Bauschlicher et al. (1990a)	Comparisons with Balasubramanian and Feng (1990b) on M_4, M = Cu-Au.
Bauschlicher et al. (1990b)	M_4, M_5, M = Cu-Au.
Bauschlicher et al. (1990c)	AgO, AgS.

Table 7.7. (continued)

Bowmaker and Schwerdtfeger (1990)	ZnX, X = F-I. Ground-state properties and UV spectra. Monotonous k_2 decrease suggested for MX, M = Zn-Hg.
Bravo et al. (1990)	AgO_2 potential-energy surfaces. O_2^--production in olefin oxidation explained.
Bruno et al. (1990)	PtL_2, L =$-CH_2-PH_2-BH_2-PH_2CH_2-$. Bonding and PES.
Christiansen (1990)	Al^{n+}, n=0-2. Core polarization potentials. PP MC.
Dai and Balasubramanian (1990)	EH_3^{n+}, E = As-Bi, n = 0, 1. Also EH, EH_2.
K.K. Das and Balasubramanian (1990a)	Rh_3. X^2A_3 (D_{3h}).
K.K. Das and Balasubramanian (1990b)	Au_2 low-lying states. X O_g^+ is 96% $^1\Sigma_g^+$. R_e 251.8 pm, ω_e 193 cm^{-1}, D_e 2.05 eV (exp. 247, 191, 2.30).
K.K. Das and Balasubramanian (1990c)	Tc^++H_2,Ru^++H_2.
K.K. Das and Balasubramanian (1990d)	LaH. Low-lying states.
K.K. Das and Balasubramanian (1990e)	GeH_n^{q+}, n = 1-3, q = 0,1.
K.K. Das and Balasubramanian (1990f)	YNH, NYH. Linear $X^2\Sigma^+$ YNH lowest.
K.K. Das and Balasubramanian (1990g)	NbH. X $^5\Delta$.
K.K. Das and Balasubramanian (1990h)	Rh_3.
Dolg et al. (1990a)	GdO. $X^9\Sigma^-$. Bond-length expansion 1.6 pm.
Dolg et al. (1990b)	EuO. $X^8\Sigma^-$.
Feng et al. (1990)	Xe-I^+ collision system. Transfer of translational and electronic energy calculated.
Fernandez Pacios (1990)	Modified Ar-core PP for 3d metals. Improved s^2d^n-s^1d^{n+1} HF-level energies.
Flad et al. (1990)	Adsorption of Ag_n^{q+} on AgBr surfaces.
Haberlandt (1990)	NiH.
Igel-Mann et al. (1990)	$(XY_m)_n$, X=In, Sn, Sb; Y=H, O, F, S; n≤6. $In(C_5H_5)$. Ground-state properties.
Illas et al. (1990)	Rh, RhH, Rh_2.
Jarret-Sprague et al. (1990)	HXO_3, X=As, Sb. Structure and frequencies.
Karna et al. (1990)	CHX_3, X=F-I. Static polarizability α, first and 2nd hyperpolarizabilities β and γ. Geometries, dipole moments.
Katsuki (1990)	Ag, AgH using a spectral representation PP.
Kaupp et al. (1990a)	$M(CH_3)_n$, M=Mg, Zn, n=1, 2. Ground-state properties. Chemical properties of Mg and Zn compared.

Table 7.7. (continued).

Knight et al. (1990)	PdH_2^+. X $^2A_1$.
Koga and Morokuma (1990)	C-H activation in CH_4 by $RhCl(PH_3)_2$.
Krauss and Stevens (1990)	Rb_2, Cs_2 and their anions.
Kyle et al. (1990)	$Cu_4I_4(NH_3)_4$ as model for luminescence in $Cu_4I_4(C_5H_5N)_4$.
LaJohn (1990)	M_2, M_2^+, M=Li-Cs. Includes core-valence correlation potentials.
Langhoff and Bauschlicher (1990)	NbN. X $^3\Delta$. Results compared with isoelectronic ZrO, Nb is $5s^1$ and has more stable 4d orbitals.
Li and Balasubramanian (1990)	Mo + H_2. Insertion (C_{2v}) mode easier than collinear ($C_{\infty v}$ one.
Lin and Ortiz (1990)	CrH^-, MnH^-, FeH^-. IP.
Z.-X. Ma and S.-S. Dai (1990a)	BaCl. X $^2\Sigma$ and A states.
Z.-X. Ma and S.-S. Dai (1990b)	$TiCl_2$.
Z.-X. Ma et al. (1990)	BX_3, X=F-I. PES reassigned, including SO.
Marino et al. (1990)	Cluster models for PbI_2.
Merchan et al. (1990)	Cu_2, CuH.
Musolino et al. (1990)	Sb_2, Sb_4 using several DFT PP. PES interpreted.
Nagase and Kudo (1990)	Bicyclo [2.2.0] hexaplumbane. M_6H_{10}, M=Ge-Pb. Geometries (C_2) and frequencies.
Nagase et al. (1990)	HM=MH, M=As-Bi. Double bonds found, even for Sb and Bi. Geometries (C_{2h}) and frequencies.
Nakatsuji and Ehara (1990)	CsXe. Collision-induced 6s-5d absorption spectra from a quasistatic model.
Nakatsuji and Nakai (1990)	O_2-Ag_n, n=2, 4, as models for oxygen chemiabsorption on silver.
Nakatsuji and Saito (1990)	Excited states of $[MoO_{4-n}S_n]^{2-}$ and $MoSe_4^{2-}$.
Nakatsuji et al. (1990)	^{95}Mo NMR chemical shifts in $[MoX_{4-n}Y_n]^{2-}$, X, Y = O, S, Se. E(d-d*) important. No SO.
Nicolas and Spiegelmann (1990)	M-C_2H_4, M = Cu-Au. Bonding and excited states.
Ohanessian et al. (1990)	MH^+, M = Ba, La, Hf-Hg. Bonding analysed, compared with 3d and 4d analogs.
Ohanessian and Goddard (1990)	Review on bonding in MH^+, M = 3d, 4d or 5d metal.
Pacchioni and Bagus (1990)	CO/Pd_n, n = 2, 8 as models for chemisorption. R PP of Hay and Wadt (1985ab) compared with NR PP of Huzinaga.

Table 7.7. (continued).

Paniagua and Illas (1990)	H/Rh_n, n = 3, 4, as models for chemisorption.
Partridge et al. (1990)	$(MM')^q$, $(MM'M'')^q$, q = -1, 0, +1, M = Cu-Au IP and EA.
Pepper and Bursten (1990)	U_2. X $^{13}\Delta_g$ at R_e = 300 pm, D_e = 160 kJ/mol.
Plass et al. (1990)	Cu_2X_2, Cu_4X_4, X = Si, Sn.
Poulain et al. (1990)	$M + H_2$, M = Ni, Ru, Rh, Pt.
Ramírez-Solís and Daudey (1990)	CuCl.
Ramírez-Solís et al. (1990)	CuI. SO included.
Rochefort et al. (1990)	Chemisorption and diffusion of H in and on cluster models of Pd, Rh and bimetallic PdSn, RhSn and RhZn catalysts. LSD potential.
Rosi and Bauschlicher (1990)	Bonding of La^+ and La^{2+} to C_2H_2, C_2H_4 and C_3H_6.
Rosi et al. (1990)	M^{n+}-C_2H_6 and $M(CH_3)_2^{n+}$, M = Y - Ag, n = 0,1.
Sawamura and Ermler (1990)	$(PbI_2)_7$ cluster models. Quantum confinement effects in layered clusters.
Schwerdtfeger (1990)	$M(CH_3)_2^{n+}$, M = Au - Pb, n = -1 - +2. R/NR. Force constant maximum at $HgMe_2$. Decrease at $TlMe_2^+$ relativistic, further decrease at $PbMe_2^{2+}$ both R and NR.
Schwerdtfeger et al. (1990a)	TlMe, $TlMe_2^+$, $TlMe_3$, $TlMe_4^+$, $TlMe_2Br$. Frequencies reported here.
Schwerdtfeger et al. (1990c)	Au(I) complexes. AuL, AuL_2^-, L = H, F-I, CN, SCN, CH_3 PH_3^+. Two-coordination, 5d participation and Cl NQCC of $AuCl_2^-$ increased by relativity.
Sellers (1990a)	Nb_n, n = 1-4, Nb-N_2. Cations included.
Sellers (1990b, 1991)	Pd_n + H, O, N, S; n = 10...22. Chemisorption models.
Sellers and Ove (1990)	Anisotropic PP for modelling partially filled d shells. CoH, Co_2.
Sodupe et al. (1990)	Ground and low-lying states of FeH. X $^4\Delta$.
Spiegelmann et al. (1990)	The $ArKr^*$ exciplex. SO included.
Strömberg et al. (1990)	$M(H_2O)_6^{2+}$, M = Cd, Hg. $Hg(H_2S)_6^{2+}$. Quasioctahedral, T_h energy minima.
Sumathi and Balasubramanian (1990)	H_2Te, H_2Po and their cations. TeH and PoH. SO important for Po. Dipole moment changes sign from H_2Te to H_2Po.
Tobisch and Rasch (1990)	Pt, PtH, PtH_2.
Trinquier (1990)	XH_n (n = 1, 2, 4), X_2H_4, X = Sn, Pb. <u>Trans</u>-bridged forms, rather than $H_2X = XH_2$ predicted to be stable.
Trinquier and Barthelat (1990)	XF_2, X_2F_4, X = Sn, Pb. Dito.

Table 7.7. (continued).

J.-Z. Wang et al. (1990)	$Zr + H_2$.
L.-S. Wang et al. (1990a)	E_2, E_2^+ E = As-Bi.
L.-S. Wang et al. (1990b)	AB, AB^+, A = Sn, Pb; B = Se, Te.
Winkler and Vetter (1990ab)	Mössbauer IS and NQCC in $SnX_n(CH_3)_{4-n}$, X = F-I.
Andrae et al. (1991)	Ag_2, Au_2, RuH, OsH as tests of the potentials of Andrae et al. (1990). Also M_2^+, M_2^-, M = Ag, Au. No SO. (Cp. Benavides-Garcia and Balasubramanian (1991)
Andreocci et al. (1991)	Cyclic $Me_2Si(N\text{-}Me)_2M$, M = Sn, Pb. $(Me_2Sn)(NMe)_2(SnMe_2)$. PES.
Audouard and Spiegelmann (1991)	Kr_2^* and Kr_2^+ potential energy curves at MR CI level including SO.
Balasubramanian (1991a)	Pt_2H_2 potential-energy surface.
Balasubramanian et al. (1991a)	Compare the small-basis DF-LCAO calculations of Ramos et al. (1988) with large-basis correlated PP ones. For reply, see Malli et al. (1991).
Balasubramanian and Das (1991a)	HfH. Strong SO mixing found. $X^2\Delta_{3/2}$. The $^4\Phi$ states have more d, less s and go up, compared to ZrH.
Balasubramanian and Das (1991b)	M_4^+, M = Cu-Au. X $^2B_{1u}$, rhombus.
Balasubramanian and Das (1991c)	Au_3 excited states.
Balasubramanian and Feng (1991a)	Ga_4, In_4.
Balasubramanian and D.-W. Liao (1991a)	Au_6 isomers. C_{5v} is 0.73 eV below D_{6h}.
Balasubramanian and D.-W. Liao (1991b)	Bi_2, Bi_2^-. Bi_2 $X^1\Sigma$ R_e 276 pm (exp. 265.96). Important SO increase of the EA.
Balasubramanian and Ma (1991)	WH_2, WH_2^+ potential surfaces. WH_2 more stable than MoH_2 by 0.5 eV, compared to $M(^7S) + H_2$.
Balasubramanian et al. (1991b)	E_3, E_3^+, E = P-Bi. The different photo fragmentation patterns of Sb_n and Bi_n explained: IP(Bi) < IP(Bi_2) but IP(Sb) > IP(Sb_2).
Balasubramanian and Tao (1991)	EH_n, EH_n^+, E = In, Tl; n = 1-3.
Balasubramanian et al. (1991c)	GaAs + X, InSb + X, X = Cl, Br. Models for halogen-etching.
Barthelat et al. (1991)	NbH_3 and TaH_3 non-classical (dihydrogen) and classical, respectively.
Basch (1991)	M_2^{2+}, M = Pt, Au, Hg. $R_e(Hg_2^{2+})$ 285 pm!
Bauschlicher and Langhoff (1991)	M^+, M^{2+} complexes (M = Y, La) with C_2H_2, C_2H_4, C_3H_6.
Bauschlicher et al. (1991a)	Bonding of Nb^{2+} to CH_2, C_2H_2 and C_2H_4.

Table 7.7. (continued).

Bauschlicher et al. (1991b)	Zr_2. New spectral assignments.
Benavides-Garcia and Balasubramanian (1991)	OsH. $X(^4\Pi + {}^4\Delta)$.
Bock et al. (1991)	SiI_2 PES.
Breidung et al. (1991)	AsH_nF_{3-n}, AsH_nF_{5-n} vibrational spectra.
Castillo et al. (1991)	The $HCuCH_3$ reaction intermediate.
Cauletti et al. (1991)	$SnCl_2$. PES.
Chang (1991)	$C_{60}M$, M = Cs, Ba, La, Eu, U. $(COT)_2An$, An = U, Np, Pu, including SO. Magnetic moment and optical spectra calculated.
Chang et al. (1991)	$C_{60}M$, $C_{60}M^+$.
Cheng and Balasubramanian (1991)	TaH.
Christiansen (1991)	PP MC on Sc and Y.
Czuchaj et al. (1991)	NaHg potential curves, TP.
Dai and Balasubramanian (1991a)	$Os^+ + H_2$.
Dai and Balasubramanian (1991b)	$Re + H_2$, $Re^+ + H_2$.
Dai and Balasubramanian (1991c)	IrH. Results compared with RhH.
Dai et al. (1991a)	$Ta + H_2$, $Ta^+ + H_2$.
Dai et al. (1991b)	Pd_3^+. X^4B_2, nearly D_{3h}.
K.K. Das and Balasubramanian (1991a)	Ag_n, Au_n EA calculated, n = 3,4.
K.K. Das and Balasubramanian (1991b)	LaH_2. X^2A_1.
K.K. Das and Balasubramanian (1991c)	LaH^+, LaH_2^+. $X^2\Delta$, X^1A_1, respectively.
K.K. Das and Balasubramanian (1991d)	RhH^+, $X^2\Delta$.
K.K. Das and Balasubramanian (1991e)	HfH_2. X^1A_1. Results compared with ZrH_2.
K.K. Das and Balasubramanian (1991f)	$InSb_2$, $SbIn_2$, $GaAs_2$, $AsGa_2$ and their cations.
K.K. Das and Balasubramanian (1991g)	Ru_2. $X^7\Delta_u$.
K.K. Das and Balasubramanian (1991h)	RhH_2^+.
Dolg et al. (1991a)	$Ce(C_8H_8)_2$. X $4f^1e_{2u}^3$ singlet. First triplet 0.5 eV higher.
Dolg et al. (1991b)	HgH_n(n = 1,2), TlH_n(n = 1,3), PbH_n(n = 1,2,4), BiH_n (n = 1,3,5), PoH_n(n = 1,2), AtH. RnF_n(n = 2,4,6,8). NR/QR/SO comparisons reported. Relative chemical stability for various n analysed.
Dolg et al. (1991c)	CeO. 4f in core or in valence space.
Dolg et al. (1991d)	LnX_2, LnX_3, Ln = La... Lu, X = F-I. Atomization energies compared to exp.
Dolg et al. (1991e)	$LnHe^{3+}$, Ln = La...Lu. The La, Gd, Lu ones stable, Eu and Yb ones metastable.
Faegri and Bauschlicher (1991)	ScNi, YNi, ScPd, YPd. $X^2\Sigma$.

Table 7.7. (continued).

Fernandez Pacios and Botella Olcina (1991ab)	Improved Ar-core PP for Sc-Cu.
Flurer and Busch (1991)	M_2X^+ ions, M = Cu, Ag, X = H, CH_3, O, CO. Mass spectroscopic data interpreted.
Focher et al. (1991)	The eigenvalue for the last valence electron compared to experimental IP_n, Z = 1-94. LDF-based QRPP of Bachelet et al, (1982) used.
Gayen et al. (1991)	Cluster models for GaAs surface passivation by sulfur.
Hay (1991a)	$Pt(PH_3)_2 + H_2$ revisited. If 5s and 5p shells are in core, too large E_{corr} obtained, due to missing 6s, 6p nodes.
Huzinaga (1991)	Review.
Illas et al. (1991)	Cu_5O as model for O chemisorption on Cu(100). 3d correlation decreases the interaction.
Kaupp et al. (1991a)	MH, MH^+, MH_2, M=Ca-Ba. CaH_2 linear, SrH_2 and BaH_2 bent. Both core polarization and direct d-AO contributions to the bending.
Kaupp et al. (1991b)	MX_2, M=Be-Ba, X=F-I. All Be and Mg halides, $CaCl_2$-CaI_2 and SrI_2 linear. CaF_2, $SrCl_2$, $SrBr_2$ and BaI_2 are borderline. SrF_2 and BaF_2-$BaBr_2$ bent. Bending force constant (> or < 0) correlates with d character.
Klobukowski (1991)	XH, X=N-Sb. $^3\Sigma^-$ and $^1\Sigma^-$ states. Compared to the nodeless PP, the model potential with nodal wave functions is useful for SO.
Koga and Morokuma (1991a)	Review on catalytic elementary reactions and catalytic cycles of transition-metal complexes.
Koga and Morokuma (1991b)	CO insertion into the Pd-R bond of $HPd(R)(CO)(PH_3)$, R = H, CH_3.
Jarid et al. (1991)	CrF_4, CrF_5, RuF_4 and RuF_5. High-spin T_d, D_{3h}, D_{4h} and C_{4v} geometries predicted, respectively, at CI level.
Lee and Lee (1991)	MP2 with V_{SO} for HX, XX', X=Br, I. PbH_4.
Ma and Balasubramanian (1991)	WH. SO effects separated. Results compared with MoH.
Mains and White (1991)	Rh_n, $Rh_x(CO)_y$, RhH, RhH_3, RhC, RhCH, RhO, RhO_2. PP and AE results compared.
Marino (1991)	Summary of the cluster-model work on PbI_2, BiI_3 and Cs-activated Be-surfaces.
Marino and Ermler (1991)	$Be_{45}X_2$, X=Cs, OCs, HCs surface models. Cesiation lowers surface work function by 2.2 eV.
Martinez-Magadan et al. (1991)	ZnH_2^{n+}, n=0-2. Reaction surfaces.

Table 7.7. (continued).

Morokuma and Borden (1991)	$(H_3P)_2Pt(C_2H_4)$: a study of alkene pyramidalization.
Nakatsuji and Saito (1991)	RuO_4, OsO_4 excited states. Ru-O bond weaker than Os-O one. E(LUMO) -4.1 and -2.9 eV, respectively, explaining why RuO_4 is a stronger oxidation agent. First allowed excitation energies 3.22 and 3.90 eV, respectively.
Nguyen et al. (1991)	M_2E_3 and $M_2E_3H_2$ propellanes, M = C - Sn, E = O, S.
Novaro and Jarque (1991)	Pd-H_2. Results compared with matrix spectroscopy. R/NR.
U. Meier et al. (1991)	GaAs, $GaAs_2$, Ga_2As_2, As_2 and As_4 at MRD-CI level. Ions included.
Ortiz and Ballone (1991a)	PP for various non-local density functionals applied on M, M^+ and M_2, M = Be-Ba, Zn-Hg. IP_n and atomic excitation energies stable. D_e of M_2 vary strongly.
Ortiz and Ballone (1991b)	M_2^{2+}, M = Ag, Cd, Au, Hg. DFT PP. Gradient corrections remove binding for Au. M = Cd and Hg predicted to be metastable.
Ortiz and Ballone (1991c)	M_2, M = Be-Ba, Cd, Hg. LDA PP.
Pak et al. (1991)	LiBe, with full SO CI.
Pitzer and Winter (1991)	SO integrals.
Pyykkö and Zhao (1991a)	Bonding trends in XAu_n^{m+}, X = B-N, Al-S; n = 4 - 6. CAg_6^{2+}. At QR HF level, radial bonding dominant.
Pyykkö and Zhao (1991b)	$(Cl\ M\ PH_3)_2$, M = Ag, Au. The weak, "aurophilic" Au...Au attraction ascribed to correlation effects, not hybridization, by a HF/MP2/MP3 comparison. BSSE not considered. [See Li and Pyykkö (1992)].
Pyykkö and Zhao (1991c)	The large range of uranyl bond lengths interpreted as a frozen soft mode of a UO_6^{6-} octahedron. The D_{2h} structure of a $(OAnO)_2^{n+}$ dimer reproduced.
Sakaki and Ieki (1991)	Oxidative addition of SiH_4 to $Pt(PH_3)_2$. MP4.
Savin et al. (1991)	Visualisation of the electron density in Sn(II) compounds: SnO, Sn_2O_2, Sn_2H_4, Cu_4Sn_4. The $5s^2$ lone pair seen.
Schwerdtfeger (1991a)	$(TlH)_2$ model for $(Tlcp)_2$. A weak Tl(I)...Tl(I) attraction found at correlated level, none at HF level. TlH studied at seven different levels, up to QCI.
Schwerdtfeger (1991b)	Au and Au_2. Au EA increased 1.07 eV by relativity. Total EA 2.133 (exp. 2.309(5)) eV, IP_1 8.930 (9.226) eV. Au-Au 253.7 (247.2) pm.

Table 7.7. (continued).

Schwerdtfeger and Dolg (1991)	AuLa, AuLu. D_e tripled by relativity. In AuLa, Au $5d^{9.91}$, not much d transfer. Cp. Watson et al. (1987) for solid AuLu.
Schwerdtfeger et al. (1991)	PdH, PdF.
Seijo et al. (1991)	MX_2, M = Mg-Ba, X = F-I. Geometries and frequencies obtained at HF level.
Smith and Carter (1991)	Interactions of NO and CO with Pd and Pt atoms. MCO linear, X $^1\Sigma$. MNO bent. Pd and Pt prefer CO and NO, respectively.
Sodupe and Bauschlicher (1991)	$M^+ + C_2H_2$, M = Y-Ag. Y^+-Mo^+ insert into the π bond, Tc^+-Ag^+ have electrostatic bonding.
Sodupe et al. (1991b)	$Cl_4W{=}CH_2 + C_2H_4$. Formation of the metallacyclobutane exothermic.
Sodupe et al. (1991c)	Collinear reaction of Fe^+ with H_2.
Song and Hall (1991)	$WOCl_2(NH_3)_3$, $MoOCl_2(PH_3)_3$: no evidence for bond-stretch isomers.
Trinquier (1991)	X_2H_4, X = Sn, Pb. A singly-bridged local minimum.
Wang and Ermler (1991)	$Cs_{11}O_3^{n+}$ cluster model for cesium suboxide, n = -1, 0, +1.
Wexler et al. (1991)	$(C_6H_6)Ta(OH)_2$. Structure and bonding.
Albright and Tang (1992)	$Ta(CH_3)_5$, TaH_5. C_{4v} preferred to D_{3h}.
Allouche et al. (1992)	BaH. SO included.
Anchell et al. (1992)	PdH, Pd_nH_2 (n = 2,6).
Andrae et al. (1992)	OsH. Results compared with Benavides-Garcia and Balasubramanian (1991).
Andreocci et al. (1992)	$Sn(C{\equiv}CMe)_4$. PES.
Armstrong et al. (1992)	$LiMPh_3$, M=Sn, Pb. Sn-Li>Pb-Li.
Balasubramanian et al. (1992)	Hg_2. 12-VE PP. Many excited states given.
Balasubramanian and Feng (1992a)	$M_2 + H$, M = Ni, Pd. C_{2v} ground state. SO for Pd. Cp. B and F (1990a) on Pt_2H.
Barandiarán and Seijo (1992)	E_2, E = N-Sb. ScO, ScS. MnO, CuO.
Bauschlicher et al. (1992b)	MCH_2^+, M=Y-Ag.
Benavides-Garcia and Balasubramanian (1992)	GeX_2, GeHX, X=Cl-I. X $^1A_1$. Singlet-triplet separation.
Bender et al. (1992)	$Os(CO)_4(C_2H_4)$, an osmacyclopropane. GVB. $Os(CO)_4$, $H_2Os(CO)_4$.
Blomberg et al. (1992b)	$CH_4 + Pd_3$.
Boatz et al. (1992)	CdAr potential-energy surfaces.
Boehm and Banerjee (1992)	ReO_2, ReO_4^{n-}, n = 0,1.
Boldyrev and Simons (1992)	TeF_8^{2-} electron detachment energy 5 eV.
Boldyrev et al. (1992)	ICCH, ICCI, $IF_n(CCH)_{3-n}$, $I_4(CC)_4^{4+}$, $I_4(CC)_4F_4$. HF. New iodonium compounds predicted.

Table 7.7. (continued).

Breidung and Thiel (1992)	MI_3, MI_5, M = Sb, Bi. Ground-state properties.
Casarin et al. (1992)	$M(TAA)^{p+}$, M=Ni, Pd; TAA = tetraazaannulene. PES.
Colmenares-Landin et al. (1992)	Ru + H_2.
Cundari (1992a)	TM imido complexes, $L_nM{=}NR$. M=Ti-Hf, ..., Rh, Ir.
Cundari (1992b)	$(NH_2)_2Zr{=}NH$, **1**. **1** · H_2.
Cundari (1992c)	$H_2M{=}NH$ + CH_4 reaction, M = Ti-Hf. $X_2Zr{=}NH$, X = $-NH_2$, -Cl.
Cundari and Gordon (1992a)	Olefin metathesis catalysts: $M(OH)_2(NH)(=CHR)$, M = Mo, W, Re; R = H, CH_3. $MCl_2(XH)(CH_2)$, $M(OH)_2(XH)(CH_2)$.
Cundari and Gordon (1992b)	Transition metal alkylidenes: $H_2M{=}CHX$, M = Ti-Hf. H_3M = CHX, M = Nb, Ta.
Czuchaj et al. (1992a)	CdHg potential-energy curves and transition moments.
Czuchaj et al. (1992b)	KHg potential-energy curves and transition moments.
Dai and Balasubramanian (1992a)	M_3 + H, M = Pd, Pt. X $^2A_2$, C_{3v}. SO
Dai and Balasubramanian (1992b)	Zr_4. X D_{2h} rhombus, ^1A_g or $^3B_{1u}$, 5s-to-4d and 5p promotion observed.
Dai and Balasubramanian (1992c)	Rh_3. X S=6 C_{2v}. Low barrier to D_{3h}.
Dai and Balasubramanian (1992d)	M_4, M = Ge-Pb. X D_{2h} rhombus ^1A_g. SO for Pb_4, increases R by 0.5 pm, lowers E by 0.2 eV, changes atomization energy from 148 to 56 kcal/mol. Pb $6s^{1.94}$, nearly "inert pair".
Dai and Balasubramanian (1992e)	Os + H_2. X $^3B_1$, C_{2v}. (cp. linear RuH_2 quintet states). SO effects on bond angle up to 10°. Os ^5D ground state doesn't insert into H_2, the ^3F does.
Dai and Balasubramanian (1992f)	M_4^+, M=Ge-Pb. SO.
Dai et al. (1992a)	Ge_3. X $^1A_1$ or $^3B_2$.
Dai et al. (1992b)	IrH^+.
Dixon et al. (1992)	$CH_2X{-}CH_2X$, X = Br, I.
Dmitriev et al. (1992)	P- and PT- odd terms for HgF and PbF.
Dolg et al. (1992a)	Yb and YbO. An $f^{13}\sigma^1$ 0^- ground state still found, instead of f^{14} $^1\Sigma^+$.
Dolg et al. (1992b)	YbH, YbF. SO included.
Dolg et al. (1992c)	Ln_2, Ln=La-Lu. The 4f AO in core, 5s5p5d6s AOs in valence space.
Eckert et al. (1992)	H_2 rotation barriers in $M(CO)_3(PR_3)_2H_2$, M = Mo, W.
Fanizzi et al. (1992)	Pt(II) coordination in Pt(N-N)(L)X_2(N-N a bidentate N-donor ligand, L and X monodentate): 5-coordinate tbp for L = strong π-acceptor. Otherwise CN = 4.
Fernandez Pacios (1992)	New PP with [Ar] core for Sc-Cu: improved s^2d^n-s^1d^{n+1} -d^{n+2} energies.

Table 7.7. (continued).

Flad et al. (1992)	Cartesian Gaussian projection operators for quantum Monte Carlo. Li-Cs, Be-Ba, MM' (M = Li-K).
Foucrault et al. (1992)	Rb_2, Cs_2 at 1-VE level, including core-valence correlation potentials.
Gayen and Ermler (1992)	Cluster models for K adsorption on Ag.
Goursot et al. (1992)	M_2, M_4, M_4CO, M = Rh, Pd. Chemisorption analysed.
Gropen et al. (1992)	PtH. Two lowest states. R/NR. Results compared with PT ones.
Hagelberg et al. (1992)	Sb_4.
Hay (1992)	Oxidative addition and reductive elimination of H_2 and alkanes.
Haynes et al. (1992)	MH_7L_2, M = Tc, Re; L = PH_3. Classical (M-H) hydrides preferred by Re, non-classical (M-$H_2(\eta^2)$) ones by Tc. Cp. Pyykkö (1988a), p. 585.
Hickman et al. (1992)	XeHe and XeAr excited states and cations. SO. The ab initio CI curves improved by fits to empirical parameters.
Igel-Mann et al. (1992)	X_2, XH, XY, XY_m, X = In, Sn, Sb; Y = F, O, S. $(XY_m)_n$. Effect of the X $5s^2$ inert pair discussed. Electron-density pictures.
Jonas et al. (1992)	TiH_6^{2-} D_{3h} < Oh by 3 kcal/mol. VH_6^- C_{3v} < D_{3h} << O_h. MPn unreliable. QCISD(T) or CCSD(T) preferred.
Kalinkin et al. (1992)	Cluster model for Bi_{12} Ge O_{20}.
Kaupp and Schleyer (1992)	MX_2, M = Ca-Ba; X = Li, BeH, BH_2, CH_3, NH_2, OH, F. Most Ca compounds linear and Ba compounds bent at SCF level. QR SCF.
Kaupp and v. R. Schleyer (1992b)	Shapes of group 1-3 metal compounds $M^{n+}L_m$, M = K-Cs, Ca-Ba, Sc-La; L= NH_3, H_2O, HF. d AOs important.
Kaupp and v. R. Schleyer (1992c)	$(CH_3)_n$ PbF_{4-n}, $(CH_3)_nPbF_{2-n}$. Why are organic Pb(IV) and inorganic Pb(II) more stable?
Kaupp et al. (1992a)	MCp_2^+, M = Sc, La. Bending attributed to dσ. Also MH_2^+, MF_2^+ models.
Kaupp et al. (1992b)	MCp_2, M = Ca-Ba, Sm, Eu, Yb. M = Ba linear in HF, bent in MP2. All systems floppy.
Kaupp et al. (1992c)	$CaX_2(L)$, X=H, F; L=Ne-Xe, CO, N_2.
Kawamura-Kuribayashi et al. (1992)	$(SiH_2$ $Cp_2)$ ZrR^+: Silylene-bridged zirconocene catalyst for olefin polymerization. R = CH_3, C_2H_4, C_3H_7.
Kim and Balasubramanian (1992a)	GaBr. 15 states.
Kim and Balasubramanian (1992b)	GaCl
Kippels et al. (1992)	Harmonic force fields for $M(CH_3)_2$, M = Zn-Hg. HF and MP2.

Table 7.7. (continued).

Klobukowski (1992a)	$M^{2+}(H_2O)_n$, M = Ca, Sr; n = 1-6. SCF + MP2. Experimental gas-phase hydratisation energies reproduced.
Klobukowski (1992b)	HX, X_2, X - Cl, Br. ECP methods (without inner nodes) and model potentials (with inner nodes) compared.
Krogh-Jespersen et al. (1992)	$(NH_3)_5Ru(II)S(CH_3)_2$. HF, MP2, MP3. Bonding and electronic spectrum.
Kudo and Nagase (1992)	$X_4H_6^{m+}$, X = Ge-Pb, m = 0,1.
Laasonen et al. (1992)	$La@C_{82}$.
Lao and Christiansen (1992)	Ne ground state, quantum Monte Carlo. Valence E_{corr} 0.313(3)a.u.
Lee and Lee (1992)	Polyatomic program including double-group symmetry. HX, X_2 (X, X=Br, I), CH_3I. PES.
Li and Pyykkö (1992)	Au_2^{2+}, $(ClAuPH_3)_2$, $SeAu_2$, $Se(AuPH_3)_2$. The "aurophilic" Au(I)...Au(I) attraction still attributed to correlation, strengthened by relativity.
Liao and Balasubramanian (1992a)	Group III-V tetramers and their cations: Al_2P_2, Ga_2As_2, In_2Sb_2 and Tl_2Bi_2. Also AlP - TlBi. SO. TlBi D_0^0 only 0.53 eV.
Liao and Balasubramanian (1992b)	M_6, M_6^+, M = Cu-Au. All M_6 ground states capped pentagonal, C_{5v}.
Lin and Hall (1992a)	Classical and nonclassical hydrides, IrH_5L_2(L = Be, PH_3, PMe_3). Correlation important, MP4 close to MRCI, CISD worse.
Lin and Hall (1992b)	Dito, $ML_{7-n}H_n$, $ML_{8-n}H_n$ (n = 2-7, M = Mo, W, Tc, Re, Ru, Os, Rh, Ir; L = PH_3, CO.
Lin and Hall (1992c)	$M(CO)_6$ + CO, M = Ta, W. SCF.
Lin and Hall (1992d)	$M(CO)_6$ + G, G = CO, PH_3; M = Cr-W, V-Ta. Substitution reactions.
Lin and Hall (1992e)	$ML_{8-n}H_n$, n = 4-7, L=PH_3. Stability of non-classical isomers.
Lin and Hall (1992f)	M_8C_{12}, M = Y.
Lundell and Kunttu (1992)	EHE^+, E = Kr, Xe. $D_{\infty h}$. IR frequencies given.
Marino et al. (1992)	LiBe valence and Rydberg states. SO.
Márquez and Fernández Sanz (1992a)	$(CO)_5Mo{=}MH_2$, M = Ge, Sn. CASSCF.
Márquez and Fernández Sanz (1992)	$MoSnH_2$.
Maseras et al. (1992)	$Rh(PH_3)_3Cl$.
Maseras and Morokuma (1992)	NiH_2, $[Os(PH_3)_4H(H_2)]^+$. Effect of the formally empty metal np AOs on population analysis. "Natural population analysis" compared to Mulliken one.
Matsunaga et al. (1992)	Heteroatom 6π benzene analogues $X_3Y_3H_6$, X, Y = B-Ga, C-Ge, N-As, O-S, Zn.

Table 7.7. (continued).

Miralles et al. (1992)	$[Cu_2Cl_6]^{2-}$ singlet-triplet gap.
Mösges et al. (1992)	$M(NH_2)_2(HF)_4$, M = Ca-Ba. H $Ba(C_4H_4N)$. $M(C_4H_4N)$, M = Na-Cs.
Müller and Reinhold (1992)	$R_3P...HX$, R=H, CH_3; X = Cl-I. HF, MP2. No trace of ion-pair complexes $R_3PH^+...X^-$.
Nakamura et al. (1992)	MeCu, Me_2Cu^- addition to acetylenes.
Nakatsuji et al. (1992a)	Dative metal-metal bonds found in $(OC)_5Os-M(CO)_5$, M = Cr, W. Results compared with $(OC)_5M-M(CO)_5$, M = Mn, Re.
Nakatsuji and Nakai (1992)	End-on O_2-Ag "dipped adcluster" chemisorption model.
Ortiz et al. (1992)	$An(CH_3)_3$, An = U-Pu. Pyramidal, C_{3v} structures found, even for the free molecule. 6d important.
M. Otto et al. (1992)	XN_3, X = F-I.
P. Otto et al. (1992)	$(MI)_n$ cluster models (M = In, Tl) for the orthorhombic crystal. $(CaSi)_n$ and $(RbI)_2$ also considered.
Pacchioni and Bagus (1992)	Pd-PX_3, L-Pd-PX_3, X = H, -Me, -OMe. $(CO)_3$Pd-PX_3. σ donation, π^* back donation analysed.
Pápai et al. (1992)	$M(CO)_n^{m+}$, n = 1, 2; m = 0,1. DFT.
Perry et al. (1992)	MR_1R_2, M=Co-Ir, R=H, CH_3.
Probst (1992)	Hydration of M^{2+}, M = Zn-Hg, Mg. $[M(H_2O)_n)]^{2+}$, n = 1-6.
Ramirez-Solis et al. (1992)	CuCl. Diagonal and transition dipole moments.
Reinhold et al. (1992)	L-$HgCH_3$, L = C≡CH, $CH=CH_2$, CH_2-CH_3, CH_3. Weak C-C bond or longer chain (C_2 versus C_1) weaken the <u>trans</u> C-Hg bond. Correlations with ^1J(HgC) and group electronegativity.
Reynolds (1992)	$C_2H_4Br^+$, $C_4H_8Br^+$ isomers.
Riehl et al. (1992)	Ir(III)$L_2ZZ'X$, L = PH_3, Z = H, CH_3; X = H, Cl, NH_2, OR. Stability and bonding analysed.
Saethre and Gropen (1992)	X_4^{n+}, n = 0-2, X = S-Te. d AOs required for agreement with experimental (n=2) geometries. SCF.
Sakai et al. (1992)	NaI ground and first excited state.
Sargent and Hall (1992)	Oxidative addition of H_2 to <u>trans</u>-$IrX(CO)(PR_3)_2$, X=H^-, Cl^-, Ph^-; R = H, Me.
Sargent et al. (1992)	Oxidative addition of H_2 to IrCl(CO)(dppe), dppe = 1, 2 -bis(diphenylphosphino) ethane.
Schleyer et al. (1992)	$H_3X-X'H_3$, X = C-Pb. No systematic relativistic effect on the rotation barrier.
Schmidt et al. (1992)	R-C≡E, E = N-Sb, R = H, F, Me, Ph.
Schneider and Thiel (1992)	MH_3X, M = C-Sn, X = F-I. Anharmonic force fields. HF.

Table 7.7. (continued).

Schröder et al. (1992)	FeF^+ X $^5\Sigma$.
Schwerdtfeger (1992a)	Comments on MH_n^{m+}, M = In, Tl; n = 1-3; m = 0,1.
Schwerdtfeger and Boyd (1992)	$H_3PAu-AuPH_3$.
Schwerdtfeger et al. (1992a)	XH_3 (X = N-Bi) inversion barriers and other ground-state properties. HF, MP2, R/NR and QCI for Bi.
Schwerdtfeger et al. (1992b)	AuL_3, AuL_4^-, Au_2L_6, L = H, F-I. AuF_6^-. Relative stability of AuL_4^- over AuL_2^- increased by relativity, as suggested by Pyykkö (1978).
Schwerdtfeger et al. (1992c)	MX, MX_3 (M=B-Tl; X = H, F-I). AuH, HgH_2. PbX_2, PbX_4; BiX, BiX_3, BiX_5 (X=H, F). Energetics of the valency change from Pb(IV) to Pb(II) etc. R/NR. Relativity energetically favours the lower valency, however the $6s^2$ pair is not more "inert" than ns^2, n<6.
Sellers and Sudhakar (1992)	Hg clusters and their interaction with H_2O. Water-Hg, Hg-Hg potentials.
Seijo et al. (1992)	Valence E_{corr} for I^-, I and I^+. CISD. Correct nodal structure required.
Seitz-Beywl et al. (1992)	Li^+ and I^- interactions with Pt_n surface models, n = 5, 9.
Sodupe et al. (1992)	$[Sr(CO_2)_n]^+$, n = 1, 2.
Takeda and Shiraishi (1992)	$(SnH_2)_n$ polystannane.
Tornieporth-Oetting et al. (1992)	I_2^{m+}, m = -1, 0, +1. $I_2N_3^+$. A I-I-N_3 chain structure lowest, a C_{2v} one next. MP2.
Trinquier (1992)	$X_2H_5^+$, X = Ge-Pb. Doubly bridged, $H_2XH_2XH^+$ isomer lowest for Sn and Pb.
Vitale et al. (1992)	$Cu_4I_4L_4$, L = NH_3, C_5H_5N. I-to-pyridine and I-to-Cu transitions studied.
Vijayakumar and Balasubramanian (1992)	Tl_n^{m+}, n=2-5, m=0,1. Including SO. Tl_4 is D_{4h}, X $^1A_1$. Tl_3 is near D_{3h}, X $^4A_2$.
Wallace (1992)	SO CI potential curves for CuF, CuCl and AuF.
Wang and Carter (1992)	Pt_3. Ten states within 6.6 kcal/mol: one linear, two D_{3h}, seven distorted D_{3h}.
Wehman-Ooyevaar et al. (1992)	$MCl(H)(Me)_2(NH_3)...NH_3$ and $MCl(Me)_2(NH_3)...NH_4$, M = Pd, Pt.
Wiest et al. (1992)	$L-ReO_3$, L= cp, CH_3, CF_3, F, Cl.
H.-X. Zhang and Balasubramanian (1992a)	$M^+ + H_2$, M = Ni-Pt. For Pt, SO stabilizes the small-angle minimum.
H.-X. Zhang and Balasubramanian (1992b)	E_4, E = P-Bi. SO effects stabilize Bi_4 by 0.82 eV.

Table 7.8. Molecules treated by the Perturbative Hartree-Fock-Slater (P-HFS method).

Reference	Comments
Ziegler (1985c)	Proton affinity of d^8 metal pentacarbonyls (Cr^{2-}, Mn^--Re^-, Fe-Os, Co^+) and d^{10} tetracarbonyls (Fe^{2-}, Co^--Ir^-, Ni-Pt, Cu^+).
Dyke et al. (1986a)	As_2, As_4 PES.
Dyke et al. (1986b)	Sb_2, Sb_4 PES.
Louwen et al. (1986)	Trans-$MCl_2(EH_3)_2$ PES. M=Pd, E=N, P; M=Pt, E=N.
Boerrigter (1987)	Thesis. A summary on SO effects in X_2^+, X=F-Br, and bonding in $An(COT)_2$ and AnX_4.
Boerrigter et al. (1987)	SO effects in excited states of X_2^+, X=F-Br. A localised hole found for the $^2\pi_u$ state of Br_2^+.
Dyke et al. (1987); Fehér (1988)	MO, MO^+, M=Sr, Ba. PES.
Ziegler (1987)	Review on periodic trends. Dimer D_e is $Mo_2>W_2$ and $Mo_2<W_2$ for NR and R, respectively. Becke's non-local correction used.
Ziegler et al. (1987a)	Multiple M-M bonds in M_2, $M_2(OH)_6$ (M=Cr-W), $M_2Cl_4(PH_3)_4$ (M=V-Mn, Nb-Tc, Ta-Re). Relative bond strengths discussed.
Ziegler et al. (1987b)	Relative bond strengths of M-R bonds, R=H, CH_3. $RRe(CO)_5$, $RIr(CO)_4$ R/NR.
Ziegler et al. (1987c)	$M(CO)_6$ (M=Cr-W), $M(CO)_5$ (M=Fe-Os), $M(CO)_4$ and $M(PF_3)_4$ (M=Ni-Pt). M-CO bond strengths 4d<5d<3d and 5d<4d<3d for R and NR, respectively.
Allen et al. (1988); Fehér (1988)	UO, UO_2. PES interpreted. Bond-length **expansion** by 7.5pm found for UO_2.
Boerrigter et al. (1988a)	Bonding in $An(COT)_2$, An = Th-Pu, COT = C_8H_8. Relative importance of $6d\pi$, $5f\pi$ and $5f\delta$ bonding discussed. Rel. contractions of An-C reported. PES interpreted.
Boerrigter et al. (1988b)	AnX_4, An=Th, U; X=F, Cl. T_d geometry found. Rel. contractions reported. PES interpreted.
Ziegler et al. (1988a)	Relative strengths of M-R bonds, R=H, CH_3, in cp_2 MR, M=Y, La, Tc, Re. For early metals H≈Me, for late metals H>Me.
Ziegler et al. (1988b)	M-L bond strengths (L=OH, OCH_3, SH, NH_2, PH_2, CH_3, SiH_3, CN and H) in Cl_3ML (M=Ti-Hf). $LCo(CO)_4$.
Ball et al. (1989)	$W(SH)_6^{2-}$, $Cu(PH_3)_2^{2+}$ and their complex. Metal-metal interaction 100kJ/mol of total 1233.

Table 7.8. (continued).

Grabandt et al. (1989)	InF, InF^+. PES and ground-state properties.
Tschinke (1989)	W_2. Cl_3MR, R=H, CH_3; M=Th, U; Ti-Hf. $RM(CO)_5$, M=Mn-Re, $RM(CO)_4$, M=Co-Ir.
Ziegler et al. (1989a)	$[Pt(CN)_4]^{2-}$, $Tl_2Pt(CN)_4$. Bonding and optical spectrum. NR/QR/QR+SO. Tl behaves as a 6s donor and $6p_z$ acceptor.
Ziegler et al. (1989bc)	Reviews.
Ziegler et al. (1989d)	Cp ML (M=Rh, Ir; L=CO, PH_3), $M(CO)_4$ (M=Ru, Os and their insertion into CH_4. 5d bonds stronger due to relativity.
Lelj and Rosa (1990)	Bonding in MIn, M=Cu, Ag, Au. Au-In < Ag-In.
Folga et al. (1991)	L_2 Lu-H + H_2 exchange reaction. Experimental L = cp or cp* modelled by L=Cl. Activation energy, enthalpy and entropy obtained.
Vanquickenborne et al. (1991)	Reassignment of AnX_4 PES, An=Th,U; X=F,Cl. (Modification of Pierloot et al. (1991) for the solids).
van Wezenbeek et al. (1991)	Relativistic bond lengthening of UO_2^{2+} and UO_2, because depopulation of 6p upon bond shortening leads to smaller $\langle h_m \rangle$.
Folga and Ziegler (1992)	X_2Lu-H + D_2 -> X_2LuD + HD, X_2LuCH_3 + H_2 -> X_2LuH + CH_4. $(Cp^*)_2$ Lu modelled by Cl_2Lu. Four-centre transition state.
Kirchner et al. (1992)	High-energy O_2-Pt(111) scattering. PtO. R/NR, significant effects found.
van Daelen et al. (1992)	Adsorption of S on Ir_4. Influence of Mg^{2+} studied.
van Wezenbeek (1992)	Thesis on uranium compounds.

Table 7.9. First-order pertubation theory on molecules.

Reference	Comments
Meath (1966)	BP contributions to interatomic forces for degenerate states. An $\alpha^2 R^{-3}$ dispersion term found.
Meath and Hirschfelder (1966a)	BP contributions to intermolecular forces.
Chang (1967)	Moderately long-range intermolecular forces. SO effects included.
Walker and Richards (1970)	SO of diatomics at HF level. UHF calculations of core-polarisation effects in atoms.
Barron and Buckingham (1973)	SO coupling allows, besides E1, also M1 and E2 transitions of molecules. New singlet-triplet intensity term found.
Beck et al. (1974)	Fine structure of the a $^3\Sigma_u^+$ state of He_2.
Bendazzoli and Palmieri (1974)	GTO SO calculations for polyatomics. CO_2^+, N_3, H_2CO. SOO (spin-other-orbit) important.
Abegg (1975)	GTO SO for diatomics.
Dunning et al. (1978)	GaKr, $GaKr^+$ potential curves and transition moments, including an SO term.
Michels et al. (1978)	Noble-gas dimer ions. SO effects near dissociation limit.
Gribov et al. (1984)	PT for relativistic effects in molecules.
Almlof and Faegri (1986)	ZR_4, Z=C-Pb, R= H, $-CH_3$. Bond-length contraction studied.
Bauschlicher and Langhoff (1986)	ZnO, ZnS. D_e increased by 0.02 eV.
Chong et al. (1986)	CuH, ZnH spectroscopic constants.
Langhoff and Bauschlicher (1986)	CuO and CuS. X $^2\pi$ and $A^2\Sigma^+$.
Langhoff et al. (1986)	Cu_2, Cu_3 ground-state properties.
Pettersson and Langhoff (1986)	GeH.
Thakkar (1986)	$\langle h_m \rangle$, $\langle h_d \rangle$ for diatomics, H_2...RbF.
Werner and Buckingham (1986)	GeH. Effects on R_e and dipole moment.
Yarkony (1986)	Line strengths of spin forbidden transitions at BP level. Example NF b $^1\Sigma$-X$^3\Sigma$.
Alvarez Collado (1987)	RbF HF potential curve.
Grein and Peyerimhoff (1987)	Ne_2 low excited states with semiempirical SO.
Grein et al. (1987)	Ne_2 with ab initio SO.
Matsushita et al. (1987)	SeO. Radiative lifetimes from a$^1\Delta$ and b $^1\Sigma$ to X$^3\Sigma$.
Pettersson et al. (1987)	MH^+, M=Sc-Cu, Y-Ag.
Raseev et al. (1987)	Spin polarisation of molecular photoelectrons from HBr and HI.

Table 7.9. (continued).

Alvarez-Collado and Buenker (1988)	SeS transition probabilities. MRD-CI.
Banichevich et al. (1988)	Potential curves and predissociation of HBr^{2+} and DBr^{2+}.
Bauschlicher et al. (1988)	Cu_n^{m-}, n=1-3, m=0,1. (NR reference).
Blomberg et al. (1988)	$PdCO$, Pd_2CO. All-electron CPF level. Relativistic contributions to CO binding 11 and 14 kcal/mol, respectively, originate from smaller $4d^{10}$-$4d^9 5s$ splitting. Pd and PdH tests.
Blomberg and Wahlgren (1988)	Pd atom. 4s and 4p orbital relaxation shown to be important in 1st-order PT estimates of relativistic effects.
Buenker and Chandra (1988)	CI calculations including Breit-Pauli terms. NBr, SeS.
King and Furlani (1988)	Computation of 1- and 2-electron SO integrals for GTO:s.
Langhoff et al. (1988)	ScX, X=F-Br.
Lefebvre-Brion et al. (1988)	SO effects in HCl autoionization.
Senekowitsch et al. (1988)	H_2Se vibrational transition probabilities.
Vrbik et al. (1988)	Quantum Monte Carlo including $h_m + h_d$. Ground-state energy of LiH.
Blomberg et al. (1989)	$LPdH_2$, $L=C_2H_4$, CO, N_2, PH_3, H_2O, Cl^-. Ligand effect on Pd-H bonding investigated. Only relativistic H-Pd-H exists: Low and Goddard (1984b), Balasubramanian et al. (1988b).
Carlacci (1989)	SO effects in organic molecules.
Frey and Davidson (1989)	ScCO, Sc atomic states.
Marian et al. (1989)	NiH.
Pan and Zhao (1989)	The usual mass-velocity term, h_m, is OK in 1st-order PT, contrary to claims of Farazdel and Smith (1986).
Thümmel et al. (1989)	MgO. Spin-forbidden transitions and BO breakdown.
Yarkony (1989)	Quenching of He $2\ ^3S$ in helium gas.
Balasubramanian (1990g)	Stability of He_n^+, n=3,4, including differential relativistic effects.
Daskalopoulou et al. (1990)	Xe_2^+, Xe_3^+ MRCI.
Gemein and Peyerimhoff (1990)	$HeAr^+$ potential curves for X $^2\Sigma$ and A $^2\pi$.
Graff and Wagner (1990)	Long-range forces for $O(^3P) + OH(^2\pi)$.
Kölmel and Ahlrichs (1990)	$(CuX)_n$, X=H, F, Cl, n=1,2. Cu_2, Cu_2^+. $[Cu(HNNNH)]_2$, $[Cu(HN_5H)]_3$: models for "supershort" (245, 235pm) Cu-Cu distances.
Matsuoka (1990b)	BP integrals for spherical Gauss-Laguerre functions.
Schwerdtfeger et al. (1990b)	CuF ^{63}Cu NQCC.
Staemmler (1990)	$HeAr^+$. SO.

Table 7.9 (continued).

Strömberg and Wahlgren (1990)	Au_2, Hg_2^{2+}. Ground-state properties.
Yarkony (1990)	The decomposition reaction $HN_3(S=0)$-> $N_2(S=0)$ + $NH(S=0,1)$. Large CI with BP terms. Landau-Zener treatment at the crossing.
Banichevich et al. (1991)	Potential curves and predissociation of HBr^{2+} and DBr^{2+}.
Blomberg et al. (1991a)	M +H-CH_3, M+CH_3-CH_3, M=Fe, Co, Ni, Rh, Pd. E_{tot} at minima and at TS lowered by 2-4 and 6-10 kcal/mol for 3d and 4d metals, respectively.
Blomberg et al. (1991b)	$LRhH_2$ (L=Cl^-, PH_3, CO), (OC)MH_2 (M=Rh, Ru, Ru^+), M-CH_4 (M=Rh, Rh^+): Importance of the ligand in activating a C-H bond.
Bär and Ahlrichs (1991)	AlCu. R_e contraction 0.08a.u., D_e increase 0.15eV.
Ciullo et al. (1991)	NiN_2, $Ni(PH_3)_2N_2$: end-on and side-on preferred, respectively.
Faegri and Bauschlicher (1991)	YNi, ScPd, YPd: results compared with PP.
Ishii et al. (1991)	Free-radical g-values by FPT.
Parlant et al. (1991)	Spin-forbidden decay of HS^{2+}.
Roth et al. (1991)	$MgFe^+$ and its reactions with hydrocarbons. X^6.
Sodupe et al. (1991a)	$Sr(H_2O)_n^+$. $^-$ Model for gas-phase clusters.
Åkeby et al. (1992)	Sc_2 X $^5\Sigma$.
Andersson and Roos (1992)	Ni atom valence states. CASPT2 + $\langle h_m + h_d \rangle$ from Martin and Hay (1981).
Banichevich et al. (1992)	Predissociation of HBr^+ and DBr^+. BP MRD-CI.
Bauschlicher et al. (1992a)	Ni_2, Ni_2^+. D_0 calculated at MCPF level.
Bauschlicher et al. (1992b)	MCH_2^+, M = Sc-Cu.
Blomberg and Siegbahn (1992)	CrN, CrO, FeN. Ground-state properties.
Blomberg et al. (1992a)	M + CH_4, M = Y-Pd. Lowest repulsion toward methane in the d^{n+2} state, strongest bonds to the $d^{n+1}s$ state. For Rh both are low. Only Pd has a bound η^2 precursor.
Blomberg et al. (1992b)	Pd_2 + CH_4, Pd_2 + H_2.
Blomberg et al. (1992c)	MC_2H_4, M = Y-Pd.
Gropen et al. (1992)	PtH. Results compared with PP ones.
Hippe and Peyerimhoff (1992)	CuO ground and excited state SO splittings. Occupation of Cu 3d states crucial.
Koseki et al. (1992)	The effective charges in $h_{SO}=(\alpha^2/2)Z_{eff}r^{-3}\mathbf{l}\cdot\mathbf{s}$ determined for Li...Cl, used for diatomics.

Table 7.9. (continued).

Partridge et al. (1992)	Metal ions bound to He, Ne, Ar. SO-corrected NR. MAr^+ D_0 for M = V, Cr, Co and Ni about 20 % below experiment. Also ML_2^+.
Reuter and Peyerimhoff (1992)	Vibrational structure of X $^2A_1$ and A $^2B_1$ electronic states of CH_2^+.
Siegbahn and Blomberg (1992)	C-C bond activation in ethane, cyclopropane and cyclobutane by Y-Pd atoms.
Vahtras et al. (1992a)	SO in O_2, CH_2.
Vahtras et al. (1992b)	2nd-order SO effects in Cr_2.

Table 7.10. Density functional calculations. PP calculations are treated in Table 7.7. GTO calculations using transformed Dirac Hamiltonians are listed in Table 7.3.

Reference	Comments
March (1986)	Discusses bond lengths of CH_4-PbH_4 in relativistic TF theory.
Dietz et al. (1992)	A mean-field model for Be and LiH, derived from QED.

Table 7.11. Semiempirical methods.

Reference	Comments
Minaev and Terpugova (1969)	Quote inclusion of SO at CNDO or EHT level for CT complexes.
Hinkley et al. (1972)	SO splittings from MINDO. Diatomics.
Lohr (1972)	Spin-forbidden electronic excitations in transition-metal complexes.
Wittel (1972)	Different π_g and π_u SO splittings in I_2^+ attributed to σ_g repulsion from below. See also Jungen (1972).
Masmanidis et al. (1975)	SO coupling in organic molecules using CNDO/S.
Mingos (1976)	EHT on Au_n^{q+}, n = 6...13, and $[Au_6(PPh_3)_6]^{2+}$. Predicts the stability of the unknown $[CAu_6(PPh_3)_6]^{2+}$, made in 1988 by Schmidbaur et al.
Minaev (1980)	INDO-level TP for O_2 M1 transitions a $^1\Delta$ - X $^3\Sigma$ and b $^1\Sigma$ - X $^3\Sigma$. External heavy-atom effects discussed.
Minaev and Muldakhmetov (1984)	INDO/S + SO CI interpretation of forbidden transitions in CBr, HOO and O_2.
Dewar et al. (1985a)	MNDO parameters for Hg.
Dewar et al. (1985b)	MNDO parameters for Pb.
Dewar and Jie (1985)	AM1 parameters for Hg.
Krogh-Jespersen (1985)	REX calculations on cis-platinum hydrolysis. MCD intensities calculated via PT.
Barra et al. (1986, 1988)	PNC effects on NMR cemical shifts. REX.
Boudreaux et al. (1986)	$Pt_2(P_2O_5H_2)_4^{4-}$ bonding and spectra.
Gleghorn (1986)	Reaction of C_6H_6 with MCl^+ or M^{2+}, M=Cd, Hg. REX.
Jostes et al. (1986)	$MO_{4-n}S_n^{2-}$, M=Mo, W. Spectra interpreted. IEHT.
Larsson and Pyykkö (1986)	"ITEREX": a charge-iterative version of the Relativistic Extended Hückel program REX. XeF_n, n=2, 4, 6. UF_6. $UO_2X_4^{2-}$, X=F, Cl.
Lohr and Jia (1986)	REX on LnX_3. DZ fits given for Ln=La, Nd, Gd, Lu and X, X=F-I.
Lyudchik et al. (1986)	Bond angles discussed. Inclusion of SO at EHT level using a $h_{SO}=\mathbf{cl}\cdot\mathbf{s}$. $PtCl_6^{2-}$.
Z.-X. Ma and S.-S. Dai (1986)	HX, X_2, X = F-I. REX energies.
Pyykkö (1986b, 1988b)	ITEREX: a charge-iterative REX. Diskette included in (1988b).
Rösch and Pyykkö (1986)	Nuclear spin-spin coupling tensors in XeF_n, n = 2, 4, 6, MF_6, M = S-Te, U. ITEREX.
Trunschke and Miessner (1986)	CO + Pt_n, n = 1, 3, 4. REX.
van der Waals (1986)	SO coupling in lower excited states of d^0 MO_4^{n-} anions.

Table 7.11. (continued).

Wilson et al. (1986)	NMR spin-spin coupling in Zintl anions. $Sn_2Bi_2^{2-}$, Sn_8Pb^{4-} etc. REX.
Boca (1987)	A QR CNDO/1. Geometries and IP for 50 compounds, from H_2 to $PtCl_4^{2-}$.
Culberson et al.(1987)	An INDO model for LnX_n, n=2-4, and $Ce(NO_3)_6^{2-}$. Geometries.
Dixon and Tuckett (1987)	SO splitting in $(t_2)^5$ $^2T_2$ states of MX_4^+ ions M=C-Ge; X=F-I. MNDO.
Edlund et al. (1987)	REX interpretation of ^{207}Pb NMR chemical shifts in a PbH_3^- model.
Firth and Grice (1987)	SO interaction for the $^2H+X_2$ surface, X=F, Cl. DIM (diatomics in molecules).
Kertesz and Guloy (1987)	EHT band-structure study on chains, close-packed layers and honeycomb networks of Hg^q, as function of the charge q. Break-up into Hg_4^{2+}.
Krogh-Jespersen and Altonen (1987)	Hydrolysis of cis-platinum and acetamide. REX.
Lohr (1987)	A crystal version, "REXBAND", of the relativistic extended Hückel method REX. Te and Po.
Pyykkö et al. (1987)	Interpretation of the relativistic contribution to the NMR chemical shift $\sigma(^1HX)$, X = F-I, successful. CH_3X, HC≡CX only qualitatively understood. REX.
Schall et al. (1987)	LaF low-lying states. A ligand-field model.
Tatsumi and Nakamura (1987a)	Unusual Th-C-C angles in $(cp)_2Th(CH_2CH_3)_2$. "Agostic" Th...H reproduced. QR EHT.
Tatsumi and Nakamura (1987bc)	$(cp)_2AnR_2$, An = Th, U. Also -metallacyclopentadiene and -cyclobutadiene complexes.
Boca (1988a)	The QR-CNDO/1 applied on $[Co(NH_3)_6]^q$, $[MCl_4]^q$ (M=Ni-Pt) and their solvation.
Boca (1988b)	A QR-INDO/1 method, including the monocentric repulsion terms. MCl_4^{2-}, M=Ni, Pd, Pt, E110. Geometries for hydrides and halides.
Faiez and Ruiz Lopez (1988)	SO coupling constants from INDO-level finite-perturbation theory. ClF_4.
Gavezzotti et al. (1988)	Compares REX and EHT results with PP ones for Pt_n, n=1-7.
Jokisaari et al. (1988)	REX calculations of σ and J tensors in CX, XCX', X=O-Te.
Jostes (1988)	Iterative EHT energy parameters for Hf-Hg.
Marian et al. (1988)	ThO. REX compared with ab initio.
Pyykkö (1988b)	Review on semiempirical relativistic methods. ITEREX diskette included.
S. Wang et al. (1988)	A qualitative MO dimer model for organometallic $(AuTl)_\infty$ chains.

Table 7.11. (continued).

Azuma et al. (1989)	NbN X $^3\Delta$ - $^1\Delta$ cross terms from SO and hfs.
Boca (1989)	CNDO applied on XY diatomics (X,Y group 1, 11 elements).
Böhm et al.(1989)	Cluster models for magnetic anisotropy of amorphous iron, Fe_n, n=12-14, treated at ZDO level, including SO.
Borkovskii and Lyudchik (1989)	SO effects on uranyl complexes: $UO_2F_5^{3-}$, $UO_2X_4^{2-}$, X=Cl, Br.
Janiak and Hoffmann (1989a)	Tl(I)-Tl(I) interaction in an H-Tl... Tl-H model. EHT.
Janiak and Hoffmann (1989b)	1-dimensional, mixed-valent, halogen-bridged gold chains. EHT.
Kotzian et al. (1989)	A SO-INDO/S-CI method, tested on diatomic hydrides and oxides of C, N, O; HF^+-HI^+, TiO.
Minaev et al. (1989)	MINDO/3 - CI + SO. EH^q, q = -1, 0, +1, E=B...S. Intensity-borrowing in SO-allowed electronic lines discussed.
Pellow and Vala (1989)	SO splitting of alkali and noble metal atoms in rare-gas matrices.
Pyykkö et al. (1989)	Chemically realistic ITEREX and REX parameters for An = Th-Np. Applications on $An(C_8H_8)_2$, $An(cp)_4$, ThO_2 versus UO_2^{2+}.
Anderson et al. (1990, 1991)	QR INDO/1 model for 4d transition metals. Geometries for hydrides, oxides, halides etc.
Boca (1990a)	CNDO/1, including SO. Applications on AH, AH_2, AH_3, MH, InX and HgI_2.
Boca (1990b)	Jahn-Teller stability or instability of octahedral copper and gold complexes.
Boca and Breza (1990)	Models for Y-Ba-Cu-O superconductors.
Borkovskii et al. (1990)	$[Ce(H_2O)_n]^{3+}$, n=8, 9. Iterative MWH + SO for the f-d bands.
Breza and Boca (1990a)	Cluster models for $YBa_2Cu_3O_y$ (y=6,7). QR INDO.
Breza and Boca (1990b)	QR-INDO on the Tl-Ba-Ca-Cu-O system cluster models $[Tl_4Ba_{12}Ca_{6n-6}Cu_{2n}O_{16+7n}]^{2n-8}$, n=1-3.
Dai and Ma (1990)	REX on HX, XX', InX, X=F-I.
Gleghorn and Hammond (1990)	Erratum to earlier REX work on M_2H_6, M=Ge-Pb.
Janiak and Hoffmann (1990)	M(I)-M(I) interactions, M=In, Tl, in molecules and solids.
Mingos and Kanters (1990)	EHT on bonding in mono- and dicarbido gold clusters, $[X(AuPH_3)_m]$, X = B-N, C_2.
Mukherjee et al. (1990)	Au_2^{2+} at tight-binding (EHT) level: X $^1\Sigma_g$ ground state repulsive, Σ_u excited state bound. Longer Au_m^{2+} chains, n = 3-6, also considered.
Nizam and Bouteiller (1990)	MNDO on cluster models of PbF_2.

Table 7.11. (continued).

Novak (1990)	REX/EHT on five mixed, chiral halomethanes CXYZU, X- = H, F-I.
Pedash et al. (1990)	Inclusion of SO in the π-electron approximation. Singlet-triplet splittings for aromatics.
Pineda de Castro and Müller (1990)	REX on M_6X_{12} and FeM_6X_{12} cluster models, M = Zr, Th; X = Br, I. Bonding analysed.
Stewart (1990)	Review on MOPAC. Includes MNDO up to Pb, PM3 up to I.
Tatsumi et al. (1990)	The U-S bonds in $[U(SCH_2CH_2S)_4]^{2-}$ involve U 7s, 7p and 6d but little 5f and weak U-S π interactions. QR EHT.
Assefa et al. (1991); Assefa (1992)	Models for $Tl[Au(CN)_2]$, $Tl_2Pt(CN)_4$. Bonding and luminescence.
Aucar and Contreras (1991)	MNDO-RPA calculations of nuclear spin-spin coupling constants. Atomic DF $<r^{-3}>$ and $<\delta(r)>$ used. XH_4, X = C-Pb. Also XH_3^-, XMe_4, H_3XXH_3,...
Jové et al. (1991); Pyykkö and Jové (1991)	Mössbauer NQCC in neptunyl compounds interpreted by REX.
Kotzian and Rösch (1991)	INDO/CI studies of low-lying levels of PrO and TmO.
Kotzian et al. (1991)	INDO/S-CI on $[Ce(H_2O)_6]^{3+}$.
S. Lee (1991)	Structures of heavy main-group elements from a EHT-level band structure 2nd moment model.
Lohr (1991)	REXBAND on DOS of UB_n, UC, UBC, UPt_3.
Nogueira and Guenzburger (1991)	Valence-orbital IP expansions as functions of atomic charge for Hf-Hg from atomic DFT. R/NR.
Pastor et al. (1991)	Metastability of Pb_3^{2+} understood using a parametrized Hamiltonian.
Boca and Pelikán (1992)	Review on quantum chemistry of coordination compounds.
Boca et al. (1992a)	QR INDO/1 cluster models for $(GaAs)_n$, n $\leq$ 80. Comparisons with EHT band structures and ESCA.
Boca et al. (1992b)	Ge_x, Ge_xGa_y and Ge_xAs_y cluster models.
Breza (1992)	Cluster models for H_2 in Pd. QR CNDO.
Estiu and Zerner (1992)	$(CO)Rh_n$, n = 1-15. INDO. Transition from <u>bridge</u> to <u>on</u> <u>top</u> CO with larger n, related to charge shift.
Jahns et al. (1992)	$[(Cp^*_2M)_2\ C_6H_4]$, M = Sc, Lu. Agostic (M...H) interactions found for M = Lu. 5d important. INDO.
Janiak and Hoffmann (1992)	In(I)...In(I) and Tl(I)...Tl(I) attractions in molecules and solids. Assigned to hybridisation. EHT.
King (1992)	Discusses 6d-5f hybridisation of An=Th-Pu in actinyls and actinocenes.
Kotzian et al. (1992)	LnO, Ln=La...Lu. Energies, oscillator strengths, SO splittings. INDO. 5d population constant, 1.1 electrons.

Table 7.11. (continued).

Kotzian and Rösch (1992)	$[Ce(H_2O)_n]^{3+}$, n = 8,9. The 4f-5d spectrum interpreted.
Nogueira et al. (1992)	Bonding and g-tensor for [Ir(II)$(CN)_5]^{3-}$, $[Ir(II)(CN)_{6-x}Cl_x]^{4-}$, x = 1, 2. IEHT. VOIP for Ir given.
Pastor and Reindl (1992)	Ground states of Pb_n^{2+} clusters using a parametrized many-electron Hamiltonian.
Roszak and Lipinski (1992)	INDO including SO. Triplet lifetime of formaldehyde, pyridine etc. SO splitting of X_2, X = Cl-I.
Schwerdtfeger et al. (1992a)	XH_3 inversion barriers (E_a), X = N-Bi. REX/EHT, MP2. 6s radial contraction at C_{3v} increases E_a.
Solà et al. (1992)	ZnO, HgO. Semiempirical VB.
Thiel and Voityuk (1992)	MNDO for d orbitals. Cl-I.
G. S. Wu et al. (1992)	QR CNDO applied on main-group diatomics, LnX_3, Ln = La-Lu, X = F-I.

Table 7.12. Relativistic crystal field theory.

Reference	Comments
Gerasyuk et al. (1986)	O_h and C_{4v} sites for Ce^{3+} in CaF_2.
Pastusiak and Kuriata (1986)	Relativistic CFT for $4f^7$ ions. Interpretation of tetragonal 2nd-order spin-lattice coefficients.
Andriessen and Postma (1987)	Crystal-field model for Tl^0 and Pb^+ $6p^1$ centers.
Makhyoun (1987); Makhyoun and El-Ezaby (1988)	Derives effective ligand-field parameters for $5f^1$ systems from SO-perturbed QR MS Xα calculations.
Schall et al. (1987)	Diatomic LaF. A ligand-field model for the low-lying states.
Tuszynski and Dixon (1987)	Gd^{3+} in C_{3h} symmetry. A study of crystal fields, SO and residual interactions.
Siu (1988ab)	S ground-state splitting of Mn^{2+}.
Siu (1988c)	Covalency effects in relativistic crystal fields.
Vokhmin and Ionova (1988)	Electrostatic and SO parameters for f electrons.
Ammerlaan and van Oosten (1989)	Model for Pt(-I), $5d^9 6s6p$, in Si.
Bartram et al. (1989)	Pb(0) in SrF_2.
Chatterjee and Buckmaster (1989)	New electric-field effective operators.
Tuszynski and Dixon (1989a)	Relativistic effects in 4f and 3d complexes
Tuszynski and Dixon (1989b)	Zero-field splittings in 4f and 3d complexes.
Yu (1989)	Cubic zero-field splitting of a d^5 ^6S-state ion.
Yu (1990)	Rank-four spin-Hamiltonian parameters of a $3d^5$ ion.
Blanchard and Girault (1991)	Cation vacancies in II-VI compounds.
Boulanger et al. (1991)	TP of Mn^{2+} d^5 $^4T_1$-$^6A_1$ transitions in II-VI compounds. Ligand SO important.
Chatterjee and Buckmaster (1991)	Relativistic effective Hamiltonians for S-state ions. EPR of Gd^{3+}.
Goodman et al. (1991)	Crystal-field levels for Ln = Pr, Nd, Ho in Ln Ba_2 Cu_3 O_7.
Wang and Yu (1991)	Zero-field splitting of a ^6S-ion in tetragonal symmetry.
Ning et al. (1991)	Cubic zero-field splitting of CaF_2 : Mn^{2+}.
Balcar and Lovesey (1992)	Magnetic inelastic neutron scattering intensities for Pr^{3+} and Tm^{3+} (f^2 and f^{12}, respectively).

Table 7.12. (continued).

Gajek and Mulak (1992)	Ab initio fundamentals of $5f^n$ ion angular overlap model (AOM) for halide ligands. Both σ, π and δ contributions necessary.
Spain and Morse (1992)	Ligand-field theory for $d^n\sigma^m$ states of MM', M = Ni, Cu, Pt, H.
Yu and Rudowicz (1992)	Zero-field splitting of ^6S-state Mn^{2+} and Fe^{3+} in cubic and tetragonal fields.

Table 7.13. Relativistic theories of molecular properties. For parity non-conservation effects, see table 5.17.

Reference	Comments
Hameka and Goodman (1965); Lohr (1966)	Raise the question of correct operators for spin forbidden molecular transitions. At Pauli level, <r> is OK, <p> must be replaced by <π>.
Englman (1966)	Operators for spin-forbidden transitions. The Dirac level.
Chiu (1968)	Dirac- and Pauli-level operators for radiative transitions of molecules. A thorough analysis.
Ginsburg and Goodman (1968)	Two-electron SO terms in S-T TP. Formaldehyde at CNDO level.
McGlynn et al. (1969)	SO effects in triplet-state spectroscopy. Book.
Tterlikkis et al. (1969)	Knight shifts and nuclear spin-spin coupling tensors in a Dirac OPW basis.
Walker and Richards (1970)	SO of diatomics at HF level.
Barron and Buckingham (1973)	SO-allowed M1 and E2 transitions of molecules.
Bendazzoli and Palmieri (1974)	SO of CO_2^+, NNN, H_2CO.
Abegg (1975)	SO of diatomics.
Turro and Devaquet (1975)	S-T transitions in pericyclic organic reactions.
Masmanidis et al. (1975)	SO coupling in organic molecules. CNDO/S.
Teo and Lee (1979)	Relativistic effects in the EXAFS of W.
Lefebvre-Brion et al. (1985)	SO autoionization effects in HI.
Barra et al. (1986,1988)	PNC effects on NMR chemical shifts.
Dodelson (1986)	Ortho-para H_2 transition rate 10^{-12} a^{-1} in vacuum.
Rösch and Pyykkö (1986)	Time-reversal symmetry aspects in the relativistic theory of nuclear spin-spin coupling.
W.Q.Chen and Cook (1987)	Quasirelativistic treatment of nuclear motion in atoms and molecules.
Dagdigian and Campbell (1987)	Spin-orbit effects in gas-phase chemical reactions.
Pyper (1988)	Relativistic analogues of the NR hfs operators.
Z. C. Zhang and Pyper (1988)	Relativistic analogues of NR hfs operators. Assumes that nuclear magnetization resides on nuclear surface. Individual contributions diverge, their sum not.

Table 7.13. (continued).

Rutkowski and Schwarz (1990)	PT appproach to molecular structures, force constants or polarisabilities.
Rehr et al. (1991)	Theoretical XAFS standards for K-shell Cu, Pt, $GeCl_4$.
Avery and Antonsen (1992)	Magnetic interactions and 4-currents.
Heifets (1992)	3rd-order PT formulae for g-tensors.

8. SOLID-STATE THEORY

The chemical bonds in solids are not unrelated to those in molecules. Therefore we give below a summary of relativistic solid-state calculations on electronic and geometrical structures in Table 8.1. Table 8.2. gives an idea of relativistic theories of various solid-state phenomena.

Table 8.1. Band-structure calculations.

Reference	Comments
Loucks (1966)	R/NR Fermi surfaces for W. Differences from Mo mainly relativistic.
Koelling and Freeman (1976)	Review on An, An intermetallics.
Overhof et al. (1976)	Band-structure study of the optical gap in expanded fluid mercury. Closes at 5.5 and 9.3 g/cm^3 for sc and fcc, respectively. R KKR.
Elyashar and Koelling (1977)	Nb.
Overhof et al. (1978)	RbAu, CsAu. R KKR. "Significant charge transfer to gold found". PES interpreted.
Weinberger (1982b)	Au, Pt and $d^n s^1$ impurities in them. SO-split DOS given for the impurity.
Koelling et al. (1983)	CeO_2, PrO_2. Metal d and f character found in the O2p band.
Dakshinamoorthy and Iyakutti (1984)	Ac Fermi surface, superconductivity and resistivity at high p. RAPW.
Bachelet and Christensen (1985)	GaAs, Ge. Direct gap reduced to half by relativity. Atomic effect depressed <u>or</u> amplified in solids.
Bhattacharyya et al. (1985)	$MoSi_2$, WSi_2. E_{coh} and ν_{opt} larger for W.
Ebert et al. (1985a)	Ag_xPt_{1-x} alloys. SO splitting of the d shells discussed.
Rabe and Joannopoulos (1985)	SnTe, PbTe. Rhombohedral (distorted NaCl) and NaCl structures, respectively, reproduced. R/QR/NR comparisons. NR SnTe a semimetal.
Springelkamp et al. (1985)	ß-NaSn.Contains tin tetrahedra, isoelectronic to P_4: a $(Na^+)_4(Sn_4^{4-})$ semiconductor.
Wei and Krakauer (1985)	Pressure-induced metallization of BaSe and BaTe. QR/NR.
Brooks et al. (1986)	Review on Ac-Am, ThN-AmN.

Table 8.1. (continued).

Christensen et al. (1986)	Pb. NR structure diamond, R : observed fcc. LMTO. SO effects on bcc/hcp/fcc also considered, about ± 1 mRy. The fcc- hcp transition raised by 100 kbar by SO.
Hybertsen and Louie (1986)	Inclusion of V_{SO} in PP work. Atomic splittings are enhanced for highest occupied p states of Ge, Ar, Kr, Xe.
Koelling (1986)	Why does density-functional theory work for excitation energies? A: The orbitals are localized. Ce, U systems.
Kubo and Yamashita (1986)	Pb under high pressure.
Moriarty (1986)	Phonon spectrum of bcc Ba. Partial filling of 5d band essential.
Pyper (1986); Wood and Pyper (1986)	A relativistic ab initio method for ionic solids. Free-ion DF basis. MgO, NaCl, LiF, NaF, AgF, PbF_2. Dispersion forces appended. Good agreement with experiment for D_e, R_e, bonding.
Schadler et al. (1986)	Ce, Pu. Fully relativistic calculation including spin polarization. Zeeman splitting in B_{ext} included.
Watson et al. (1986)	5d-5d metal alloys, isoelectronic with Re: WOs, TaIr, HfPt. E_{coh} increases with Z_2-Z_1. Right structure obtained.
Weinert et al. (1986)	4f core hole energies in Au.
S.C. Wu et al. (1986)	Ag 4d and Au 5d SO splittings only weakly affected in Ag-Au alloys.
Boring et al. (1987)	UMn_2, UFe_2. Magnetic behaviour.
Brooks (1987)	PuE, E = S, Se, Te predicted to be "relativistic [intrinsic] semiconductors" with a filled $5f_{5/2}$ and empty $5f_{7/2}$ band.
Cortona and Sommers (1987)	Spin-polarized calculations on rare earths.
Fritsche et al. (1987)	Ferromagnetic Fe, Ni, Pd.
Goalwin and Kunz (1987)	MI excitonic spectra, M=Li-Cs.
Harrison and Straub (1987)	Discuss bonding mechanisms in d- and f-shell solids. AnAs, An = Th-Cm.
Hashizume (1987)	Solid Ar.
Jaffe and Singh (1987)	Inclusion of h_{SO} in tight-binding calculations.
Johansson et al. (1987, 1990)	An metals and intermetallic compounds.
Kelly and Brooks (1987)	Cohesive properties of AnO_2, An=Th, U, Pu. LMTO.
Kertesz and Guloy (1987)	Stability of Hg^q chains, close-packed layers and honeycomb networks as function of the charge q.
Kubo (1987)	Sr, Yb under normal and high pressure.
Lohr (1987)	A crystal version of REX. Te and Po. Cubic structure of the latter attributed to SO.

Table 8.1. (continued).

Nemoshkalenko et al. (1987)	Pseudopotentials for transition metals.
Norman (1987)	DFT of f electron systems.
Ohlsén and Calais (1987)	Effect of SO found dominant on g-tensor anisotropy in Rh, Pd, Ir and Pt.
Ostanin et al. (1987)	Mo.
Pyper et al. (1987)	Relativistic effects on interionic potentials in PbF_2. The Pb^{2+}-Pb^{2+} interaction is reduced by a factor of 3. The electron-gas method gives too large relativistic corrections by 2-3.
Qi et al. (1987)	Experimental evidence for no 5d holes in Au, $5d_{5/2}$ holes in Pt. For violet $AuAl_2$ and $PtAl_2$, comparable $d_{3/2}$ and $d_{5/2}$ and dominant $d_{3/2}$ holes, respectively.
Schadler (1987)	Fully relativistic magnetic moments. Gamma-Ce, fcc-Pu.
Terakura et al. (1987)	Alloy phase stability of Cu-Ag, Cu-Au and Ag-Au.
Tréglia and Ducastelle (1987)	PtNi. SO induced ordering of the alloy.
Watson et al. (1987)	Au-5d metal alloys.
Weinberger and Gonis (1987)	Actinides.
Zhu et al. (1987)	E_{coh} of Mo, W, $MoSi_2$ and WSi_2. W>Mo but relativistic effects were not separated.
Albers (1988)	Linear Pt-Br chains. LMTO.
Boring et al. (1988)	Np.
Cardona et al. (1988)	Zinc-blende-type semiconductors. SO splitting effects classified. LMTO.
Davenport et al. (1988)	Cu_3Au. Non-overlapping 3d and 5d bands. SO effects discussed.
Ebert (1988); Ebert et al. (1988a)	Spin-polarized relativistic LMTO calculations.
Eppenga et al. (1988)	Semiconductor SO splittings from Augmented Spherical Wave calculations.
Ginatempo and Staunton (1988)	Disordered alloys containing heavy elements. Cu_3Au.
Gonze et al. (1988)	Bi, including SO coupling.
Herbst and Wilkins (1988)	2p and 3d excitation energies in Ac-Am.
Jeong et al. (1988)	Relativistic (SO) effects on the surface electronic structure of Mo(011).
Liu et al. (1988)	WC. Cohesive properties calculated: both W-C bonds and a metallic component.
Mazin and Savrasov (1988)	Xe. Pressure-dependence of the gap.
McAdon and Goddard (1988ab)	1D Cu-Au, Li, Na. Charge or spin density waves, Peiers distortions.

Table 8.1. (continued).

Moriarty (1988)	High-pressure phases of Hg, to 1TPa = 10 Mbar. NR Hg is hcp, like Zn or Cd, R Hg has the observed ß-Hg structure. E_{coh} 1.21, 0.27 and 0.67 eV for NR, R, exp., respectively.
Nizam et al. (1988)	Periodic-HF on ß-PbF_2. QR PP. DOS compared with PES.
Pospelov and Novikov (1988)	SO in As and Sb.
Saalfrank et al. (1988)	Te_∞ chains of trigonal tellurium. Cohesive properties, including interchain interactions.
Weinberger et al. (1988)	Ordered and disordered Cu_3Au. Itinerant Au 5d states in ordered phase.
Yasui (1988)	Orbital and SO magnetic susceptibilities in bcc V, Nb and W.
Anisimov and Korotin (1989)	FePd, FePt, CoPt, MnAl.
Ebert (1989)	Core states in spin-polarized LMTO calculations. Fe, Co, Ni.
Eriksson et al. (1989a)	$AnIr_2$, An = Th-Am. SO-induced volume-increase for Pu is substantial, due to filling of narrow $5f_{5/2}$ band.
Eriksson et al. (1989b)	$AnRh_3$, An = Ac-Cm.
Fernando et al. (1989)	Full-potential linear augmented STO method. Bcc W, fcc Pt.
Florio et al. (1989)	Random Pd-Pt alloys.
Godwal and Jeanloz (1989)	Equation of state of gold up to 200 GPa and 5000 K. LMTO.
Hafner (1989)	Review on solid and liquid sp-bonded systems, including binary alloys and Zintl compounds.
Hamann (1989)	BaSe, as test for generalized norm-conserving pseudopotentials,
Jeong et al. (1989)	Symmetry effects in hydrogen chemisorption electronic structure.
Kim et al. (1989a)	Optical properties of Mo.
Kim et al. (1989b)	Optical properties of Nb.
Krewer and Feder (1989)	Scattering of Dirac electrons from non- spherical potentials. Application on LEED of W(001).
Krutzen and Springelkamp (1989)	Spin-polarized fully relativistic calculations. Omits the orbital contribution. Several LDF used. Ni and Gd.
Liberman and Zangwill (1989)	4p-4f resonance transitions in Ce.
B. Lindgren (1989)	Reviews calculations of magnetic hfs in Fe, its surfaces and compounds. Several LDF used. Sresses the importance of the correct hyperfine integral.

Table 8.1. (continued).

Z.W. Lu et al. (1989a)	La, fcc and bcc. The 5p must be included in valence space. Several LDF tested.
Z.W. Lu et al. (1989b)	HgSe, HgTe. Semimetals, in contrast to the semiconducting Zn, Cd chalcogenides. Cohesive properties reproduced.
Masovic (1989, 1990)	The phase V of CuI. Includes SO.
Nemoshkalenko et al. (1989)	Lu. Energy spectrum and optical properties of single crystals.
Oja et al. (1989)	Indirect nuclear spin-spin coupling in Cu. QR.
Ostanin and Shirokovskii (1989)	Optical absorption of Mo.
Ostanin and Shirokovskii (1989b)	Optical absorption in Nb and Ta.
Richter and Eschrig (1989)	Spin-polarized relativistic LCAO formalism. Ni.
Saalfrank et al. (1989)	Pb (100), (110) and (111) surfaces at HF level. No SO.
Smelyanskii et al. (1989)	U band structure.
Solov'ev and Likhtenshtein (1989)	Linearized approaches to spin-polarised calculations for An.
Solov'ev et al. (1989)	Spin-polarized relativistic calculations for Fe-Ni, Pu, Am.
Sticht (1989)	Band structures for heavy-fermion systems.
Strange et al. (1989)	Relativistic spin-polarized multiple-scattering theory. Ferromagnetic Fe.
Svane (1989)	LMTO and Green-function calculations of ^{119}Sn Mössbauer isomer shifts. Minimum for Sn s character for a tin impurity in the middle of d-transition-metal series. Maximum for sp metals.
Takeuchi et al. (1989)	Equilibrium properties of Ag and Au. R/NR.
Takizawa et al. (1989); Takizawa (1990)	Phase stability of the nine AB alloys, A=Ni-Pt, B = Cu-Au. Relativistic 5d-to-6s population shifts important.
Tamura and Feder (1989)	A layer-KKR method for crystal surfaces. Pt(111).
Tegze and Hafner (1989)	Metallic and semiconducting alkali metal-lead compounds. The composition range $Na_{15}Pb_4$, NaPb, $NaPb_3$ considered. The orbitals of the Pb_4^{4-3} Zintl anion are strongly delocalized. Low ionicity.
Turner and Harmon (1989)	HgI_2. Covalent, rather than ionic bonding, Hg charge < +0.1. Directional Hg6s-I5p_z bonds give a small elastic constant in the ab plane.
X.W Wang et al. (1989)	PdH_n, n=1-4.
Watson et al. (1989)	Alloys of Ti-Hf with Tc-Pd or Re-Pt.

Table 8.1. (continued).

Wei and Zunger (1989)	Negative SO bowing in semiconductor alloys.
S.C. Wu et al. (1989)	Relativistically allowed photoemission from Cu {001} interpreted.
J.H. Xu et al. (1989)	The rutile dioxides MO_2, M = Nb, Ru, Ir.
Arola et al. (1990a)	Disordered $Au_{70}Pd_{30}$.
Arola et al. (1990b)	Disordered $Cu_{75}Au_{25}$.
Blaha et al. (1990)	A full-potential, linearized augmented plane wave program.
Elsässer et al. (1990)	Ground-state properties of the 4d and 5d metals Rh-Ag, Ir-Au. NR/QR a_o, B_o and E_{coh} given.
Eriksson et al. (1990)	Cohesive properties of Ln and Ln-like An elements.
Fernando et al. (1990)	Cohesive properties of 5d metals, Hf-Au. Full versus muffin-tin potentials. Relative energies of fcc, bcc and hcp.
Gonze et al. (1990)	As, Sb, Bi.
Hafner and Jank (1990)	Liquid Al-Tl. Relativistic 6s stabilization leads to a pseudogap between 6s and 6p.
Jank and Hafner (1990a)	Liquid Si-Pb. R and NR interatomic potentials compared. Photoemission spectra compared with DOS.
Jank and Hafner (1990b)	Liquid Ca-Ba, Zn-Hg. Incipient d-band effects seen in alkaline earths. Hg pair correlation function clearly requires relativity.
Jank and Hafner (1990c)	Review on polyvalent liquid metals.
K.J. Kim et al. (1990)	$AuGa_2$, $PtGa_2$. Optical properties discussed.
Krutzen and Inglesfield (1990)	Calaverite, $AuTe_2$: both the periodic average structure and the incommensurate one. Te p - Au d hybridisation.
Leiberich et al. (1990)	In NQCC.
MacLaren et al. (1990)	Fe, using several LDF. Some give correct bcc structure. LMTO.
Nemoshkalenko et al. (1990)	Th.
Ostanin and Shirokovskii (1990)	Simplified method for ferromagnets.
Pyper (1990)	Ab initio calculation of interionic potentials in solids. DF ionic functions.
Sakisaka et al. (1990)	SO effects in bulk Fe. Comparison with PES. Experimental zeta parameter 0.110 eV band-structure value 0.045.
Schmid et al. (1990)	Si, Ge, GeSi. Effect of inversion asymmetry on SO splitting.
Sklyadneva and Chulkov (1990)	Hf. Surface and bulk electronic structures.
Smelyansky et al. (1990)	Os Fermi surface.

Table 8.1. (continued).

Söderlind et al. (1990)	Relativistic effects on the thermal expansion of the actinides, Th-Pu. A 5f SO-induced increase. 5f contribution to cohesion separated.
Solov'ev et al. (1990)	α-δ transition of Pu.
Tamura and Feder (1990)	Pd(110) surface.
Walzer (1990,1991ab)	Binary intermetallic compounds classified using radial and energy quantities derived from PP.
Wang and Davenport (1990)	The s-d promotion energy and spin-polarization energy of transition metals.
Wei and Zunger (1990)	Atomic and diatomic hydrogen in fcc Pd.
Weinberger et al. (1990)	Fe in Au.
Yamagami and Hasegawa (1990)	α-U.
Zhong et al. (1990)	Two-step (QR+SO) inclusion of relativistic effects in orthogonalized LCAO calculations with a GTO basis. Ni, Nb and Ce band structure.
Ahuja et al. (1991)	Pt Fermi surface. R/NR.
Aprá et al. (1991)	AgCl. QR-PP-HF binding energy, a_o, bulk modulus and electron density.
Chulkov et al. (1991)	Metal surfaces.
Cortona (1991)	Spin-polarized LD calculations.
Costa Cabral et al. (1991)	Monte Carlo simulation of CsAu melt
Deiseroth et al. (1991)	NaHg. Contains chains of square-planar 6p-bound Hg_4 units. Nearly neutral atoms.
Eriksson et al. (1991)	UNiSn. Magnetic properties.
G.-Y. Guo et al. (1991)	Fe, fcc ground state still predicted. Experimental : bcc.
Gyorffy et al. (1991)	Review on relativistic density functional theory for solids. Mentions magneto-crystalline anisotropy, magneto-optic (Faraday and Kerr) effects, Fano effects, corrections to London moment in superconductivity and new magnetic phase transitions.
Hjelm and Calais (1991, 1992)	Zeeman splitting for Pd and Pt in external **B**.
Hörmandinger et al. (1991)	Spin-orbit effects in $Bi_2Sr_2CaCu_2O_8$.
Kokko (1991)	LMTO calculations on monovalent metals and their alloys. K, Ag-Au, Cu-Au.
Kübler and Harmon (1991)	"Electronic structure in the 1990s": Proceedings of the A. J. Freeman seminar. 37 contributions.
S. Lee (1991)	Structures of heavy main-group elements from an EHT, 2nd-moment argument.
Y. Li et al. (1991)	Noble gases Ne-Xe, and NaCl. QR.

Table 8.1. (continued).

Liu et al. (1991)	High-pressure phases of Pb: fcc -> hcp around 14 GPa, hcp -> bcc around 109 GPa reproduced. Method of Hybertsen and Louie (1986). SO lowers the bcc and raises the hcp wrt fcc, however less than in Christensen et al. (1986).
Lohr (1991)	Uranium borides, carbides UPt_3. REXBAND.
Z.W. Lu et al. (1991)	Random $Ag_{0.5}Pd_{0.5}$ and $Ag_{0.5}Au_{0.5}$ alloys. In the latter, s charge transfer $Ag^{+0.025}Au^{-0.033}$, but d charge transfer $Ag^{-0.015}Au^{+0.012}$ (signs corresponding to ionic charge).
Mansfield and Needs (1991)	Surface energy and stress of Pb (111) and (110) surfaces.
Méndez and Dominguez-Adame (1991)	A numerical method for 1D relativistic band structures. Mathieu potential $V(x) = V_0 \cos 2x$.
Min and Jang (1991)	Effect of SO on the electronic structure of magnetic materials. Fe-Ni, Ce-Gd.
Nikolaev and Ionova (1991)	Th-Am, fcc and bcc.
Ostanin and Shirokovskii (1991)	Simplified method for ferrimagnets and antiferromagnets. Dirac-KKR. Theory only.
Schober et al. (1991)	Inter-conversion coefficients for valence electrons of hcp-Tc and bcc-U.
Solovyev et al. (1991)	Spin-polarized LMTO. Volume-dependent electronic sructure and magnetic moment of Pu.
Takizawa et al. (1991)	CuPd, CuPt alloys. The bcc, respectively $L1_1$ structures reproduced.
Tománek et al. (1991)	H on Pd (001), Pd (110) and bulk Pd. PP used for both Pd and H!
Wang and Chou (1991)	Structural properties of hcp Y.
Watson et al. (1991ab)	s-d promotion and E_{coh} in d transition-metals.
Wills et al. (1991)	High-pressure phases of Ce. Both 4f and 5d contributions found important.
S.C. Wu et al. (1991)	Relativistic effects on the Cu(111) surface electronic structure.
Yamagami and Hasegawa (1991)	Itinerant 4f electrons in CeNi.
Yasui et al. (1991)	Orbital and SO magnetic susceptibilities in fcc Rh, Ir, Ni-Pt and Cu-Au.
Agrawal and Agrawal (1992)	AlAs and CdTe. Elastic properties and PES.
Alouani et al. (1992)	$Pt_2Br_6(NH_3)_6$. Dimerisation of the halogen-bridged linear chains into Pt(II) and Pt(IV).
Blaha and Schwarz (1992)	Solid Cl_2, Br_2 and I_2. Geometry optimised. NQCC.

Table 8.1. (continued).

Chang and James (1992)	HgI_2.
Cortona (1992)	Cohesive properties of the alkali halides, MX. R/NR for RbBr, CsX, MI. Of the CsI dissociation energy (to atoms), 7 % is "relativistic".
Ebert and Akai (1992)	Spin-polarized relativistic treatment of dilute and concentrated, disordered $Fe_x Co_{1-x}$ and $Co_x Pt_{1-x}$.
Eriksson and Wills (1992)	Am. High-pressure 5f delocalization.
Eriksson et al. (1992a)	Th. High-pressure fcc-bct transition.
Eriksson et al. (1992b)	Ce crystal structures under pressure. The α' phase stabilised by 4f, the bct also by 5d electrons.
Ettema et al. (1992)	SnS. α and ß phases.
Felser-Wenz et al. (1992)	Ba, BaO, BaS and BaF_2. Ba 5d population larger than 6s or 6p one.
García et al. (1992)	Gradient-corrected functionals give no consistent total-energy improvement over LDF for Ge, GaAs, Nb and Pd. R/NR for Ge, Nb, Pd.
Gordienko et al. (1992)	Silver azide, AgN_3.
G.Y. Guo et al. (1991b)	Magnetocrystalline anisotropy of a Fe monolayer on Cu, Ag or Au.
Hasegawa and Yamagami (1992)	PuE, E = S, Se, Te.
Katsnel'son et al. (1992)	α-δ transition of Pu as a Mott transition in the 5f system.
Körling and Hägglund (1992)	Cohesive and electronic properties of 3d, 4d and 5d metals. LSD and gradient-corrected potentials compared.
Markowsky and Podgorny (1992)	Optical properties of MTe, M = Zn-Hg.
Mattheiss (1992)	MSi_2, M = Cr-W. Structures.
Methfessel et al. (1992)	Surface energies of 4d metals, Y-Ag. NR/QR.
Neumann et al. (1992)	KMO_3, M = Nb, Ta.
Orita et al. (1992)	I_2 under pressure. Mechanism of insulator-to-metal transition.
Orlando et al. (1992)	Tetragonal and cubic ZrO_2 using a PP version of the crystal HF program.
Rao et al. (1992)	Th : a 5f metal at ultrahigh pressures. The 6p band must be in valence space.
Schick et al. (1992)	Fully relativistic spin-polarized technique for isolated impurities in crystals. Applications on U, Np, Pu in Pd.
Sigalas et al. (1992)	Band structure and total energy of fcc and bcc 3d, 4d and 5d metals. Relativistic effects worsen agreement with experiment (due to cancellation of errors).

Table 8.1. (continued).

Takeda and Shiraishi (1992)	$(SnH_2)_n$ polystannane.
Tamura (1992)	Dirac-Green functions for general, magnetically polarized cell potentials.
Tegze and Hafner (1992)	A_3B, A = Li-Cs, B = Sb, Bi. Small ionic gap. The ionic ASb compounds contain Sb spirals. The ABi, ABi_2 are metallic.
Trubitsin et al. (1992)	Relativistic, spin-polarized treatment of antiferromagnetic Cr.
Walzer (1992ab)	Pseudopotential approach for binary intermetallic compounds. Structures, melting points.
X.-D. Wang et al. (1992)	Relativistic MS formalism for space-filling potentials.
Wills and Eriksson (1992)	Th, Pa, U. Strong 5f effects on the structure. QR approximation increases the volume by about 5%. This SO effect was attributed to 6p.
Wills et al. (1992)	Elastic constants of $_{55}Cs$ - $_{80}Hg$.

Table 8.2. Relativistic theories of solid- and liquid-state phenomena.

Reference	Comments
Mott (1949)	Interprets earlier x-ray spectra of Pt as evidence of 5d-band SO in the metal. The holes near top are $5d_{5/2}$, can receive electrons from $2p_{3/2}$ ($\Delta j=+1$) but not from $2p_{1/2}$. Hence L_3 seen, L_2 not. See van der Laan and Thöle (1988).
Elliott (1954)	Spin-orbit coupling in band theory.
Jortner (1962)	Halide-ion SO splitting in KI or CsI and in solution.
Ruvalds and Falicov (1968)	SO hybridisation in ferromagnetic Ni.
Tterlikkis et al. (1969)	Knight shifts and indirect nuclear spin-spin coupling tensors in Rb and Cs. Dirac OPW.
Shiba (1976)	SO effects, due to the surface, on the Knight shift and susceptibility of normal and superconducting small particles. Without SO, no shift for even number of electrons.
Sone (1977)	SO effects on spin susceptibility of small particles.
Feder et al. (1983)	Relativistic multiple scattering of electrons by ferromagnets.
Ebert et al. (1985b)	Relativistic theory of nuclear spin-lattice relaxation in metals. $Ag_x Pt_{1-x}$.
Anholt and Meyerhof (1986)	Relativistic heavy-ion collisions with solid targets.
Szpunar (1986)	Method for obtaining orbital moments in complex crystal structures. SO. Fe, Co, Ni.
van der Laan et al. (1986)	Experimental identification of SO-split states in a solid. Ce materials.
Blügel et al. (1987)	3d and 4d impurities in Ni. Quasirelativistic analogs to the M1 hfs terms derived.
Gaylord and Kevan (1987)	SO-induced surface resonance on W(011).
Kaveh and Mott (1987)	SO effects in Si:Sb induce a low-temperature metallic phase, separated from the high-temperature phase.
Lee (1987)	Relativistic corrections to density of states and conductivity of s-dimensional semiconductors. Electron-gas model.

Table 8.2. (continued).

Lefebvre et al. (1987)	Scheme for possible stereochemical rules of Sb $5s^2$ lone pairs: i) Low-lying inactive, ii) Hybridizes with chalcogen ligand p-AOs, active. iii) High-lying inactive, partially depleted.
Misra and Callaway (1987)	Relativistic theory of neutron form factors. The Dirac expression reduced to spin, orbital and spin-orbit terms.
Pankratov (1987)	Dirac theory for semiconductors with heterogeneous structures.
Pilkuhn and Soerensen (1987)	Dirac equation for electron channeling.
Sacchetti (1987)	Relativistic and solid-state effects on x-ray scattering.
Thole and van der Laan (1987,1988)	Systematics between valence band SO and x-ray absorption branching ratio.
Abramovich and Nemtsov (1988)	Multiple-wave scattering and transition radiation of relativistic electrons in crystals.
Band et al. (1988)	Atomic mechanisms for mixed-valence states in Ln, An.
Bychkov (1988)	Energy spectra for 2D systems with SO interaction in an inclined magnetic field.
K.C. Das et al. (1988)	Spin and SO contributions to magnetic susceptibility of divalent hcp metals.
Ebert and Gyorffy (1988)	Scattering solutions of the Dirac equation for nonspherical targets.
Ebert et al. (1988b)	Circularly polarized x-ray absorption by ferromagnetic Fe.
Ebert et al. (1988c)	Relativistic effects on magnetic moments and hyperfine fields of Fe, Co and Ni.
Jansen (1988ab, 1989)	Magnetic anisotropy in transition metals using density-functional theory. Both 1- electron SO and h_{Br}-derived terms considered.
Rashba and Sherman (1988)	SO splitting in 2D quantum wells, due to k^3 terms in the bulk dispersion law. Estimate for GaAs.
Shilkova and Shirokovskii (1988a)	Dipole transition matrix elements in crystals. Outer parts of Wigner-Seitz cell reduced to muffin-tin sphere surface by Green's theorem for the Dirac operator.
Shilkova and Shirokovskii (1988b)	Electron velocity in crystals. Vanadium as example.

Table 8.2. (continued).

van der Laan and Thole (1988); van der Laan (1989)	Core-valence x-ray absorption branching ratio related to valence-state SO. A "local probe" for metal compounds and alloys. Basic idea: absence of a $2p_{1/2}$ edge indicates absence of $5d_{3/2}$ holes in the valence band, transitions to $5d_{5/2}$ being forbidden.
Ando (1989)	Spin-orbit effects on electron localization in two-dimensional square lattices.
Diener and Grafenstein (1989)	Relativistic Kohn-Sham formalism and the microscopic stress tensor.
Ebert et al. (1989)	Relativistic description of hyperfine interaction in magnetic systems.
Feng (1989)	Conductance fluctuations in disordered metals with SO scattering and Zeeman splitting.
Ginatempo et al. (1989)	Relativistic theory of photoemission from crystalline metals and alloys. Cu, Ag, Au, ordered and disordered Cu_3Au.
Reizer (1989ab)	Effects of relativistic electron-electron interaction on superconductivity, specific heat etc.
Strange et al. (1989b)	A first-principles theory of magnetocrystalline anisotropy in metals. Fcc Ni.
Tripathi et al. (1989, (1990)	Effect of electron-phonon interaction on the Knight shift. Spin, orbital and SO-contributions.
Caldas et al. (1990)	Anion antisite defects As_{Ga} and Sb_{Ga} in GaAs.
Connerade and Karnatak (1990)	Centrifugal-barrier double-well atomic potentials and valence changes in solids.
Ferrari and Russo (1990)	Zitterbewegung-like discussion of two-band systems.
Krewer et al. (1990)	Spin-polarized electron diffraction from Pb(110).
Matsumoto et al. (1990, 1991)	Formalism for paramagnetic spin susceptibility of metals. SO-induced anisotropy. Applications on Sc, Co, Y.
Mishra et al. (1990)	The Knight shift in simple metals (Li-Cs, Be, Mg, Zn, Al, Ga) separated into spin, orbital and SO contributions, using the theory of Tripathi et al. (1982).
Bates et al. (1991)	Vibronic reduction factors for second-order spin-orbit coupling.
Brouder and Hikam (1991)	Multiple-scattering theory of magnetic x-ray circular dichroism. SO and spin-polarization included. Application on Fe.

Table 8.2. (continued).

Coffey et al. (1991)	The Dzyaloshinskii-Moriya interaction in cuprates (SO-induced anisotropic exchange interaction between electron spins).
K.C. Das et al. (1991)	Total magnetic susceptibility in metals.
Ebert et al. (1991b)	Theory of magnetic x-ray dischroism.
Ebert et al. (1991a)	Magnetic moments and hyperfine fields of 5d-impurity atoms in ferromagnetic Fe.
Gay and Richter (1991)	SO-induced orbital angular momentum in monolayers.
Ginatempo and Gyorffy (1991)	Spin-polarized photoemission from non-magnetic metals.
Hota and Tripathi (1991a)	Theory of spin, orbital and spin-orbit Knight shifts in PbTe.
Hota and Tripathi (1991b)	g-factors of $Pb_{1-x}Sn_xTe$.
Jablonski (1991)	Elastic electron backscattering from gold. A NR TF potential compared to a R DS one.
Jagannathan (1991)	Multiple SO scattering and anisotropic spin interactions in metals.
Jiang et al. (1991)	The superconducting $\langle I^2 \rangle$ parameter for hcp transition metals Sc...Os.
Kulakowski and Lacroix (1991)	SO contribution to the magnetic susceptibility in degenerate narrow bands.
Lander (1991)	Spin and orbital magnetic moments in An compounds. $V_{CF} \approx V_{SO}$. (CF=crystal field).
H.-S.Li et al. (1991)	Intra-atomic exchange integrals between 4f, 5d and 6s in Ln^{3+}. Magnetic Ln-Ln and Ln-M(3d) couplings.
Lindhard (1991)	Radiation from ultrarelativistic electrons moving parallel to a crystal axis.
Lipnitskii et al. (1991)	The Pb(001) surface.
Macedo and Chalker (1991)	SO effects in disordered conductors. Quaternions used.
Movaghar and Cochrane (1991)	Connection between Hall coefficient and magnetic susceptibility. SO.
Mustre de Leon et al. (1991)	Theory of XAFS (x-ray absorption fine structure). Applications on Cu, Ge, Pt, Br_2, $GeCl_4$.
Rozing et al. (1991)	Two-photon momentum distribution for positron annihilation. W.
Shachal and Manassen (1991, 1992)	SO-induced scanning tunneling microscopy observation of individual paramagnetic spins.
Sinkovic et al. (1991)	Diffraction of spin-polarized photoelectrons in magnetic materials.
Staunton et al (1991)	Theory of magnetocrystalline anisotropy.

Table 8.2. (continued).

Stern and Entin-Wohlman (1991)	Interplay of SO and Zeeman leads to damped conductivity oscillations as function of B_{ext}.
Strange et al. (1991)	Dichroic x-ray fluorescence. Fully relativistic multiple-scattering theory for Fe.
Ando and Tamura (1992)	Conductance fluctuations in quantum wires with SO scattering.
Blügel (1992)	Ferromagnetism of 5d-metal monolayers, e.g. Ir on Ag or Au, or Os on Ag.
Bonesteel et al. (1992)	Role of SO coupling in anisotropic superexchange (Dzyaloshinskii-Moriya interaction). La_2CuO_4.
Bouchaud and Sornette (1992)	SO effects on magnetoconductance.
Chao and Chuang (1992)	SO effects on strained semiconductor quantum wells.
Chatterjee et al. (1992)	Tight binding model within a fibre bundle formalism.
Ebert (1992)	Review on (SO-induced) relativistic effects in magnetic solids.
Ebert et al. (1992)	Spin-polarized relativistic treatment of disordered alloys. Fe_xCo_{1-x}, Co_xPt_{1-x}.
Edelstein (1992)	SO contribution to the Hall effect.
Hafner and Jank (1992)	Liquid As, Sb and Bi. Relativistic effects lead to s-p splitting in the DOS. Structure factors S(q) calculated.
Hernandez and Sanquer (1992)	SO decreases magnetoconductance.
Hörmandinger and Weinberger (1992)	Spin polarized relativistic approach to magnetocrystalline anisotropy energy of Fe.
Jagannathan (1992)	Nature of middle-range spin-spin interactions in metallic alloys. Anisotropic SO-induced terms included.
Kurdak et al. (1992)	SO effects on quantum interference effects in quasi-1D wires and rings.
Oreg and Entin-Wohlman (1992)	SO scattering in low-D disordered mesoscopic systems.
Papanikolaou et al. (1992)	SO scattering cross sections for 4sp and 5sp impurities in a Mg host. For Cu and Ag impurities, d contributions found.
Romanov (1992)	SO splitting in cylindrical quantum wires.
Sahnoune et al. (1992)	SO scattering effects on magnetoresistance. Scales between Au and Ag in Ca-Al as Z^6, instead of theoretical Z^8.
Shen et al. (1992a)	Ground-state wavefunction for a gas of spin-($\frac{1}{2}$) anyons in a **B**.
Shen et al. (1992b)	Second virial coefficient for a 2D spin-($\frac{1}{2}$) anyon gas.

Table 8.2.(continued).

Smith et al. (1992)	MCD of L_2 and L_3 edges of Fe and Ni.
Strange et al. (1992)	Relativistic theory of x-ray fluorescence from magnets.
Tan and Thouless (1992)	Total energy for fermions an a 2D lattice in a **B**.
Xia and Chang (1992)	Magnetic coupling in Gd_mY_n superlattices.
Zeyada (1992)	Effect of SO coupling on diamagnetic susceptibility of thin Cu films.

9. RELATIVISTIC EFFECTS AND HEAVY-ELEMENT CHEMISTRY

Perhaps the most dramatic impact of relativity on chemical thought is the insight that the chemical differences between row 5 (Z=41-54) and row 6 (Z=73-86) contain large, if not dominant, relativistic contributions. The further development of this story is outlined in Table 9.1.

As to particular properties, references on bond lengths and other ground-state properties are summarized in Table 9.2. The magnetic-resonance parameters are discussed in Table 9.3. and the molecular electric dipole and higher multipole moments, charge distributions and polarizabilities in Table 9.4. Data on molecular energy levels and energy-transfer are summarized in Table 9.5. and those on molecular ionization potentials and electron affinities in Table 9.6.

In principle, only the papers comparing the corresponding relativistic and non-relativistic calculations are included in this chapter. For the other relativistic molecular calculations, see Ch. 7.

Table 9.1. "Relativity and the periodic system": Periodic trends, reviews and pedagogical papers.

Reference	Comments
Bohr and Coster (1923)	X-ray spectra and the Periodic System. A screened Sommerfeld relativistic term introduced.
Sugiura and Urey (1926)	Comment on FS. While the lanthanides were known on row 6, the actinides were not known on row 7 in 1926. This was explained by lack of occupied 5f states, first predicted to occur at Z=95.
Wu and Goudsmit (1933)	Contrary to Sugiura and Urey (1926), the (NR) 5f one-electron states in a TF potential become occupied already at Z=92, 93, suggesting a new f-element series.
Goeppert Mayer (1941)	(NR) solution in a TF potential predicts occupied 5f states around Z=91-93. Explains similarity of $_{93}$Np to $_{92}$U.
Fricke and Greiner (1969)	Atomic ground states for Z=160-170. E164 a $(8p_{1/2})^2$ noble gas, E170 a $8p^6 9s^2$ noble gas.
Dehmer (1973)	Atomic SO splitting arises in the K-shell region. Z-dependence analysed.
Keller Jr. (1976)	Predicted properties for superheavy elements.
Mann (1976)	Review on superheavy elements E103-E172.
Desclaux and Pyykkö (1980b)	Popular review on relativistic effects in chemistry.
Ellis (1985); Ellis and Holland (1986)	Reviews on molecular cluster compound calculations.
Fazzio et al. (1985)	Discuss the trends for Cu, Ag and Au impurities in Si.
Rabe and Joannopoulos (1985)	SnTe is rhombohedral (distorted NaCl), PbTe is 'NaCl'.
Romanovskaya (1986)	History of the QM interpretation of periodicity. Relativistic effects discussed on pp. 80-85, 95-107.
Watson et al. (1986)	ZrPd bonds less strongly than HfPt.
Balasubramanian and Pitzer 1987)	Review on relativistic quantum chemistry.
Kotochigova and Tupizin (1987)	MCDF R/NR studies of the 4f-shell collapse between Ba and Ce.
Kutzelnigg (1987)	Reviews methodology for relativistic molecular work.
Lohr (1987)	Te and Po. Cubic structure of the latter attributed to large SO. "REXBAND".
Norman (1987)	DFT of f electron systems.
Weinberger and Gonis (1987)	Review on actinides.

Table 9.1. (continued).

Wulfsberg (1987)	Inorganic chemistry textbook. Ch.11.7. "Relativistic effects on orbitals".
S. B. Zhang et al. (1987)	"Nodal radii" for s, p and d orbitals of Li-La, Hf-Rn. Relativistic contraction up to 10.4 and 5.9% for s and p, respectively. No "gold maximum".
Zhu et al. (1987)	E_{coh} for Mo and W 7.8 and 9.7 eV (exp. 6.82 and 8.90, respectively). No NR reference calculation.
Ziegler (1987)	Review on periodic trends.
Dai and Ma (1988b)	Reviews on relativistic quantum chemistry.
Ermler et al. (1988a)	Review on relativistic effects in atoms and molecules. Especially SO effects and PP methods.
Langhoff and Bauschlicher (1988b)	Review on transition-metal hydrides, halides, oxides, dimers and trimers.
Malli (1988)	Review on relativistic quantum chemistry.
Marian et al. (1988)	Bonding in diatomic ThO analysed.
Miyoshi et al. (1988)	The EA of WF_6 1.52 eV smaller than that of MoF_6.
Moriarty (1988)	NR Hg is hcp like Zn and Cd, R Hg is ß-Hg. See Table 8.1.
Pyykkö (1988a)	Relativistic effects in structural chemistry.
Zel'dovich et al. (1988)	Magnetic or nuclear-spin effects in chemistry.
Balasubramanian (1989c)	Review on relativity and chemical bonding.
Balasubramanian (1989e)	Review on heavy p-block diatomic hydrides, halides and chalconides.
Balasubramanian (1989f)	Coinage metal clusters.
Burns and Bursten (1989)	Review on f-element organometallics.
Dolg et al. (1989b)	Ln compounds.
Glebov et al. (1989)	Element 104 ground state $6d7s^27p$. The $6d^27s^2$ lies 0.5 eV higher.
Kratz et al. (1989)	Chemical properties of E105. The anionic halide complexes rather resemble those of Nb and Pa than Ta.
Z.W.Lu et al. (1989b)	HgSe, HgTe are semimetals but the Cd chalcogenides semiconductors.
Mackay and Mackay (1989)	Introduction to inorganic chemistry. Ch. 16.10.: Relativistic effects.
Malli (1989)	Review on 5d and 5f elements.
Novaro(1989)	Activation of small molecules by transition-metal atoms: a review.
Schwarz et al. (1989)	Analyse the radial distribution of direct and indirect relativistic effects. Direct ones come from the K-shell region. Indirect ones arise from all shells and influence all shells. The "gold maximum" of 6s contraction understood.

Table 9.1. (continued.)

Schwerdtfeger (1989)	AuX_2^- and AuX_4^- complexes compared. Larger stability of Au(III) attributed to relativity.
Sen et al. (1989b)	A "Z-transition state" concept for LDF energy differences of isoelectronic atoms and molecules.
Takeuchi et al. (1989)	Equilibrium properties of silver and gold. R/NR.
Takizawa et al. (1989)	Phase stability of AB, A=Ni-Pt, B=Cu-Au. The absence of Pt-based alloys, like AgPt, related to more s, less d (larger d hole) and hence larger Pt-Pt cohesion. NR AgPt would exist. Au is a counterexample with large E_{coh} and many alloys.
Ziegler et al. (1989bc)	Reviews on periodic trends, especially among nd and 5f metal compounds.
Balasubramanian (1990b)	Review on heavy p-block dimers and trimers.
Baerends et al. (1990)	Suggest the use of different radii, r and r_{FW}, for discussing relativistic orbital contraction.
Elsässer et al. (1990)	Ground-state properties of 4d and 5d metals.
Eriksson et al. (1990)	Cohesive properties of Ln and Ln-like An. Lr found to be the first 6d metal.
Hoffman (1990)	Chemistry of the transactinides.
E.Johnson et al. (1990)	IP_n and radii of Ti-Hf and E104. MCDF.
Massey (1990)	Inorganic chemistry text. Relativistic effects quoted on pp. 58, 61, 158, 180, 206.
Milman et al (1990)	Trends amond d transition metal atoms discussed using 4-component PP DFT.
Ohanessian and Goddard (1990)	Review on bonding in MH^+, M=3d, 4d or 5d metal.
Schwarz (1990)	Relativistic effects in chemistry.
Zhuikov et al. (1990)	E104 atomic ground state s^2pd.
Bonacic-Koutecky et al. (1991)	A review on small group 1, 2 and 11 clusters.
Bursten and Strittmatter (1991)	A review on bonding in An-cp complexes.
Ellis et al. (1991)	A review on TM clusters and their interaction with H and O.
Jolly (1991)	Inorganic chemistry text. Relativistic effects on pp. 22-23.
Koga and Morokuma (1991)	Homogeneous catalysis by transition-metal complexes.
S.Lee (1991)	Structures of heavy main-group elements. EHT-level band-structure 2nd-moment model.
Liu et al. (1991)	Role of SO in the fcc->hcp->bcc high-pressure transition. Smaller than in Christensen et al. (1986).

Table 9.1. (continued).

Norrby (1991)	A pedagogical review on relativity and chemistry.
Pepper and Bursten (1991)	Review on theoretical actinide chemistry: hydrides, halides, oxides and organometallics.
Pyykkö (1991a)	Relativistic effects on periodic trends.
Sabirov and Bagatur'yants (1991)	Review bonding of f-element molecules.
Schwarz et al. (1991)	A nonsingular PT analysis of relativistic changes of molecular structure.
Smith and Carter (1991)	Atomic Pd likes CO but Pt likes NO.
Takizawa et al. (1991)	The different structures of CuPd and CuPt reproduced.
Balakrishnan et al. (1992)	D_0 of H_2, H_2^+. Latest experiment, supports theory.
Bauschlicher and Langhoff (1992)	Review on 3d and 4d TM mono- and dihydrides.
Hafner and Jank (1992)	Structure factors and DOS of liquid Sb and Bi.
Hay (1992)	Oxidative addition and reductive elimination of hydrogen and alkanes.
Ionova and Gerasimova (1992)	Review on actinyl chemistry.
Ionova et al. (1992)	Redox potentials of $M^{n+}(aq)$ ions, M = V-105, 103-105, estimated from MCDF.
Kaupp and v.R. Schleyer (1992c)	Why are organic Pb(IV) and inorganic Pb(II) the more stable oxidation states?
Koga and Morokuma (1992)	Review on hydrogen transfer from transition metal hydrides.
Mamaev et al. (1992)	Reviews calculations on CH_4 activation by group 10 metals. Claims tunneling dynamics relevant.
Neumann et al. (1992)	KMO_3, M=Nb, Ta. The latter has a larger gap and larger E_{coh}.
Ryzhkov et al. (1992)	Is E104 a member of group 4?
Schmidbaur et al. (1992)	Review on the "aurophilic", Au(I) ... Au(I) attraction.
Schädel (1992)	Chemical properties of elements 103-105.
Tegze and Hafner (1992)	ASb (A=Na-Cs) are ionic, contain Sb spiral chains. ABi (A=Li, Na) are metallic. Difference attributed to p AO size.
Tyson et al. (1992)	Experimental evidence for Au 5d loss, 6s gain and Ag 4d gain, 5s loss in Au-Ag alloys.

Table 9.2. Bond lengths. Many of these papers also give data on k_2 and D_e. C is the relativistic bond-length contraction, $C = R_{NR} - R_R$.

Reference	Comments
Huzinaga et al. (1984)	I_2, XeF_2 (see volume 1).
Chong et al. (1986)	CuH, ZnH.
March (1986)	Bond lengths of CH_4 to PbH_4 in R TF theory.
Petterson et al. (1987)	C for MH^+, M=Sc-Cu.
Sakai and Miyoshi (1987)	WF_6^{n-} C/pm 2.7, 2.5 and 1.6 for n=0, 1 and 2, respectively. QR PP HF.
Schwarz (1987)	Analysis of relativistic effects on bond lengths.
Schwerdtfeger et al. (1987)	C for HX^{n+}, X=Br, I; n=-1, 0, +1.
Allen et al. (1988)	UO_2 bond length **expansion**, C=-7.5 pm.
Langhoff et al. (1988)	ScF , C=0.1 pm ScCl, 0.16 pm ScBr, 0.74 pm (1st. order PT).
Pyykkö (1988a)	Table IV gives existing values of C until early 1988.
Jansen and Hess (1989c)	AuH X $^1\Sigma$ C=20 pm.
Marian et al. (1989)	NiH X $^2\Delta_i$ C=1.5 pm.
Moullet et al. (1989)	Cs_2, Cs_2^+. C=16 and 21 pm, respectively.
Schwerdtfeger et al. (1989a)	C for Tl-H and some Tl-C bonds.
Schwerdtfeger et al. (1989b)	AuL, L=H, F-I, Li, Na, S. Ions of Au_2, AuH. Largest C (109 pm) for AuH^+, smallest (16 pm) for AuF.
Schwerdtfeger et al. (1989c)	PbH^+, PbH_2, PbH_4. C=4.7, 3.7, and 7.0 pm.
Strömberg et al. (1989)	CdH^+ HF C=5 pm, HgH^+ 30, 31 and 31 pm for HF, CAS and CCI, respectively. MCl_2 HF C 4 and 14 pm for M=Cd, Hg.
Tschinke (1989)	W_2 C=4 pm.
Dolg et al. (1990a)	GdO. Rel. expansion, C=-1.6 pm.
Dolg et al. (1990b)	EuO. Small expansion.
Katsuki (1990)	AgH. C=4.2 pm.
Kellö and Sadlej (1990a)	HX, X=Br, I. C=0.26 and 0.90 pm, respectively. Also frequencies.
Lelj and Rosa (1990)	CuIn, AgIn, AuIn C=2, 11 and 32 pm, respectively. P-HFS.
Schwerdtfeger (1990)	$AuMe_2^-$ - $PbMe_2^{2+}$. C=14.8, 14.4, 10.5 and 1.6 pm, respectively. Effects on k_2 and D_e also discussed.
Schwerdtfeger et al. (1990c)	AuL, AuL_2^-, L=H, F-I, CH_3, CN, SCN. $Au(PH_3)_2^+$. C vary from 20 to 30 pm.
Strömberg and Wahlgren (1990)	At PT level, Au_2 C is 22 and 20 pm for HF and CPF, respectively. For Hg_2^{2+}, 30 pm for both.

Table 9.2. (continued).

Dolg et al. (1991d)	MH_n, M=Hg-At. RnF_n.
Dolg et al. (1991a)	CeO. QR/NR expansion 4 pm.
Dyall et al. (1991b)	MH_4, M=C-Pb. DF-LCAO.
Faegri and Bauschlicher (1991)	ScNi, YPd. CASSCF C= 1 and 9 pm, respectively. SCF 5 and 8 pm.
Lee and Lee (1991)	SO effects on R_e for HX, XX' and PbH_4. C_{SO}=-0.3 pm for HI, -1.8 pm for I_2.
Schwerdtfeger (1991a)	TlH C using seven levels of correlation. HF 2.9, QCI 2.2 pm.
Schwerdtfeger (1991b)	Au_2 C=25 pm.
Schwerdtfeger and Dolg (1991)	AuLa, AuLu. C=41 and 36 pm respectively.
van Wezenbeek et al. (1991)	UO_2, UO_2^{2+} -7.4 and -2.6 pm, respectively. Bond **expansion** due to $\langle h_m \rangle$ of the (diagonal and off-diagonal) 6p hole.
Åkeby et al. (1992)	Sc_2 $X^5\Sigma_u$. Sign(C) depends on approximation.
Barandiarán and Seijo (1992)	HF C for As_2, Sb_2, MnO and CuO 0.3, 3.2, 0.2 and 1.9 pm, respectively.
Dai and Balasubramanian (1992e)	OsH_2. SO effects on the bond angle up to 10°.
Dyall (1992a)	XH_2 C = 0.004, 0.30, 1.10 and 4.44 pm for X = Si, Ge, Sn and Pb, XH_4 C = 0.7, 2.1, 7.3 pm for X = Ge-Pb, respectively. Bond angle effects on XH_2 and vibrational frequencies also studied.
Gropen et al. (1992)	PtH two lowest states. PT C for $^2\Sigma$ and $^2\Delta$ levels.
Häberlen and Rösch (1992)	AuH_4 AuCl, Au_2.
Ishikawa et al. (1992a)	AuH^+. SCF-level C 101 pm!
Kirchner et al. (1992)	PtO C for various states.
Lee and Lee (1992)	SO effect on ground-state properties of HX, XX' (X=Br, I): $C_{SO} < 0$.
Malli (1992)	ThPt C 89 pm.
Matsuoka (1992b)	HX, HX^+, H = I, At.
Rutkowski et al. (1992)	H_2^+ using double-PT. Effects on R, k, D_e.
Schwerdtfeger et al. (1992b)	R/NR R, k, D_e for AuL, AuL_2^-, AuL_3, AuL_4^-, Au_2L_6 (L = H, F-I). AuF_6^-.
Schwerdtfeger et al. (1992c)	TlX, TlX_3, X = H, F-I. AuH, HgH_2. PbX_2, PbX_4, BiX, BiX_3, BiX_5, X=H, F.
Visser et al. (1992a)	MH_4, M = C-Pb. Effect of H_{Br} studied.

Table 9.3. Magnetic resonance parameters.

Reference	Comments
Tterlikkis et al. (1969)	Knight shifts and spin-spin coupling tensors in Rb and Cs metals.
Shiba (1976)	SO effects on small-particle Knight shifts.
Ebert et al. (1985b)	Relativistic theory of nuclear spin-lattice relaxation in metals.
Barra et al. (1986,1988)	PNC effects on NMR chemical shifts estimated by REX.
Larsson and Pyykkö (1986)	Assign for the first time the An NQCC in actinyl ions, $OAnO^{n+}$, to the hole in the 6pσ semicore orbital. REX.
Rösch and Pyykkö (1986)	Time-reversal aspects of nuclear spin-spin coupling. Applications on heavy-element fluorides.
Wilson et al. (1986)	Spin-spin coupling in Zintl anions using REX.
Edlund et al. (1987)	A heavy-atom shift of the heavy atom ("HAHA") contribution identified for ^{207}Pb NMR chemical shift in a PbH_3^- model using REX.
Ohlsén and Calais (1987)	Effect of SO dominant in g-tensor anisotropy of platinum-group metals.
Pyykkö et al. (1987)	The NMR 'heavy-atom chemical shift' in HX ascribed to SO-induced spin-density in π and Zeeman effects between σ and σ^*. The perpendicular shift, $\sigma_\perp$ dominant. REX.
Winkler et al. (1987)	Mössbauer isomer shifts of ^{119}Sn in halides, hydride and $SnMe_4$.
Berksoy and Whitehead (1988b)	$SnCl_2Ph_2$. Sn and Cl NQCC.
Blügel et al. (1988)	3d and 4d impurities in nickel. Derive the quasirelativistic analogues to the M1 hyperfine contact, orbital and dipolar terms.
Jokisaari et al. (1988)	NMR parameters for CX and XCX', X=O-Te by REX.
Kutzelnigg (1988)	Origin and meaning of the Fermi-contact interaction.
Pyper (1988)	Relativistic analogues of the NR hfs operators.
Angstl (1989)	Effects of mass-velocity corrections on molecular g-tensors.
Bowmaker et al. (1989)	X_2^n NQCC, n=-1,0,+1, X=Cl-I.
Oja et al. (1989)	Indirect nuclear spin-spin coupling calculated for metallic copper. Seen as magnetic ordering at 58 nK. QR.
Svane (1989)	^{119}Sn Mössbauer isomer shifts for tin impurities in d- and sp-metals and tin compounds.

Table 9.3. (continued).

Kellö and Sadlej (1990b)	q_x in HX, X=Cl-I. Nuclear Q obtained.
Mishra et al. (1990)	Knight shift in simple metals.
Nakatsuji et al. (1990)	^{95}Mo NMR chemical shifts.
Schwerdtfeger et al. (1990c)	$AuCl_2^-$ ^{35}Cl NQCC increased by 85%.
Winkler and Vetter (1990ab)	Mössbauer IS and NQCC in $SnX_n(CH_3)_{4-n}$, X = F-I.
Aucar and Contreras (1991)	MNDO-RPA calculations of nuclear spin-spin coupling constants for group 14 (C-Pb) hydrides, halides and methyl compounds.
Hota and Tripathi (1991a)	Theory of spin, orbital and spin-orbit Knight shifts of ^{207}Pb in PbTe.
Hota and Tripathi (1991b)	g-factors of $Pb_{1-x}Sn_xTe$.
Ishii et al. (1991)	Free-radical g-values by FPT.
Jové et al. (1991), Pyykkö and Jové (1991)	Mössbauer NQCC in neptunyl compounds interpreted by REX. The 6pσ semicore hole important.
Schwerdtfeger et al. (1991b)	CuF q_{Cu} decreased 19%.
Blaha and Schwarz (1992)	NQCC of solid Cl_2, Br_2 and I_2. Intermolecular effects on η.
Heifets (1992)	3rd-order PT formulae for g-tensors.
Schwerdtfeger et al. (1992b)	MS Xα NQCC for AuCl, $AuCl_2^-$, AuX_4^-, X = F-I.

Table 9.4. Electric dipole moments, Q_1, higher multipole moments, Q_L, and molecular charge distributions.

Reference	Comments
Werner and Buckingham (1986)	GeH dipole moment.
Chapman et al. (1987a)	SO decreases the HI dipole moment at R_e by 3.6%.
Lee and McLean (1987)	AgH, AuH dipole moments decreased by relativity.
Schwerdtfeger (1987)	TlH Q_1, Q_2.
Chapman et al. (1988b)	Dipole moments of MH, M=Ge-Pb. μ(PbH)/D 0.937 and 0.637 for X $^2\pi_{\frac{1}{2}}$ and $^2\pi_{3/2}$, respectively.
Laaksonen et al. (1988)	HCl dipole moment increased by 0.015 D. Cp. Kellö and Sadlej (1990a).
Sundholm (1988)	Fully numerical DS R/NR Q_1, Q_2 for H_2^+, H_2, LiH, Li_2, BH, CH^+.
Marian et al. (1989)	NiH dipole moment decreased -0.3D.
Schwerdtfeger et al. (1989b)	Q_1 of AuL, L = H, Li, Na, F-I, O, S. R/NR.
Schwerdtfeger et al. (1989c)	Q_1 of PbH, PbH_2. R/NR.
Baeck and Lee (1990)	Relativistic effects on Q_1 of BH^+-FH^+ by DF-LCAO.
Kellö and Sadlej (1990a)	Dipole moments of HX, X=Cl-I and of AgH, decreased by relativity. Effects on dipole polarizability also studied.
Sumathi and Balasubramanian (1990)	Signs of H_2Te and H_2Po dipole moments opposite.
Dolg (1991d)	Q_1 of MH, M=Hg-At. NR/QR.
Kellö and Sadlej (1991)	Molecular Q_2 of MH, M=Cu-Au.
Sadlej (1991)	AuH. Relativity decreases Q_1 from 1.21 to 0.62 a.u. Polarizability and Q_2 also studied.
Sadlej and Urban (1991)	AgH. Dipole moment.
Schwerdtfeger and Dolg (1991)	AuLa. Opposite Q_1! Relativistic changes about +1.04 and +0.79 D, respectively.
Dyall (1992a)	XH_2 dipole moments, X = Si-Pb. $(\_Q_1/D)/Z^2 = 0.00010$.
Häberlen and Rösch (1992)	AuH, AuCl Q_1 decreased by relativity.
Kellö and Sadlej (1992a)	XCN Q_1, Q_2 and α, X = F-I. QR CI. R/NR.
Kellö and Sadlej (1992b)	PbH_4, BiH_3, PoH_2, AtH Q_1 and α_1.
Sadlej (1992a)	Q_1 and α_1 of SbH_3, H_2Te, HI. SCF-level R/NR + NR-MBPT.
Sadlej (1992b)	Q_1 and α_{zz} of XX', X = F-I.

Table 9.5. Molecular energy levels and energy transfer. Chemical reactions.

Reference	Comments
Lohr (1972)	Spin-forbidden electronic excitations in transition metal complexes.
Salem and Rowland (1972)	Intersystem crossing in diradical reactions discussed.
Shaik and Epiotis (1980)	Spin inversion in triplet Diels-Alder reactions discussed.
Z. Wu et al. (1985)	Spin-rotation coupling in MX (M=K-Cs, X=Ar-Xe) is mainly due to noble-gas SO.
Fisher and Michl (1987)	External and internal heavy-atom effects on spin-forbidden proton tunneling in 1,3-perinaphtadiyl.
Zel'dovich et al. (1988)	Magnetic or nuclear-spin effects in chemistry.
Yarkony (1990)	The decomposition reaction HN_3 (S=0) -> N_2 (S=0) + NH (S=0,1). Landau-Zener treatment at the singlet-triplet crossing.

Table 9.6. Molecular ionization potentials and electron affinities.

Reference	Comments
Sakai and Miyoshi (1987)	First and second EA of MF_6, M = Cr-W. Relativity decreases both for WF_6 by 1.1 and 1.2 eV, respectively; the electrons go mainly into a 5d AO on W.
Rubio et al. (1989)	Spherical DS models for the IP_n of Cu_N and Ag_N clusters, N≤25.
Boldyrev and Simons (1992)	TeF_8^{2-} electron detachment energy 5 eV.

Corrections to Volume I

P. 13, Table 2.2., entry for Dirac (1928a), reads $R = B^{-1/2}P$, should read $R = r^{-1}B^{1/2}P$.

P. 24, Table 2.4.: Lapidus (1983) treats a "hydrogen atom" with a 1D δ-function potential.

P. 25, Table 2.4.: Spector and Lee (1985) treat a 1D KG hydrogenic atom

P. 43, Table 4.5.: Band et al. (1984) optimised the Slater α for DS.

P. 75, Table 5.4.: Add Dzuba et al. (1983a) and (1983b) for the IP of Cs and Fr, respectively.

P. 117, Table 7.3.: Add Pyykkö and Desclaux (1977b) for $(114)H_4$.

P. 126, Table 7.6.: Bursten et al. (1985): $An(C_5H_5)_4$.

P. 134, Table 7.7.: Andzelm et al. (1984): reads 'diminish' should read 'increase'.

P. 141, Table 7.8.: The reference Louwen et al. (1984b) is the present Louwen et al. (1986).

Reference 828 (Dirac 1979) has been published as abridged version in Europhys. News 8(1) (1977) 1-4.

Reference 1167 (Goldman and Drake 1984): p. **L**197.

Reference 1278: The authors are: Gurchumeliya, A.D., Ivanova, E.P., Tsirekidze, M.A. and Tsirekidze, T.A. (1985b).

Reference 1591 (Kahn 1984): Volume 25.

Reference 1910 (Lyudchik and Borkovskii 1984): The journal is Dokl. Akad. Nauk **Belor.** SSR.

Reference 2038 (Mendoza and Zeippen 1982): $3p^2$.

Reference 2073 (Migdalek and Baylis 1984a): Page **L**459.

Reference 2593 (Scharf et al. 1985): Page 447.

Some comments on notations and terminology

In the Bibliography, Smith (1975) and Smith (1975a) are synonymous. The references are in alphabetic order according to:
1) The first author (including initials), 2) The second author, 3) The third author, etc., 4) For each of these, the year, 5) For the same author(s) and year, the letters a, b, c, ...

We have adopted the IUPAC notations 1 to 18 for the groups in the Periodic System (1 for H and Li, 4 for Ti, 12 for Zn, 14 for C, 18 for Ne). The elements Li - F are called "2nd-row" ones, Na - Ar "3rd-row" ones etc.

No apologies are offered for using for ions both the notation Cu^+ and Cu II in a work on the borderline of chemistry and physics.

List of acronyms and symbols.

A	Magnetic vector potential.
$\underline{A}$	Hyperfine coupling tensor.
$\boldsymbol{\alpha}$	Dirac matrix.
α	Fine structure constant (1/137.035 989 5(61), 1986).
AE	All-electron.
AL	Average level.
α_L	Electric polarizability of multipolarity L.
An	An actinide (Ac - Lr).
AO	Atomic orbital.
APW	Augmented plane-wave method.
B	Magnetic field.
ß	Dirac matrix.
BP	Breit-Pauli.
c	Speed of light.
CASSCF	Complete active space SCF.
CC	Coupled cluster.
CCSD	Coupled cluster method with single and double substitutions.
CEPA	Coupled electron-pair approximation.
CFT	Crystal field theory.
CG	Cowan-Griffin (approximation).
CI	Configuration interaction.
CN	Coordination number.
CNDO	Complete neglect of differential overlap.
CP	Core polarization.
Cp	Cyclopentadienyl, C_5H_5.
Cp*	$C_5(CH_3)_5$.
CT	Charge transfer.
D_e	Dissociation energy.
DF	Dirac-Fock. (<u>Not</u> "density-functional").
DFT	Density functional theory.
DOS	Density of states.
DS	Dirac-Slater.
DVM	Discrete Variational Method.
DZ	Double-zeta (radial function).
E	Electric field.
EA	Electron affinity.
EAL	Extended average level.
ECP	Effective core potential.
EHT	Extended Hückel theory.
EM	Electromagnetic.
ESR	Electron spin resonance.
EXAFS	Extended x-ray absorption fine structure.
FAKE	Fast, Accurate Kinetic Energy method.
FEM	Finite-element method.
FFT	Fast Fourier transform.
FPT	Finite perturbation theory.
FS	Fine structure.
FW	Foldy-Wouthuysen.
g	The electron g-factor.
$\underline{g}$	The electron g-tensor (in ESR).
γ_L	Electric screening constant of multipolarity L.
GTO	Gaussian type orbital.
GVB	Generalized valence bond.

h_{Br}	Breit Hamiltonian.
h_D	Dirac Hamiltonian (see eq.(2.4)).
h_d	Darwin term at the NR limit.
h_m	The mass-velocity term.
h_p	Pauli Hamiltonian.
HF	Hartree-Fock.
HFR	Hartree-Fock with relativistic correction terms.
Hfs	hyperfine structure.
HFS	Hartree-Fock-Slater.
HOMO	Highest occupied MO.
IEHT	Iterative EHT
INDO	Intermediate neglect of differential overlap.
IP	Ionization potential.
IS	Isomer shift.
χ_L	Magnetic susceptibility of multipolarity L.
KG	Klein-Gordon.
KKR	Korringa-Kohn-Rostocker band-structure method.
L	Multipolarity; orbital angular momentum.
Λ	Electronic orbital angular momentum around the molecular axis for linear molecules.
LCAO	Linear combination of atomic orbitals.
LDA	Local density approximation.
LDF	Local density functional.
LEED	Low-energy electron diffraction.
Ln	A lanthanide (La - Lu).
LMTO	Linear Muffin-Tin Orbital method.
LSD	Local spin density.
LUMO	Lowest unoccupied MO.
MBPT	Many-body perturbation theory.
MCD	Magnetic circular dichroism.
MCDF	Multiconfiguration Dirac-Fock.
MCHF	Multiconfiguration Hartree-Fock.
Me	Methyl (CH_3-).
MINDO	Modified INDO.
MNDO	Modified NDO.
MO	Molecular orbital.
MP(n)	Møller-Plesset PT (of order n).
MRD-CI	Multireference CI.
MRCI	Multireference CI.
MS	Multiple Scattering.
MWH	Mulliken-Wolfsberg-Helmholtz (= EHT).
N	Number of electrons.
NMR	Nuclear magnetic resonance.
NQCC	Nuclear quadrupole coupling constant.
NR	Non-relativistic.
OCE	One-centre expansion.
ODC	Optimised Double-Configuration method.
ω_e	Vibrational frequency.
P	Parity inversion.
PES	Photoelectron spectrum, -spectroscopy.
PF	Pair function.
PK	Phillips-Kleinman.
PM3	"Parametric model 3"
PNC	Parity non-conservation.
PP	Pseudopotential.
PT	Perturbation theory.
QCI	Quadratic CI.
QED	Quantum electrodynamics.
QM	Quantum mechanics.
QMC	Quantum Monte-Carlo.

QR	Quasirelativistic ("one-component").
ϱ	Electron density.
RASSCF	Restricted active space SCF.
R_e	Bond length.
REX	Relativistic Extended Hückel.
RPA	Random phase approximation.
S	Overlap matrix.
SCF	Self-consistent field.
σ_L	Magnetic screening constant of multipolarity L.
SO	Spin-orbit.
STO	Slater-type orbital.
SZ	Single-zeta (basis).
T	Time inversion.
TD	Time-dependent.
T_e	Electronic excitation energy.
TF	Thomas-Fermi.
TFDW	Thomas-Fermi-Dirac-Weizsäcker.
TM	Transition metal.
TP	Transition probability.
TS	Transition state.
V	A potential.
VB	Valence bond.
n-VE	n-Valence-electron (/atom) PP.
WKB	Wentzel-Kramers-Brillouin ("semiclassical") approximation.
X	Electronic ground state of a molecule.
$X\alpha$	Slater's $X\alpha$ (= HFS) method.
Z	Nuclear charge.

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