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P. Pyykkö

Relativistic Theory of Atoms and Molecules

A Bibliography 1916–1985

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"...tempus item per se non est sed
rebus ab ipsis consequitur sensus..."

(Lucretius, "De rerum natura")

PREFACE

The project that finally led to this book, was originally started with Dr. Jean-Paul Desclaux. It is a pleasure to thank him for a fruitful collaboration stretching over more than a decade.

While accepting the responsibility for any remaining errors and omissions, I wish to acknowledge in particular the comments by Teijo Åberg, Viktor Flambaum, Burkhard Fricke, Franz Mark and Arne Rosén.

The Bibliography was compiled using a Fortran program, written for the DEC 20 at the University of Turku by Matti Hotokka, and adapted to the University of Helsinki Burroughs 7800 by Dage Sundholm.

Harriet Björnström did most of the typing and Käthe Ramsay cross-checked the text against the Bibliography.

Readers, interested in obtaining a Wordstar-readable, IBM PC compatible diskette file (about 520 kb on a two-sided diskette) of the Bibliography should contact the author .

Helsinki, 20 August, 1986

Pekka Pyykkö

CONTENTS

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. As a matter of policy, we have not tried to be comprehensive, concerning solutions leading to elementary particle spectra. Some of this material is included, however. 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 3119 references are given in the Bibliography. No "stars" 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. Monographs and other general references.

Reference	Area
Aglitskii and Safronova (1985)	Autoionization states.
Akhiezer and Berestetskii (1965)	QED
Armstrong (1971)	Hyperfine structure.
Armstrong (1983)	Many-body effcts in atoms.
Armstrong and Feneuille (1974)	Atoms.
Bagrov et al. (1982)	All exact solutions of Dirac and Klein-Gordon equations, known in late 1981.
Barut (1980)	QED
Baym (1969)	Dirac theory.
Behrens and Buhring (1982)	Beta decay.
Berestetskii et al. (1971)	Relativistic quantum mechanics.
Berry et al. (1980)	Foundations of atomic theory.
Bethe and Jackiw (1968)	QM.
Bethe and Salpeter (1957)	One- and two-electron atoms.
Bialynicki-Birula and Bialynicka-Birula (1975)	QED.
Bjorken and Drell (1964)	Relativistic QM.
Bjorken and Drell (1965)	QED
Bogolyubov and Shirkov (1980)	QED
Bradley and Cracknell (1972)	Symmetry in solids.
Braun et al. (1984)	Foundations of atomic theory.
Cartan (1981)	Spinors.
Condon and Shortley (1951)	Atomic spectra.
Corben (1968)	Particles with spin.
Corinaldesi and Strocchi (1963)	Relativistic QM.
Corson (1953)	Relativistic wave equations.
Cowan (1981)	Atomic structure and spectra.
Crasemann (1982, 1985)	Atomic inner-shell physics.
Das (1974)	Relativistic electron theory.
Davydov (1976)	QM.
de Broglie (1934)	Dirac theory.
Desclaux (1980, 1983a-c)	Relativistic atomic calculations.
Desclaux and Freeman (1984)	Actinoid atoms.
Dirac (1974)	QM.
Dmitriev et al. (1984)	Atomic spectra.
Drake (1982b, 1983ab)	QED effects in few-electron atoms.
Eddington (1936)	Relativistic QM.
Feshbach and Villars (1958)	Dirac and Klein-Gordon theories.
Feynman (1961)	QED.
Fock (1932)	Dirac theory.
Grant (1970, 1979, 1983a-b)	Relativistic atomic calculations.
Greiner (1981)	Relativistic wave equations.
Greiner (1983)	QED of strong fields.
Greiner and Reinhardt (1984)	QED.

Table 1.1. (continued).

Greiner et al. (1985)	QED of strong fields.
Griffith (1960)	Transition-metal ions.
Hagedorn (1964)	Relativistic kinematics.
Harriman (1978)	Relativistic electron theory and theoretical foundations of electron spin resonance.
Heitler (1954)	QED.
Hill and Landshoff (1938)	Dirac theory.
Hund (1954)	Field theory.
Itzykson and Zuber (1980)	QED.
Jansen and Boon (1967)	Group theory.
Jauch and Rohrlich (1976)	QED.
Johnson (1980, 1983)	Relativistic many-body calculations.
Kaempffer (1965)	QM.
Källen (1958, 1972)	QED.
Kelly and Kim (1985)	Relativistic and QED effects in heavy atoms (a conference).
Koster et al. (1963)	The 32 point groups.
Kovalev (1965)	The 32 point groups.
Kramers (1938)	Dirac theory.
Leushin (1968)	The 32 point groups.
Lifshitz and Pitaevskii (1974)	QED.
Lindgren and Morrison (1982)	Atomic many-body theory (mainly n.r.).
Lindgren and Rosen (1974)	Relativistic atomic calculations; hyperfine effects.
Loucks (1967)	Augmented plane-wave method.
Lurie (1968)	QED.
Malli (1982, 1983a-b)	Relativistic effcts in atoms, molecules and solids.
Mandl (1959)	QED.
Messiah (1962a)	QM.
Moiseiwitsch (1980)	Atomic collisions.
Moiseiwitsch (1985)	Scattering of relativistic electrons.
Moss (1973)	Relativistic electron theory.
Mott and Massey (1965)	Atomic collisions.
Neumann (1981)	Two-electron systems.
Nikitin and Rudzikas (1983)	Relativistic atomic calculations.
Nishijima (1969)	Field theory.
Pauli (1958)	Dirac theory.
Pauling (1960)	The nature of the chemical bond.
Penrose and Rindler (1984)	Two-spinor calculus.
Pitzer (1979)	Chemistry.
Pyykkoe (1975)	An elementary introduction.
Pyykkoe (1978, 1984)	Relativistic effcts in atoms, molecules and solids.
Pyykkoe and Desclaux(1979b)	Chemistry.
Ramana and Rajagopal(1983)	Density-functional calculations.
Richards et al. (1980)	Spin-orbit effects in molecules.
Richtmyer (1978)	Dirac theory.
Roman (1969)	Field theory.
Rose (1957)	Angular momentum.
Rose (1961)	Relativistic electron theory.
Rudzikas and Kaniauskas (1984)	Quasispin and isospin in atoms.

Table 1.1. (continued).

Safronova (1982ab, 1983ab, 1984ab)	Atomic theory.
Safronova and Senashenko (1984)	Multiply charged ions.
Sakurai (1967)	QM.
Scadron (1979)	Relativistic electron theory.
Schiff (1968)	QM.
Schmutzer (1968)	Relativity.
Schweber (1961)	QED.
Schwinger (1958)	QED (collection of reprints).
Silver (1976)	Irreducible tensors.
Slater (1960)	Atoms.
Slater (1963)	Molecules.
Slater (1974)	Local-density theory.
Sokolov and Ivanenko (1952)	QED.
Sokolov and Ternov (1974)	Relativistic electrons.
Sommerfeld (1939)	Dirac theory.
Streater and Wightman (1964)	PCT, spin and statistics etc.
Sucher (1983, 1984)	Foundations of atomic theory.
Thirring (1958)	QED.
Umezawa (1956)	QED.
Varshalovich et al. (1975)	Angular momentum.
Wentzel (1949)	Field theory.
Wigner (1959)	Group theory.
Yutsis and Bandzaitis (1965)	Angular momentum.
Yutsis et al. (1962)	Angular momentum.
Yutsis and Savukinas (1973)	Atoms.
Zapryagaev et al. (1985)	One- and two-electron atoms.

2. ONE-PARTICLE PROBLEMS

2.1. Special relativity and the old quantum theory.

The special theory of relativity of Einstein (1905) was incorporated into the old quantum theory of Bohr by Sommerfeld (1916) and collaborators (Green 1923, Sommerfeld and Heisenberg 1922). (See also Foersterling (1920), Landé (1924).

Both the relativistic stabilization and the splitting of energy levels are already found in this model of Sommerfeld (1916). For an explanation for this, quantitative, success see Biedenharn (1962, 1983) and Biedenharn and Swamy (1964). As a curiosity we mention its use by Grimm and Sommerfeld (1926) to discuss the valencies of halogens. Darwin (1920) discussed the relativistic Lagrangian.

For a fresh start from special relativity, see Horwitz and Piron (1973) and Grelland (1980, 1981).

2.2. On the Klein-Gordon equation.

For a spin-less particle in an electromagnetic field ($\mathbf{A}$, ϕ) the relativistic Hamiltonian

$$H = \{m^2c^4 + c^2(p - e\mathbf{A})^2\}^{1/2} + e\phi \tag{2.1}$$

gives the Schroedinger equation

$$(i\hbar \frac{\partial}{\partial t} - e\phi)\psi = \{m^2c^4 + c^2(i\hbar\nabla + e\mathbf{A})^2\}^{1/2}\psi, \tag{2.2}$$

whose square becomes

$$(i\hbar \frac{\partial}{\partial t} - e\phi)^2\psi = \{m^2c^4 + c^2(i\hbar\nabla + e\mathbf{A})^2\}\psi. \tag{2.3}$$

This equation is called the Klein-Gordon equation and was originally derived independently by several authors (Fock 1926ab, Gordon 1926, Klein 1926, 1927, Schroedinger 1926). Its correct interpretation was found by Pauli and Weisskopf (1934). (See also Ioannidou (1984) and Pauli (1940)).

As shown by Sucher (1963), eq. (2.2) is not Lorentz invariant, in contrast to the classical theory. This was an important motivation for finding Dirac's equation, (2.4).

For a solution of the Klein-Gordon equation in a Coulomb field, see e.g. Davydov (1976, VIII. 58) or Razumov et al. (1981). The non-relativistic limits are discussed by Case (1954), Crater and Van Alstine (1983), Schoene (1979) and Veselic (1983). for discussions of the equations of this type, see Austen and de Swart (1983), Bagrov et al. (1982), Cea et al. (1982, 1983), Daubechies (1984), Daubechies and Lieb (1983), Feshbach and Villars (1958), Fiziev (1985), Friar (1980b), Friar and Tomusiak (1984), Greiner (1981), Greiner et al. (1985), Herbst (1977), Kulkarni and Sharma (1980), and Rafelski et al. (1978).

A virial theorem was proven by Brack (1983). The analytically solvable potentials are reviewed by Bagrov et al. (1982) or Kulkarni and Sharma (1980).

2.3. The Dirac equation.

The Dirac equation

$$h_D \Psi = (c\underline{\alpha}\cdot(\mathbf{p} - e\mathbf{A}) + \beta mc^2 + e\phi)\Psi = E\Psi \qquad (2.4)$$

with

$$\underline{\alpha} = \begin{pmatrix} 0 & \underline{\sigma} \\ \underline{\sigma} & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}, \quad \Psi = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix} \qquad (2.5)$$

was constructed by Dirac (1928ab). For historical notes, see Dirac (1979), Kragh (1981), Moyer (1981a-c) and Wightman (1972). The general references to Dirac theory are given in Table 1.1.

Interpretative studies, symmetry properties and non-relativistic limits are summarized in Table 2.1., further transformations in Table 2.2., solutions for hydrogenic atoms, including the Coulomb Green functions, in Table 2.3., the solutions for other fields in Table 2.4., and the literature on the virial theorem in Table 2.5. The "H_2^+" problem of an electron or muon in the field of two nuclei is covered in Table 7.1.; the "Kronig-Penney" delta-function one is included in Table 2.4.

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
Heisenberg and Jordan (1926)	The Pauli limit.
Thomas (1926, 1927)	The "Thomas factor 2".
Pauli (1927)	The Pauli limit.
Breit (1928)	The magnetic moment of the electron.
Breit (1928b)	Interpretative.
Darwin (1928b)	The magnetic moment of the electron.
Dirac (1928ab)	The equation.
Gordon (1928b)	Current density. Conduction and polarisation terms.
Jordan and Wigner (1928)	The Pauli exclusion principle.
Nishina (1928, 1929)	Compton scattering.
Tetrode (1928)	Interpretative.
von Neumann (1928)	Interpretative.
Alexandrow (1929)	Probability density.
Fock (1929ab)	General relativistic effects.
Fock (1929c)	Interpretation of the velocity operator.
Nikolsky (1929)	Dispersion relations.
Dirac (1930b, 1934)	Negative-energy states interpreted.
Fues and Hellmann (1930)	Polarized plane waves.
Schroedinger (1930b)	Zitterbewegung.
Sen (1930,1931)	Interpretative.
Fock (1931)	Interprets the Zitterbewegung.
Huff (1931)	Magnetic field.
Laporte and Uhlenbeck (1931)	Interpretative.
Tanaka (1931)	"Electric and magnetic moments of the Dirac electron."
Moeller (1932)	Scattering of fast electrons.
Pauli (1932)	Dirac equation and geometric optics.
Wigner (1932)	Time-reversal symmetry.
Infeld and van der Waerden (1933)	General relativistic effects.
Furry and Oppenheimer (1934)	Positrons.
Heisenberg (1934)	Positrons.
Sommerfeld and Maue (1935)	N.r. limit.
Broch (1937)	Density of states.
Conway (1937, 1947, 1948)	Quaternions.
Ruse (1937)	Geometry of the Dirac equation.
Hill and Landshoff (1938)	Review of Dirac theory.
Margenau (1940)	Zeeman effect.
Papapetrou (1940)	Position operator.
Pauli (1940)	Spin and statistics.
Harish-Chandra (1945)	Algebra of the Dirac matrices.
Wigner (1947)	Relativistic wave equations.
Bargmann and Wigner (1948)	Symmetries of relativistic wave equations.
Pryce (1948)	Position and spin operators.
Rubinowicz (1948)	Momentum-space wave functions.
Becker (1949)	A two-component equation.

Table 2.1. (continued)

Johnson and Lippmann (1949, 1950)	Magnetic field.
Sewell (1949)	N.r. limit.
Foldy and Wouthuysen (1950)	N.r. limit.
Saenz (1950)	Integrals of motion.
Foldy (1952)	Interaction with EM fields.
Huang (1952)	Zitterbewegung.
Barker and Chraplyvy (1953)	N.r. limit.
K.M. Case (1954)	Generalized FW transformation.
Hirschfelder et al. (1954)	N.r. limit.
Okubo (1954)	N.r. limit.
Good (1955)	Properties of Dirac matrices.
Koba (1956)	Velocity, taking into account the positron states.
Kursunoglu (1956)	N.r. limit.
Ma (1956)	N.r.limit, especially the Darwin term.
Sucher (1956)	N.r. limit.
Cini and Toushek (1958)	The relativistic limit.
Khuri and Treiman (1958)	Dispersion relations for potential scattering.
Froeman (1958, 1960)	Pauli corrections for atoms.
Martin and Glauber (1958)	Theory of electron capture.
Prats and Toll (1959)	Construction of a central potential from phase shifts and bound states.
Bollini and Giambiagi (1961)	A generalized FW transformation.
Fradkin and Good (1961)	Polarization operators.
A.P. Stone (1961, 1963)	N.r. limit, including hyperfine effects.
Titchmarsh (1961bc)	Completeness of eigenfunctions.
Blount (1962)	Extension of the F-W transformation.
Good and Rose (1962)	Relationship between the Foldy-Wouthuysen and Lorentz transformations.
Guth (1962)	Interpretation of Zitterbewegung.
Titchmarsh (1962)	N.r. limit.
Wightman (1962)	Localizability.
Grossmann and Peres (1963)	Classical ("dequantized") theory of the Dirac electron.
Herman and Skillman (1963)	Pauli corrections for atoms.
Herman et al. (1963)	Use of the Pauli corrections in band theory.
Johnson et al.(1963)	Pauli corrections in band theory.
Pratt Jr. (1963)	N.r. limit.
Prosser (1963)	Scattering from a potential.
Rubinow and Keller (1963)	WKB solution.
A.J. Stone (1963)	Zeeman effect for molecules.
Barut (1964)	Dynamical symmetry group.
Hanus (1964)	N.r. limit.
Harriman (1964)	N.r. limit; a bibliography.
Loewdin (1964)	N.r. limit.
Yamasaki (1964, 1968)	Positron operators and Zitterbewegung.
Blinder (1965)	N.r. limit of hyperfine interaction.
Itoh (1965)	N.r. limit.
Castell (1967)	Position operator.
Joseph (1967)	Ladder operators.

Table 2.1. (continued).

Levy-Leblond (1967, 1970)	N.r. limit.
Barut (1968)	Interpretative.
de Vries and Jonker (1968)	N.r. limit.
Fong and Rowe (1968)	Position operator for free particles.
de Vries (1970)	F-W transformations.
Crowther and ter Haar (1971b)	N.r. limit.
Howard and Moss (1970, 1971)	N.r. limits for molecules.
Huzinaga and Arnau (1971)	The Pauli operators cannot be used self-consistently. (Tested on hydrogenic 1s).
Moss (1971)	N.r. limit.
Veselic (1971)	Analyticity in 1/c.
Detrich (1972)	Pauli approximation for many-electron atoms.
Wightman (1972)	Interpretative.
Jorgens (1973)	Perturbations of the Dirac operator.
Douglas and Kroll (1974)	A generalized FW transformation for variational use.
Grant (1974); Grant and Starace (1975)	Gauge invariance and radiative transitions.
Barut (1975)	N.r. limit by "dilatation".
Friar (1975)	N.r. limit.
Gurtler and Hestenes (1975)	Interpretative.
Hestenes (1975)	Interpretative.
Hunziker (1975)	N.r. limit.
F. Joergensen (1975)	The FW transformation as a "Van Vleck" transformation.
Moore (1975ab)	Zeeman effect ("g shift").
Moore (1975c-e)	N.r. limits (shown to be wrong by Tomishima (1979) and Moore and Lee (1981).
Roux and Phan (1975)	Unitary transformations of the Dirac equation.
Collier (1976ab)	General relativistic effects.
Phan and Truong (1976)	Thomas-Reiche-Kuhn sum rule (applied on elementary particles).
Cvijanovic and Vigier (1977)	Extended model for Dirac equation.
Dahl (1977)	Connection with rotations.
Drake and Glass (1977)	Hermiticity.
Feneuille and Luc-Koenig (1977)	N.r. limit.
Franzius (1977)	Separability of variables.
Hindmarsh (1977)	Position operator.
Kubo (1977)	Conformally covariant structure of the Dirac equation.
Osche (1977)	FW transformations.
Smrz (1977)	General relativistic effects.
Temchin (1977)	Two-component form.
Bachas (1978)	Supersymmetry and positron operators.
Harriman (1978)	Relativistic electron theory and ESR.
Kwon and Tabakin (1978)	Momentum-space wave functions (both Dirac and KG).
Miglietta (1978)	Two-component first-order equations.
Edmonds (1978b)	Interpretative.
Guseinov (1978)	A Levinson theorem.

Table 2.1. (continued)

Teitelboim (1978)	Connection with supersymmetry.
Bess (1979)	Diffusion model for Dirac equation.
Chatterjee and Dixon (1979); Chatterjee and Lulek (1979)	Derivation of the spin-orbit term.
Darby and Ruijgrok (1979)	A non-compact gauge group.
DiVecchia and Ravndal (1979)	Supersymmetry.
Eletskii et al. (1979)	WKB methods for $Z > 137$.
Gonsalves and Moss (1979)	N.r. limit for H_2^+.
Leon et al. (1979)	Group content of the FW transformation.
Lock (1979, 1984)	Zitterbewegung.
Moss and Trivedi (1979)	N.r. limit.
Schoene (1979)	N.r. limit.
Sebastian (1979-1984)	A FW transformation for one-photon radiative transitions.
Theis (1979)	Classical derivation of s-o coupling.
Anchiskin (1980)	N.r. limit for non-stationary, inhomogeneous EM fields.
Barut et al. (1980-1985)	Interpretative studies.
Behncke (1980)	Dirac equation with anomalous magnetic moments.
Bergou and Varro (1980, 1981)	Interaction between a free electron and an external EM plane wave.
Droz-Vincent (1980)	Relativistic theory of scattering.
Filipowicz (1980)	A quantized EM wave.
Giachetti and Sorace (1980)	A Hamiltonian formulation of two-body interactions.
Gruzdev and Sherstyuk (1980)	Dirac Green's functions for non-local potentials.
Josephson (1980)	Interpretative.
Kobe and Yang (1980)	Gauge invariant n.r. limit in a TD EM field.
Morrison and Moss (1980)	N.r. limit.
Nikitin and Nakonechnyj (1980)	A 10-dimensional invariance algebra.
Roshchupkin and Inopin (1980)	Multipole sum rules.
Snijders and Pyykkoe (1980)	An α^2 expression for E_T, formulated in terms of a "pseudorelativistic" small component.
Ternov and Bordovitsyn (1980, 1982)	Quasiclassical theory of spin.
Berezin et al. (1981)	Quaternionic solution.
Bjorken and Orbach (1981)	WKB approximation. Example: precession of an electron with anomalous magnetic moments.
Cirincione and Chernoff (1981)	N.r. limits for Dirac and KG.
Ellis (1981)	"Proper time".
Fanchi (1981)	Resolution of the Klein paradox.
Frescura and Hiley (1981)	Geometric interpretation of the Pauli spinor.
Hansen and Ravndal (1981)	Klein paradox.
Horwitz and Rotbart (1981)	N.r. limit.

Table 2.1. (continued)

Potvin (1981)	N.r. limit using free-particle basis.
Thaller (1981)	Potential scattering.
Yang et al. (1981)	Interaction with EM fields.
Barducci (1982)	Supersymmetry for particles with anomalous magnetic moments.
Caffo and Remiddi (1982)	Transition amplitudes for Dirac spinors.
Deumens (1982)	Interaction with EM fields.
Dixit and Pietenpol (1982)	S-o interaction and the centre of mass.
Ellis and Siopsis (1982)	The FW "mean-position" operator.
Gesztesy et al. (1982-1984b)	N.r. limits.
Goldman and Drake (1982)	Sum rules.
Henneaux and Teitelboim (1982)	Supersymmetry.
Herdegen (1982)	A new relativistic equations for spin-0 and -1/2 particles.
Horwitz and Arshansky (1982)	Interpretative.
Jones (1982)	Use of the Darwin Hamiltonian in a medium is illegitimate.
Keller (1982)	"Symmetry constrained" Dirac particles.
Kobe (1982); Kobe and Kennedy(1983); Kobe and Yang (1980)	Gauge invariance.
Mickelson (1982)	A relation between Maxwell and Dirac theories.
Poole and Farach (1982)	Pauli-Dirac matrix generators of Clifford algebras.
Ram (1982)	Confinement and leaks:the Klein paradox.
Roux (1982, 1984)	N.r. limit in an EM field.
Skachkova and Flesher (1982)	Hamilton-Dirac formalism for anomalous moments.
Urani and Kemp (1982)	A Dirac equation in accelerating reference frames.
Wachutka and Bross (1982)	Bivariational methods.
Yajima (1982a-c)	WKB approximation.
K.-H. Yang (1982)	Gauge invariance and FW transformations.
Yudin (1982)	WKB approximation and Coulomb excitation
Datta (1983)	Fluid-dynamical interpretation of the Dirac equation.
De Angelis et al. (1983)	Probabilistic solutions of Pauli-type equations.
des Cloizeaux (1983)	Reformulation with observable local densities and EM fields.
Gursey (1983)	Supersymmetry.
Harrell and Klaus (1983)	Large-R limit of a double-well problem.
Harris (1983)	Bounds for the eigenvalues of separated Dirac operators.
Hostler (1983, 1985)	Coulomb Green function.
Keller (1983)	Interpretative.
Ketley and Moss (1983ab); Moss (1984)	N.r. limit.
Morita (1983)	Quaternionic formulation in special and general relativity.
Olsson (1983)	Confinement and leaks: the Klein paradox
Roesch (1983a)	Use of time-reversal symmetry.
Rosen (1983)	Feynman path summation.
Salingaros (1983, 1984)	Interpretative.

Table 2.1. (continued)

Takahashi (1983)	All possible Fierz identities among the 16 elements in the Dirac algebra.
Yamada (1983)	N.r. limt.
Buenker et al. (1984ab)	An attempt to use $h=(p^2c^2+m^2c^4)^{1/2}$ and the delta-function Darwin term in SCF calculations.
Dongarra (1984ab)	Use of time-reversal symmetry.
Eschrig (1984)	Use of time-reversal symmetry.
Hamilton (1984ab)	Interpretative.
Hardekopf and Sucher (1984)	Momentum space.
Herdegen (1984)	N.r. limit.
Nam and Moravcsik (1984)	Transformation of spinors, with application on the Compton effect.
Pursey and Plebanski (1984)	SL(2,C) symmetry of the Dirac equation.
Shabaev (1984a)	Recursion relations for radial integrals
Soh (1984)	A new square root of momentum space.
Susloparov (1984)	Electric and magnetic fields.
Thaller and Thaller (1984)	Localization of Dirac particles.
Ui (1984)	Supersymmetry for a spin-orbit potential
Umezawa (1984)	Zitterbewegung.
Barut and Bracken (1985)	SO(n+2) algebras and internal geometries of relativistic systems.
Benn and Tucker (1985)	Interpretative.
Boudet (1985)	Conservation laws.
Clarkson (1985)	Clifford algebras.
Liebscher (1985)	Geometry of the Dirac equation.
Linhares and Mignaco (1985)	SU(4) for the Dirac equation.
Ma and Ni (1985)	Levinson theorem for Dirac particles.
Niemi (1985)	Supersymmetry.
Sallhofer (1985)	Elementary derivation.
Schmitt and Arenhoevel (1985)	Sum rules.
Sharma and Sharma (1985)	Perturbative solutions for two-channel equations.

Table 2.2. The Dirac equation: further transformations

Reference	Comments
Dirac (1928a)	Derives the second-order equations for spherical potentials: $\{-\frac{1}{2m}(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r}) + V + l(l+1)/2mr^2 - E - (V-E)^2/2mc^2 - \frac{1}{2mB}(\frac{\partial}{\partial r} + \frac{\kappa+1}{r})\}R = 0, \quad (2.6)$ $B = E - V + 2mc^2$ and, with the substitution $R = B^{-1/2}P$, $\{h_{nr} - E - (V-E)^2/2mc^2 - \frac{1}{2B}\frac{\kappa}{r}\frac{\partial V}{\partial r} + \frac{1}{4B}\frac{\partial^2 V}{\partial r^2} - \frac{1}{8B^2}(-3)(\frac{\partial V}{\partial r})^2\} P = 0 \quad (2.7)$
Flint (1934)	A second-order equation.
Temple (1934)	A second-order equation.
Sommerfeld and Maue (1935)	Iterated Dirac equations.
Feynman and Gell-Mann (1958)	A second-order equation for $\psi_L - \psi_S$.
Biedenharn (1962)	The equations for large and small components decoupled for a Coulomb field.
Löwdin (1964)	Partitioning.
Mott and Massey (1965)	Derive (2.7) (also in the 1949 2nd edition).
Darewych et al. (1971)	Uses the second-order equation of Mott and Massey.
Friar (1975)	Properties of the 2nd-order Dirac equation.
Cowan and Griffin (1976)	A second-order equation. Essentially (2.6), shown to work as a quasirelativistic equation.
Karwowski and Klobukowski (1976, 1978); Karwowski and Kobus (1981)	Parameterized QR Hamiltonians of hydrogen-like form for one-electron atoms.
Luc-Koenig (1976)	Uses the Mott-Massey 2nd order equation to interpret inverted spin-orbit splitting.
Rosicky et al. (1976)	Uses (2.6) in scattered-wave theory.

Table 2.2. (continued).

Reference	Comments
Koelling and Harmon (1977)	Two coupled first-order equations for a j-average with a good spin quantum number. Quote (2.6).
Gollisch and Fritsche (1978)	Essentially (2.6), used as a QR equation.
Karwowski and Klobukowski (1978)	Introduces an approximate Darwin + spin-orbit term $B^{-1}\ V\ C\ r^{-2}$ (C = constant, B as in eq. (2.6)).
Miglietta (1978)	Two-component first-order equations.
Takeda (1978)	Essentially (2.6), used as a QR equation.
Wood and Boring (1978)	Essentially (2.6), used as a QR equation.
Karwowski and Szulkin (1979, 1981)	Uses (2.6) in HF calculations on alkali-like atoms.
Barthelat et al. (1980)	An approximate second-order equation involving only dV/dr, no derivatives of ψ; exact for hydrogenic systems: $$\{-\frac{1}{2}\nabla^2 + V - E - \frac{1}{2c^2}(E-V)^2 - \kappa(1 - (1 - (Z/\kappa c)^2)^{1/2})\frac{1}{2Z}(dV/dr)\}\ \psi = 0\ . \quad (2.8)$$
Josephson (1980)	Second-order equations for H.
Sin Fai Lam (1980); Sin Fai Lam and Baylis (1981)	Uses (2.7) in electron scattering from Hg.
Szulkin and Karwowski (1981)	A QR-HF method used on alkali metals.
Wallmeier and Lutzelnigg (1981); Wallmeier (1981, 1984)	Uses the squared Dirac Hamiltonian $$h = p^2/2m + \beta V + V^2/\ 2mc^2 - E^2/2mc^2 + (\underline{\alpha}\cdot\underline{p},\ V)_+/2mc \quad (2.9)$$
Karwowski and Kobus (1981, 1985)	Uses an approximate Darwin + spin-orbit term $B^{-1}VCr^{-2}$ (C = constant, B as in eq. (2.6).
Heully (1982)	A second-order equation for Zeeman and magnetic hyperfine effects.
Schwarz and Wallmeier (1981)	A transformed Dirac Hamiltonian for LCAO calculations.
Baylis and Peel (1983, 1984)	A rediscovery of the H_D^2 of Wallmeier and Kutzelnigg (1981).

Table 2.2. (continued).

Reference	Comments
Wallmeier and Kutzelnigg (1983)	A "forth-back free-particle FW transformation" tested on H_2^+, He, Be.
Davenport (1984)	Uses the Koelling-Harmon (1977) expression.
Kutzelnigg (1984)	A critical review of various transformed Dirac equations for LCAO calculations.
Laaksonen and Grant (1984ab)	Two-dimensional, fully numerical ("2D") solutions of the second order Dirac equation $\{- c^2 B^{-1}\nabla^2 - c^2(\nabla(B^{-1})\nabla + V - E\}\psi^L = 0$ (2.10) for H_2^+ and the DF model of H_2 and HeH^+.
Almlöf et al. (1985)	Hydrogen atom with free-particle projections.
Karwowski and Kobus (1985)	A comparative study of quasirelativistic equations.
Dyall et al. (1984a-c); J. Wood (1985)	LCAO implementation of eq. (2.10).

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

Reference	Comments
Breit (1928)	The g-factor.
Darwin (1928)	Analytical solution for bound states.
Gordon (1928a)	Analytical solution for bound states.
Mott (1929, 1932)	Scattering.
Bechert (1930)	Normalisation factors. Transition probabilities.
Breit (1930a)	Magnetic dipole hyperfine integrals.
Sauter (1931b)	Use in K-shell photoeffect.
White (1931)	Pictures for $1/2 \leqslant j \leqslant 7/2$.
Furry (1934)	Approximate continuum functions. See also Sommerfeld and Maue (1935).
Bechert and Meixner (1935)	A spin-free 1/2m term discovered, see Froelich and Pilkuhn (1984)
Massey and Burhop (1935)	Auger effect treated with Coulomb functions.
Bargmann (1936)	The Fock symmetry.
Fock (1936)	The O(4) symmetry at the n.r. limit.
Lowen (1937)	Nuclear motion.
Rose (1937)	Continuum states.
Hoyle (1938)	Use in the nuclear beta decay.
Davis (1939)	Radial functions for bound states expressed through Laguerre polynomials.
Lin (1941)	Normalization factors simplified.
Sommerfeld (1941)	Searches for non-Coulomb interactions.
Christy and Keller (1942)	Fine structure with 1st-order el.-el. interaction.
Conway (1948)	Solution using quaternions.
McKinley and Feshbach (1948)	Coulomb scattering of relativistic electrons by nuclei.
Rose et al. (1952)	Uses the Coulomb function to discuss internal conversion.
Hylleraas (1955)	Uses Laguerre functions.
Brown (1950)	Hyperfine integrals proportional to $\langle r^{-2} \rangle$.
Johnson and Lippmann (1950b)	An integral of motion.
Levy (1950)	Momentum-space solution.
Rose (1951)	Incorporates finite-nucleus effects.
Lamb (1952)	Fine structure in the presence of magnetic fields.
Levinger (1952)	X-ray scattering factors for 1s electrons.
Levinger and Rustgi (1956); Levinger et al. (1957)	Dipole sum rule.
Payne and Levinger (1956)	Oscillator strengths for a K shell.
Grant (1957)	Oscillator strengths for a K shell.
Inokuti and Usui (1957)	Magnetic dipole hyperfine integrals for s-states.
Gorshkov (1961)	Perturbation theory.
Gorshkov (1964)	Coulomb functions.
Hostler (1964)	Coulomb Green functions.

Table 2.3. (continued).

Johnson et al. (1964)	Use in positron annihilation.
Garstang and Mayers (1966)	$\langle r \rangle$ and $\langle r^2 \rangle$ calculated. Screening constants discussed.
Burke and Grant (1967)	Pictures of radial distributions for Z=80.
Coulson and Joseph (1967)	Kepler problem in n dimensions.
Denti (1968)	Screening factors for many-electron atoms.
Powell (1968)	Qualitative discussion of "Relativistic Quantum Chemistry".
Sandars (1968)	Electric dipole moment of a 1s hydrogenic system.
Bartlett and Power (1969)	Dipole polarisability for 1s (Z=1).
Dogliani and Bailey (1969)	Relativistic corrections to the Thomas-Kuhn sum rule.
Szabo (1969)	Pictures of angular distributions.
Gargaro and Onley (1970)	Matrix elements for radiative interaction.
Barbieri (1971)	Superstrong magnetic fields.
Crubellier and Feneuille (1971)	$\langle r^n \rangle$ and $\langle r^{-n} \rangle$ from a factorization method.
Pyykkoe and Pajanne (1971)	Magnetic dipole hyperfine integrals for s-states.
Feneuille and Crubellier (1972)	Quaternionic solutions in the presence of magnetic charges. Cp. Hautot (1972).
Scherr (1972)	Variational inclusion of Pauli terms.
Zon et al. (1972)	Coulomb Green function and polarisability.
Barut and Rasmussen (1973ab)	The H atom as an elementary particle.
Carse and Walker (1973)	Electron scattering.
Latvamaa et al. (1973)	Second-order magnetic hyperfine effects.
Lindgren and Rosen (1973)	Electric and magnetic hyperfine integrals.
Manakov et al. (1973)	Coulomb Green function in momentum space
Pyykkoe et al. (1973)	Electric and magnetic hyperfine integrals.
Barut and Bornzin (1974)	Dynamical group for the Dirac-Coulomb problem.
Manakov et al. (1974)	Stark effect on hyperfine levels.
Manakov et al. (1974b)	Electromagnetic susceptibilities.
Walker (1974)	Electron-impact ionization.
Douglas (1975)	Magnetic hyperfine residual $(8\nu_{2s}-\nu_{1s})/\nu_{1s}$.
Glasser and Kaplan (1975)	"Superstrong magnetic fields"; see Lindgren and Virtamo (1979)
Edmonds (1975, 1978a)	Reformulation.
Kalf et al. (1975)	Spectral theory.
Moore and Moss (1975,1976)	Second-order magnetic hyperfine effects.
Moses (1975)	EM matrix elements.
Younger and Weiss (1975)	Transition probabilities.
Aashamar and Kocbach (1976)	K-shell ionization induced by protons.
Corben and Honig (1976, (1978)	Possible bound states for repulsive point Coulomb potentials with $118<Z<138$. See also Brysk and Zweifel (1981).

Table 2.3. (continued)

Epstein (1976)	A differential equation for the energy eigenvalues.
Manakov and Zapryagaev (1976)	Second-order Zeeman effect with Coulomb Green function.
Zapryagaev and Manakov (1976)	The Coulomb Green function applied to 2nd order hfs, quadratic Stark effect, oscillator strength sums and hyperpolarisabilities.
Curtis (1977)	Z expansion.
Kaneko (1977)	Multipole polarisabilities and shielding factors.
Lin et al. (1977)	Relativistic correction factors for E1 transitions.
Ranada (1977)	Non-linear terms added, to describe nuclear effects.
Angelie and Deutsch (1978)	Superstrong magnetic fields.
Auvil and Brown (1978)	An alternative, analytical solution.
Komarov and Novikov (1978)	Momentum-space representation.
Ong and Russek (1978)	Asymptotic (WKB) continuum solution.
Parthasaraty (1978)	Exact bounds for the Coulomb potential.
Sud and Sud (1978)	Asymptotic expansions for radial integrals.
Zapryagaev (1978)	Stark effect.
Gonsalves and Moss (1979b)	Hyperfine interaction.
Lindgren and Virtamo (1979); Virtamo and Lindgren (1979)	Strong magnetic field.
Moss and Trivedi (1979)	Approximate solutions using partitioning
Reitan (1979)	Electron or positron scattering.
Shinada (1979)	Strong magnetic field.
Tomishima (1979)	Points out errors in Moore (1975c-e), gives $\langle r^n \rangle$ to order α^2.
Waldenstroem (1979)	Solution of eq. (2.6). Quotes Dirac (1928a).
Zapryagaev (1979)	Zeeman effect.
Doman (1980)	Strong magnetic field.
Gruzdev and Sherstyuk (1980)	Effective-charge models for oscillator strengths.
Josephson (1980)	Interpretative.
S.K. Kim (1980)	Involutional transformations for Dirac-Coulomb waves.
Parker (1980)	Curved space-time. 1s, 2s, $2p_{1/2}$.
Savchenko (1980)	Zeeman effect.
Teodorescu (1980)	General relativistic effects.
Zapryagaev and Lavrinenko (1980)	Two-quantum transitions.
Brana and Ljolje (1981); Brana et al (1983)	Interaction with EM fields in a new formulation.
Burnap et al. (1981)	Strong Coulomb potentials.
Drake and Goldman (1981)	Discrete-basis-set solution.
Durgapal and Onley (1981)	Use of Coulomb waves in electron scattering.
Fischbach et al. (1981)	General relativistic effects.
Florescu (1981)	2s-2p excitation by proton impact.
Goldman and Drake (1981)	Two-photon decay of 2s states.

Table 2.3. (continued)

Gruzdev and Sherstyuk (1981)	Coulomb Green functions.
Klimchitskaya (1981)	Coulomb Green function and transition probabilities.
Mukoyama and Sarkadi (1981-1983)	Impact ionization from K- and L-shells.
Ranada and Uson (1981)	Non-linear, self-screening terms added.
Whittingham (1981)	Compton scattering.
Bodashko et al. (1982)	Coulomb Green functions for Breit corrections.
Cohen and Powers (1982)	A general relativistic hydrogen atom.
de Groot (1982)	Virial theorem.
Grant (1982)	Conditions for discrete-basis-set methods.
Gundersen et al.(1982)	Proton and deuteron deflection using hydrogenic wave functions.
Mukoyama (1982)	Momentum-space representation.
Ogata and Asai (1982)	Finite-nucleus effects. Application to Bremsstrahlung.
Parpia and Johnson (1982)	2E1 and M1 decay of 2s states, Z = 1-92.
Wong (1982)	Coulomb scattering.
Wong and Yeh (1982)	A simplified solution.
Yudin (1982)	Semiclassical theory of 1s-2s and 1s-2p excitations by charged particles.
Aleynikov and Klimchitskaya (1983)	"Quasi-energy levels" in alternating fields.
Areshidze and Klimchitskaya (1983)	"Quasi-energy levels" in alternating fields.
Baylis and Peel (1983,1984)	Squared Dirac operator in LCAO for 1s. See Wallmeier and Kutzelnigg (1983).
Berrondo and Recamier (1983)	Semiclassical approximation.
Briand et al. (1983, 1984b)	Spectra of hydrogen-like Kr and Ar.
Demkov et al. (1983)	Charge transfer processes, 1s - 1s.
Dul'yan and Kotsinyan (1983)	Transition probabilities due to another atom.
Gazdy (1983); Gazdy and Ladanyi (1984)	Discrete-basis-set solution.
Gol'braikh et al. (1983)	Electric polarisability.
Goldman and Drake (1983b)	Electric polarisability.
Hostler (1983, 1985)	Coulomb Green function.
Kagawa (1983)	Discrete-basis solutions for s, p and d states using a "general variation method".
Lombardi (1983)	Momentum-space representation.
Ruijgrok et al. (1983)	Interaction with a magnetic monopole.
Starchenko and Faustov (1983)	Contribution from weak interactions to hfs.
Wong and Yeh (1983a)	Zeeman and Stark effects.
Wong and Yeh (1983b)	Interaction with external fields and radiation.
Aleynikov et al. (1984)	"Quasi-energy levels" in alternating fields.
Areshidze and Klimchitskaya (1984)	"Quasi-energy levels" in alternating fields.
Barut and Gerry (1984)	Scattering states for the relativistic Kepler problem.

Table 2.3. (continued)

Bergeman (1984)	Enhanced ionisation rates at Stark-level crossings.
Dyall et al. (1984a-c)	Discrete-basis-set solution.
Hylton (1984)	Coulomb Green function.
Humphries and Moiseiwitsch (1984, 1985ab)	Electron capture between bare nuclei, Z_1 and Z_2.
Ishikawa (1984); Ishikawa et al. (1985abc)	Discrete-basis-set solution.
Kayed and Inomata (1984)	Path-integral solution.
Malli (1984)	Use as basis functions for molecules.
Shabaev (1984a)	Recurrence formulae for radial integrals.
Shabaev (1984b)	Coulomb Green functions for finite nuclei.
Shabaev (1984c)	Hyperfine structure.
Sheth (1984a)	Ionization by proton collisions.
Sheth (1984b)	Momentum-space representation.
Stanton and Havriliak (1984)	Variational safety in LCAO. 1s, $2p^*$, 2p.
Talukdar et al. (1984)	Momentum-space representation.
Xu (1984)	Energy levels by the spinor method.
Xu and Xu (1984)	General relativistic effects.
Aerts and Nieuwpoort (1985)	Discrete-basis-set solution.
Almloef et al. (1985)	Uses Sucher's projection operators for 1s states. Large deviations from the exact Dirac result.
Baryshevskii et al. (1985)	Quadrupole moment of the $2P_{1/2}$ state.
Bessis et al. (1985)	$\langle r^n \rangle$ in closed form.
Capri and Ferrari (1985)	A 1D Dirac-Coulomb problem has no bound states (resembles the Klein paradox).
Drachman (1985)	Multipole polarisabilities.
Goldman (1985ab)	Discrete-basis solutions without spurious roots.
Hess (1985)	1s (Z = 1...69) using Sucher's projection operators.
Komarov and Romanova (1985)	Discrete-basis-set solution.
A.A. Levy (1985)	New, fast solution, comparison with Klein-Gordon, Schroedinger.
Mukoyama (1985)	1s-2s excitation by heavy charged particles.
Quiney et al. (1985)	"Wrong Z" as a perturbation.
Raspini (1985)	Zeeman effect.
Su (1985)	A simplified analytical solution for bound and continuum states. Also n.r. and WKB approximations.
Sukumar (1985)	Supersymmetry.
Wong and Yeh (1985)	Coulomb Green function and Rayleigh scattering.
Wood et al. (1985)	Discrete-basis solution with a partitioning technique.
Wunner et al. (1985)	Spin-orbit anticrossings in magnetic fields. For a summary of the (mostly n.r.) work on H in magnetic fields, see Hansen and Oestgaard, Can. J. Phys. 63 (1985) 1022.

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

Reference	Comments
Darwin (1928c)	Diffraction.
Dirac (1928b)	A constant magnetic field.
Rabi (1928)	A constant magnetic field.
Klein (1929)	Potential step; "Klein paradox".
Plesset (1930)	Magnetic fields.
Nikolsky (1930)	Harmonic oscillator.
Huff (1931)	Magnetic fields.
Racah (1931ab, 1932)	Relativistic corrections to magnetic hyperfine interactions.
Sauter (1931)	Homogeneous electric field.
Sauter (1931c)	$V = V_0 \tanh(ax/2)$: the Klein paradox.
Szczeniowski (1931)	Homogeneous **E**.
Laporte (1932)	Magnetic field.
Plesset (1932)	Several simple fields.
Rosenthal and Breit (1932)	Finite-nucleus corrections to hyperfine interactions.
Wolkow (1935)	The field of an electromagnetic wave.
Heisenberg and Euler (1936)	Particle creation by a strong, infinite, homogeneous **E**.
L.I. Schiff et al. (1940)	A deep well.
Hund (1941, 1954)	Interpretation of the Klein paradox.
Massey and Mohr (1941)	Spherical well. Also scattering from n.r. Hartree fields for Kr, Xe, Au.
Pomeranchuk and Smorodinsky (1945)	Field of a finite nucleus (R = 8 fm, Z = 175) crosses $-2mc^2$.
Harish-Chandra (1948)	Magnetic monopole.
Breit and Brown (1949)	Perturbation methods.
K.M. Case (1950)	Attempts a solution for $Z > 137$ by assuming certain phases. See Greiner et al. (1985, p. 449.
Johnson and Lippmann (1950a)	Magnetic field.
Levy (1950)	Momentum-space solutions; the Yukawa potential.
Reitz (1950)	Numerical solution for a TF potential.
Acheson (1951)	Finite-nuclear-size effects on elastic scattering.
Dalitz (1951)	Scattering from a Yukawa potential.
Rose and Newton (1951)	General properties for central fields.
Bodmer (1953)	Finite-nucleus effects and isotope shifts.
Fogel (1954)	Numerical solution for a Hellmann potential.
Yennie et al. (1954)	High-energy electrons inside a nucleus.
Case (1957)	Arbitrary EM fields.
Woods and Callaway (1957)	The Kronig-Penney potential.
Werner and Wheeler (1958)	Field of a finite nucleus, $Z > 170$.
Prats and Toll (1959)	Construction of V from phase shifts and bound states.
Titchmarsh (1961)	$V=a\|x\|$.
Prosser (1963)	Scattering from a potential.

Table 2.4. (continued)

Shirley (1964)	Relativistic corrections for Moessbauer isomer shifts.
Matese and Johnson (1965)	Numerical solution for a screened Coulomb potential.
Mukherjee and Majumdar (1965)	Elastic scattering of high-energy electrons in a Sommerfeld-Maue approximation.
Redmond (1965)	A plane EM wave and a B, parallel to it.
Browne and Bauer (1966)	Scattering slow electrons in various atomic potentials.
Mande and Damle (1966)	Reproduces spin-orbit splittings by a screening parameter.
Coulson and Joseph (1967)	Kepler problem in n dimensions.
Mukherjee (1967)	Multiple scattering of high-energy Dirac particles from a TF potential.
Sen Gupta (1967)	Two beams of EM radiation.
Stanciu (1967)	$B_z(y) = B_0 \operatorname{sech}^2 (ay)$.
Wold (1967)	Effect of nuclear quadrupole moment on radial wave functions.
Davison and Steslicka (1969, 1971)	Surface states for Kronig-Penney potentials.
Pieper and Greiner (1969)	Bound states for a spherical well (cp. Massey and Mohr (1941)), and for the field of a homogeneous charged sphere, Z = 90-250.
Swamy (1969)	Exact solution for an equivalent oscillator potential.
Berrondo and McIntosh (1970)	Symmetries for combined electric and magnetic Coulomb potentials.
Glasser and Davison (1970); Glasser (1983)	Kronig-Penney model.
Crowther and ter Haar (1971a)	EM fields.
Darewych et al. (1971)	Numerical solutions in an analytical, screened Coulomb potential.
Dosch et al. (1971)	$V(x) = V_0 [\Theta(-x)/(1+\exp(-a(x+L))) + \Theta(x)/(1+\exp(a(x-L)))]$, application on the Klein paradox.
Klapisch (1971)	Atomic model potentials.
Subramanian and Bhagwat (1971,1972)	Tamm surface states for a Kronig-Penney delta-function potential.
Feneuille and Crubellier (1972)	Coulomb field plus magnetic charges.
Fisher (1972)	The Thomas precession.
Hautot (1972)	Magnetic fields.
Koenig (1972)	Atomic model potentials.
B.Mueller et al. (1972ab)	Fields of a finite nucleus.
Rosenberg and Stroke (1972)	Finite-nucleus corrections to hyperfine interaction.
Fairbairn et al. (1973)	Surface states in a Kronig-Penney model.
Soff et al. (1973)	Mixed scalar and vector potentials (both a/r).
Chatterjee and Chatterjee (1974)	Quantum defects and pseudopotentials.
Guillot and Schmidt (1974)	Spectral and scattering theory for the Dirac operator.

Table 2.4. (continued).

Sokolov and Ternov (1974)	Particle accelerators etc.
Felber and Marburger (1975)	An EM wave in an isotropic medium, a screw-symmetric $\underline{B}$, a rotating uniform $\underline{E}$.
Kalf et al. (1975)	Spectral theory for singular potentials.
Swamy and Chaffin (1975)	Exact solution for an equivalent oscillator in cylindrical coordinates.
Avron and Grossmann (1976)	Kronig-Penney model.
Barut and Krauss (1976)	Coulomb potential plus electron anomalous moment.
Critchfield (1976)	Scalar potentials proportional to r and r^{-1}.
Fano et al. (1976)	Phase shifts due to the mass-velocity term.
Kandilarov and Detcheva (1976)	Kronig-Penney model.
Narozhnyi and Nikishov (1976)	Constant **E** and an EM wave along it.
Chernoff (1977)	Singular potentials.
Cornwall (1977)	A general potential.
McEnnan et al. (1977)	Analytical, perturbation solution for a screened Coulomb potential.
Melnikoff and Zimerman (1977)	A combination of Coulomb-like and Lorentz-like potentials with SU(2) symmetry.
Pearson (1977)	Scattering theory for highly simgular potentials.
Weaver (1977)	Constant magnetic field.
Zilitis (1977ab,1981)	Relation between quantum defects and phase shifts.
Banarjee and Chakravorty (1978)	Scattering solutions for $V=-V_0(1/r-1/a)$, r<a.
Gesztesy and Pittner (1978)	Logarithmic potentials.
Kupersztych (1978, 1979)	EM waves.
Nandi and Chatterjee (1978)	An analytically soluble parametrized potential for s,p,d electrons, Z=20...83.
Rafelski (1978)	Bound states in various external fields.
Schwebel (1978)	Exact solution for Coulomb field+interaction terms reproducing the Lamb shift.
Zilitis (1978)	Coulomb field + polarisability terms.
Aharonov and Casher (1979)	Magnetic field.
Calucci (1979)	A linear potential.
Friar (1979)	Approximate wave functions for finite nuclei.
Kulkarni and Sharma (1979)	Electric and magnetic fields as Kratzer potentials.
Mottola (1979)	Normalizable solutions in the field of a magnetic monopole.
Nieto and Simmons (1979)	Limiting spectra from confining potentials.
Au and Rogers (1980)	"Scalar" fields as perturbations.
Bergou and Varro (1980, 1981)	EM waves.
Bunaciu et al. (1980, 1981)	Nuclear, internal conversion for screened Coulomb potentials.

Table 2.4. (continued)

Filipowicz (1980)	A quantized EM wave.
Gruzdev and Sherstyuk (1980, 1981)	Green's functions for non-local potentials.
Lavrov and Flesher (1980)	Green's functions for constant fields.
Bergou and Varro (1981)	A free electron and an EM wave.
Brysk and Zweifel (1981)	Possible bound states of repulsive potentials.
Freeman II (1981)	General relativistic effects.
Kalf (1981)	Non-existence of eigenvalues proven for potentials, other than Coulomb!
Karwowski and Kobus (1981)	A parameterised QR equation.
Kim and Noz (1981)	Harmonic oscillators and sympletic groups.
Ram and Arafah (1981)	Scalar potentials, $[\underline{\alpha}\cdot p+\beta m(r)-E]\psi=0$.
Rogers (1981)	Yukawa potential parameters for Z<55 to match IP_1 (exp.).
Sutherland and Mattis (1981)	Ambiguities with δ-function potentials.
Ternov et al. (1981)	Orthogonal **E** and **B**. Exact.
Thaller (1981)	Scattering from a potential.
Au (1982)	"Scalar" fields as perturbations.
Bagrov et al. (1982)	A review of all exactly soluble problems including crossed EM fields and relativistic coherent states.
Bloch (1982)	Magnetic field.
Cook (1982)	Separable solutions.
Friar and Wallace (1982)	Partial-wave representations for potential scattering of ultrarelativistic Dirac particles.
Kalckar et al. (1982)	A "Moeller box".
Khoklov (1982, 1983)	Green functions for special EM fields.
Koide (1982)	Exact solution for a spherical square-well. Cp. Pieper and Greiner (1969).
Ogata and Asai (1982)	Finite-nucleus effects.
Ram (1982)	A linear potential in K-G, Dirac. Will leak.
Roy (1982)	Disordered system of finite wells.
Achuthan and Benjamin (1983)	$E_z=E/(1-az)^2$.
Achuthan and Benjamin (1983b)	Inhomogeneous magnetic field.
Barut and Beker (1983)	A 3D harmonic oscillator.
Bernabeu and Ericson (1983)	Nuclear polarisability potential in electronic and muonic atoms.
Buehring (1983)	Approximate solutions for Hulthen potentials.
Cabo and Perez Rojas (1983)	Uniform EM field.
Krause and Kleber (1983, 1985)	Time-dependent processes; positron production.
Lapidus (1983)	One-dimensional hydrogen atom.
Laville (1983)	Arbitrary EM field.
Marciano and Muzinich (1983)	t'Hooft-Polyakov monopole.
Ram amd Leon (1983)	Power-law potential.
Sharma et al. (1983)	General even-power potential.
Bagrov and Noskov (1984); Bagrov et al. (1985)	Various EM fields.
Bhargawa and Sharma (1984)	Oscillator-plus-anharmonic potential.

Table 2.4. (continued).

Davison et al. (1984)	Linear potential well.
Gazdy and Ladanyi (1984)	Discrete-basis solution for a Hulthen potential.
Glasser and Shawagfeh (1984)	Linear potential.
Mehta and Sharma (1984)	Linear potential.
Mehta and Sharma (1984b)	Two-channel scattering solutions for a general even-power potential.
Papp (1984)	Model potentials for quarks.
Rogers (1984)	Central field plus anomalous-magnetic-moment term.
Sergeev and Sherstyuk (1984)	Perturbation theory for a Yukawa potential.
Su and Zhang (1984)	A competing scalar confining potential and an electric field.
Capri and Ferrari (1985)	A 1D Dirac-Coulomb problem has no bound states (Klein paradox).
Filipowicz (1985)	Relativistic electron in a quantized plane wave.
Franklin and Intemann (1985ab)	Several potentials with a "saddle-point variational method".
Greiner et al. (1985)	Review. Solutions in supercritical fields, i.a. (See ch. 16.5.).
Gumbs (1985)	Chains of arbitrary delta-function potentials.
Hall (1985)	General central fields f(r/b).
Ishikawa et al. (1985b)	Hg^{79+} with a finite nuleus. LCAO.
Kaminski (1985)	A relativistic "Kroll-Watson formula" for electron scattering in a laser field
Karwowski and Kobus (1985)	A screened-Coulomb model for Th.
Khalilov and Peres-Fernandes (1985)	Exact solution for a pseudoscalar wave.
Nieto and Taylor (1985)	Application of "crossed **E** and **B**" on relativistic quantized Hall effect.
Pilkuhn (1985)	Cylindrically symmetric potentials.
Schaefer et al. (1985)	Magnetic monopoles and strong charges.
Schlueter (1985)	Methods for solving the 1-electron Dirac equation for various coordinate systems and potentials.
Spector and Lee (1985)	One-dimensional hydrogen atom.
Staruszkiewicz (1985)	Dirac's electric monopole.
Yonei (1985)	Approximate numerical solutions in a T-F field of Tomishima (1969).

Table 2.5. Relativistic virial theorems.

Reference	Comments
Fock (1930b)	Derives the relativistic virial theorems $c\langle \alpha \cdot p \rangle + \langle V \rangle = 0$ (2.11) $E = mc^2 \langle \beta \rangle$ (2.12)
Gupta (1931, 1932)	Derives $c\langle \alpha \cdot \pi \rangle = -\langle r \cdot F \rangle$ (2.13)
Rose and Welton (1952)	Rederives (2.11-2.12).
March (1953)	Generalises (2.11) for continuum states. a new term arises.
Novozhilov (1956)	Continuum states.
Carr (1957)	A general v.t. for the spin-other-orbit and Darwin terms in PT: $2\langle T \rangle + \langle V \rangle + 3\langle h_{soo} + h_d \rangle = 0$ (2.14)
Novozhilov (1957)	V.t. in QED.
Schechtman and Good (1957)	Includes external EM fields. A review.
Bahcall (1961)	V.t. for many Dirac electrons in a potential.
Rosen (1966)	V.t. in field theories.
Kim (1967)	Rederives (2.11-2.12).
Gallinar (1971)	Rediscovers (2.13).
McKinley (1971)	Discusses (2.11-2.13).
Rosicky and Mark (1975)	An α^2 approximation to (2.11-2.12).
Rafelski (1977)	V.t. for interacting fields.
Oganyan (1978)	V.t. and the spectral shift function.
Rafelski (1978) p. 444	Rederives (2.13) for eigenstates of h_D.
Wood and Boring (1978)	Rediscover (2.12).
de Groot (1982)	Rederives (2.12), uses for the H atom.
Brack (1983)	Rediscovers (2.11-2.12).
Datta (1984)	Connection with "constrained-component variation".
Papp (1984b)	V.t. for the KG equation.
Sucher (1984)	V.t. for no-pair equations.
Marc and McMillan (1985)	A review.

3. QUANTUM ELECTRODYNAMICAL EFFECTS

Table 3.1. Higher-order corrections: methods.

Reference	Comments
Darwin (1920)	A retarded Lagrangian.
Dirac (1927)	QED.
Klein (1927)	QED.
Breit (1929, 1930b, 1932, 1938)	Retardation effects.
Gaunt (1929ab)	The magnetic interaction.
Oppenheimer (1930ab)	QED.
Moeller (1931, 1932)	Electron-electron interaction.
Bethe and Fermi (1932)	Electron-electron interaction.
Dirac et al. (1932)	QED.
Fermi (1932)	QED.
Bohr and Rosenfeld (1933, 1950)	QED.
Weisskopf (1934)	Electron self-energy.
Serber (1935)	QED.
Uehling (1935)	A vacuum-polarization potential.
Hulme (1936)	Electron-electron interaction for bound electrons.
Bloch and Nordsieck (1937)	Radiation field of the electron.
Breit (1938)	Approximately relativistic equations.
Primakoff and Holstein (1939)	Many-particle interactions.
Bethe (1947)	The Lamb shift.
Breit and Brown (1948)	Nuclear motion effects.
Feynman (1948)	QED.
Welton (1948)	Effects of the EM field fluctuations.
Newton and Wigner (1949)	Localised states.
Schwinger (1949)	QED.
Gupta (1950)	Longitudinal photons in QED.
Nambu (1950)	Electron-electron interaction.
Brown and Ravenhall (1951)	Electron-electron interaction.
Furry (1951)	Bound states and scattering using hydrogen-like projection operators.
Gell-Mann and Low (1951)	Bound states in QED.
Ishidzu (1951)	Effects of nuclear motion on fine and hyperfine structure.
Salpeter and Bethe (1951)	The "Bethe-Salpeter" equation.
Brown (1952)	Electron-electron interaction.
Salpeter (1952)	Mass corrections.
Chraplyvy (1953ab)	Electron-electron interaction.
Salpeter (1953)	The Lamb shift.
Wichmann and Kroll (1954)	Vacuum polarization.
Barker and Glover (1955)	A reduction from 16 to 4 components for a two-fermion system.
Kaellen and Sabry (1955)	Fourth-order vacuum polarization.
Glover and Chraplyvy (1956)	Electron-electron interaction.

Table 3.1. (continued).

Wichmann and Kroll (1956)	Vacuum polarization.
Sucher (1957)	S-matrix formalism for level-shifts.
Källen (1958)	QED.
Brown et al. (1959)	Lamb shifts for heavy atoms.
Brown and Mayers (1959)	Application on Hg.
Taylor and Payne (1960)	Retardation and K-shell x-ray intensities.
Ladik (1961b, 1965)	Radiation terms for H_2.
MacFarlane (1963)	Two-particle equations.
Gupta (1964)	Particle-particle and particle-antiparticle interactions.
Cooper (1965ab)	Coefficients for electron-electron interaction.
Erickson and Yennie (1965)	Lamb shift.
Itoh (1965)	N.r. limit.
Kossakowski (1965)	N.r. limit.
Labzovskii (1967)	Improved Breit approximation.
Breitenberger (1968)	A pedagogical introduction to magnetic interactions.
Olsen (1968)	Applications of QED.
Brodsky and Primack (1969)	Foundations of EM interactions with composite systems.
Erickson (1969)	Review on the Lamb shift.
Grotch and Yennie (1969)	Relativistic effects of order m_1/m_2 included in the wave function.
Kroll (1969)	Survey of QED.
Appelquist and Brodsky (1970)	Fourth-order corrections to Lamb shift.
Brodsky and Drell (1970)	A status report on QED.
Faustov (1970)	Magnetic moment of the H atom.
Chanmugam and Schweber (1970)	Electromagnetic many-body forces.
Labzovskii (1970b)	Lamb shifts in heavy atoms.
Wadzinski (1970)	An atomic Hamiltonian.
Brodsky (1971)	A review.
Crowther and ter Haar (1971c)	N.r. limit of el.-el. interaction.
Erickson (1971)	Lamb shift.
Fricke (1971)	A vacuum fluctuation potential.
Grotch and Hegstrom (1971)	Hydrogenic atoms in magnetic fields.
Mann and Johnson (1971)	Electron-electron interaction.
Mittleman (1971)	Three-body interaction.
Blomqvist (1972)	Vacuum polarization in exotic atoms.
Lautrup et al. (1972)	Comparisons between QED and experiment reviewed.
Mittleman (1972, 1981)	Configuration-space Hamiltonian.
Drake (1973)	Radiative decay of metastable states of the H and He sequences.
Grotch and Hegstrom(1973ab)	g-factors of many-electron atoms.
Klarsfeld and Maquet (1973)	Bethe sums for higher states (n = 1-7, Z = 1).
Kovalevskii and Labzovskii (1974)	Vacuum polarization.

Table 3.1. (continued).

Krajcik and Foldy (1974)	Composite systems.
Mohr (1974-1983)	QED effects in one-electron atoms.
Lewis and Hughes (1975)	Zeeman effect in two-electron systems.
Coester and Havas (1976)	Approximately relativistic Hamiltonians for interacting particles.
Dalgaard (1976)	Variational derivation of the Breit interaction.
Fullerton and Rinker (1976)	Vacuum polarization.
Grant and Pyper (1976)	The Breit interaction.
Huang (1976)	Vacuum-polarization potential.
Ruijgrok (1976)	A hydrogenic-atom model.
Braun and Shirokov (1977, 1981)	Energy levels and transition propabilities.
Braun and Sibirkina (1977)	Ground-state energies: radiative corrections.
Brodsky and Mohr (1977)	QED in strong fields.
Dankwort (1977)	Orbit-orbit interaction.
Detrich and Roothaan (1977, 1983)	Rederivation of the Breit interaction.
Gorelick and Grotch (1977,	One-body Dirac eq. from the Bethe-Salpeter eq.
Gorshkov et al. (1977)	Consequences of electron-electron weak interactions in atoms and ions.
Lin (1977ab)	N.r. limit for transition operators.
McEnnan and Gavrila (1977)	Radiative corrections to atomic photoeffect (hydrogenic 1s).
Rai and Ladik (1977)	Three-electron Breit-type interaction. (cp. Primakoff and Holstein (1939), Chanmugam and Schweber (1970), Mittleman (1971)).
Reinhardt and Greiner (1977)	QED of strong fields.
Barbieri and Remiddi (1978)	Solution of the Bethe-Salpeter equation for positronium.
Buchmueller (1978, 1980); Buchmueller and Dietz (1980)	Bound states in QED.
Caswell and Lepage (1978)	Reduction of the Bethe-Salpeter equation.
Ermolaev (1978)	QED effects in atomic spectra.
Leiter (1978)	Electron-electron interaction.
Marrus and Mohr (1978)	Forbidden transitions in one- and two-electron atoms.
Moore (1978, 1980)	Electron-electron interaction.
Rafelski (1978), Rafelski et al. (1978)	Bound states in external fields.
Reuse (1978)	A model for the hydrogen atom.
Huang (1979ab, 1980b); Huang and Starace (1978)	Evaluation of electron-electron interaction.
Reiss (1979)	Gauge in QED.
Sebastian (1979-1984); Sebastian and Yun (1979)	Interaction of a bound system with an EM field.
Vasil'ev and Kitanin(1979)	Renormalization of divergencies for partially filled shells.

Table 3.1. (continued)

Zemach (1979)	Quantitative properties of two-body wave equations.
Friar (1980a)	Discusses retardation operators.
Grant and McKenzie (1980)	The transverse electron-electron interaction.
Hiller et al. (1980)	Parity-violation.
Hillery and Mohr (1980)	Decay of hydrogen-like atoms in an electric field.
Sucher (1980-1984)	Foundations of atomic theory.
Kent et al. (1981)	Evaluation of various spin-orbit matrix elements using unitary groups.
Borie (1981)	Nuclear-size effects on the Lamb shift.
Sapirstein (1981)	High-order binding corrections to the Lamb shift.
Timofeeva and Labzovskii (1981)	Adiabatic S-matrix theory.
Bessis et al. (1982)	General relativistic effects.
Childers (1982)	Two-body equation for quarks.
Godefroid (1982)	Mutual spin-orbit matrix elements.
Gorshkov et al. (1982)	Parity non-conservation in polyatomic molecules.
Gross (1982ab, 1984)	Two-body and few-body problems.
Grotch and Sebastian (1982)	Magnetic dipole transitions.
Krizan (1982)	N.r. limit for a particle moving in a medium.
Kryuchov (1982)	Atoms in strong EM fields.
Martinis and Pilkuhn (1982)	Rydberg states for nuclei with spin.
Perdew and Cole (1982)	Local-density approximation for the Breit interaction.
Pilkuhn (1982, 1984)	New relativistic two-body equations for arbitrary masses, spins and EM moments.
Rosicky (1982b)	Electron-electron interaction in LCAO calculations.
Soff et al. (1982)	K-shell self-energy, up to Z=170.
Steinmann (1982)	1/c expansions in QED. Application on positronium.
Weinhold (1982)	Breit-Pauli corrections to the polarisability of ^{4}He.
Barut and Kraus (1983, 1984)	The Lamb shift.
Bhatt et al. (1983)	Compton scattering.
Borie (1983)	Vacuum polarization in antiprotonic atoms.
Crater and Van Alstine (1983)	Two-body equations.
Erickson (1983)	Status of QED precision.
Goldman and Drake (1983a)	The Bethe logarithm for two-electron ions.
Grotch et al. (1983)	Compton scattering.
Lev (1983)	Three-body problems.
Melibaev (1983)	Non-conservation of parity in x-ray spectra.
Melrose and Parle (1983ab)	QED in strong magnetic fields.

Table 3.1. (continued).

Neghabian (1983)	Vacuum polarization in strong Coulomb fields.
Neghabian and Gloeckle (1983)	Derivation of a potential from QED.
Olson and Miller (1983)	Electron-electron interaction.
Pyper (1983c)	The Breit interaction in external magnetic fields.
Riordan (1983)	"Hydrodynamic" equations for external fields.
Soff et al. (1983)	QED in high-Z systems.
Timofeeva (1983)	Level widths.
Dupont-Roc and Cohen-Tannoudji (1984)	Effective Hamiltonian approach to g-2.
Feldman and Fulton (1984)	Theory for radiative transitions.
Froehlich and Pilkuhn (1984)	Recoil corrections to the Uehling potential.
Goldman (1984)	A new approach for the Bethe logarithm.
Krolikowski (1984ab)	Electron-electron interaction.
Suarez (1984)	Feynman path integrals.
Bakalov et al. (1985)	The Hamiltonian of dd and dt .
Barut and Komy (1985)	Two-body equations in QED.
Barut and Uenal (1985)	Two-fermion equations with the most general electric and magnetic potentials.
Barut and van Huele (1985)	QED based on self energy: the Lamb shift.
Bhatt and Grotch (1985)	Recoil contributions to the Lamb shift.
Campbell (1985)	QED for Z > 170.
Dietz (1985)	The "g-Hartree" method.
Drake (1985b)	QED and heavy atoms: a summary.
Eschrig et al. (1985)	Density-functional approach to QED effects.
Giebink (1985)	Construction of 1-, 2- and 3-particle wave functions.
Greiner et al. (1985)	QED in high-Z systems: a review.
Hardekopf and Sucher (1985)	Vacuum breakdown in QED.
Hata et al. (1985)	Effect of the electron anomalous magnetic moment on fine structure.
Haywood and Morgan (1985)	Discrete basis methods for Bethe logarithms.
Hylton (1985)	Finite-nucleus corrections to the Ueling potential.
Janregui and Berrondo (1985)	"Minimal QED".
Kelly and Kim (1985)	Proceedings of a workshop on relativistic and QED effects in heavy atoms.
Mohr (1985)	QED of 1- and 2-electron atoms.
Sapirstein (1985)	Progress report on QED.
Schlueter (1985)	QED of strong fields.
Sucher (1985)	A simple model for the "continuum dissolution".
Zygelman and Mittleman (1985)	QED 3-body potentials in heavy atoms.

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

Reference	Comments
Breit and Meyerott (1947)	Nuclear motion corrections.
Brown and Arfken (1949)	Finite nucleus effects on nuclear-motion corrections.
Brodsky and Erickson (1966)	Radiative contributions for H-like atoms.
Faustov (1966)	Influence of proton structure.
Hegstrom (1969)	Shielding effects.
Iddings (1969)	Ground states of one-electron atoms.
Grotch (1970ab)	g-factors of hydrogen-like atoms in 1s states.
Hegstrom (1973)	Nuclear-mass and anomalous-moment corrections.
Douglas (1975)	The hyperfine residual $(8\nu_{2s} - \nu_{1s})/\nu_{1s}$.
Lepage (1977); Caswell and Lepage (1979)	Positronium and muonium hfs.
Bodwin and Yennie (1978)	Positronium and muonium hfs: a review.
Sapirstein (1983); Sapirstein et al. (1983)	Binding and recoil corrections.
Fischbach and Nakagawa (1984)	Apparatus dependent contributions to g-2.
Sapirstein (1984); Sapirstein et al. (1984)	Muonium and positronium hyperfine splitting.

Table 3.3. Higher-order corrections: energy levels.

Reference	Comments
Sessler and Foley (1955)	He.
Sucher and Foley (1955); Sucher (1958)	He.
Araki (1957)	He.
Kabir and Salpeter (1957)	He.
Pekeris (1958)	He.
Araki et al. (1959)	He.
Dalgarno and Stewart (1960b)	The Lamb shift of He.
Schiff et al. (1965, 1973)	He-like systems.
Garcia (1966)	H
Suh and Zaidi (1966)	$2^{1,3}S$ states of He.
Desiderio and Johnson (1971)	Lamb shift for K electrons in heavy atoms.
Fricke et al. (1972)	Ionization potentials of Fm.
Hambro (1972)	He.
Douglas and Kroll (1974)	Energy levels of helium.
Ermolaev (1973, 1975); Ermolaev and Jones (1974)	Two-electron ions.
Stroscio (1975)	A review on positronium.
Bishop (1976, 1977); Bishop and Cheung (1978-1981)	H_2^+ and H_2.
Erickson (1977)	One-electron atoms.
Gould and Marrus (1978)	Hydrogen-like argon.
Lewis and Serafino (1978)	He.
Drake (1979, 1982ab, 1983ab)	Few-electron systems.
Driker et al. (1981, 1983)	Vacuum polarization for heavy hydrogen-like ions.
Neumann (1981)	He-like systems.
Berry et al. (1982)	Two-electron systems.
Drawin (1982)	Highly ionised atoms.
Briand et al. (1983)	H-like and He-like Ar.
Ermolaev and Swainson (1983)	Two-electron ions.
Goldman and Drake (1983a)	Ground state Lamb shift of two-electron ions.
Au et al. (1984)	Retardation effects on He Rydberg states. n = 9-12, Z = 2...70.
Briand et al. (1984)	He-like Fe.
Briand et al. (1984b)	H-like and He-like Kr.
Goldman and Drake (1984); Goldman (1984)	Two-electron systems.
Hata (1984a-c); Hata and Grant (1981-1984b)	Two-electron systems.
Drake (1985)	He-like U.
Drake and Makowski (1985)	Two-electron QED for helium-like ions.
Ermolaev (1985)	S-states in 2-electron atoms.
Gould (1985)	Review on very heavy few-electron atoms.

Table 3.3. (continued).

Grant (1985)	He-like ions.
Johnson and Soff (1985)	Lamb shifts of hydrogen-like atoms, Z=1-110.
Karwowski and Styszynski (1985)	Ground-state energies of the He, Be. Ne series.
Mohr (1985a-c)	High-Z few-electron atoms.
Stamp (1985)	He-like systems.

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

Reference	Comments
Casimir and Polder (1948)	Retardation effects on London forces: $V = aR^{-7}$.
Dzyaloshinskii et al. (1961)	Review on van der Waals interactions.
Hirschfelder (1967)	A review.
Certain and Bruch (1972)	A review (see p. 119)
Varandas (1974)	The long-range coefficients W_4 and U_2.
Michels (1976)	Interaction of two H atoms.
Power (1978)	Retardation corrections.
Easa and Yousif (1982); Easa and Shukla (1983); Yousif and Easa (1982)	Long-range interactions between H, He, Li, Ne, Kr, Xe and N_2.
Fischbach and Nakagawa (1984)	Apparatus-dependent contributions.
Koga (1985)	Interaction of two ground-state H-atoms.

4. MULTIELECTRON ATOMS: METHODS

The general reviews, including ones on atoms, were already given in Table 1.1. The Table 4.1. below summarizes articles on general methods, especially angular-momentum coupling. Table 4.2. lists the published programs. The various numerical, four-component, all-electron SCF methods are included in Table 4.3., including the Dirac-Hartree ones without exchange and the Dirac-Fock (DF) and multiconfiguration, MCDF ones with full, non-local exchange as well as the random phase approximation (RPA) and other treatments of correlation. The corresponding LCAO approaches are discussed separately in Table 4.4. The various LDF (Local Density Functional) ones, including the Dirac-Slater (DS) model and the "mean-field theory" are summarized in Table 4.5. The simplest, Thomas-Fermi model is discussed separately in Table 4. 6. The independent-particle models, approximating the atomic mean field by a local one, are listed in Table 4.7.

Our usage of the terms pseudopotential and model potential is defined in Table 4.8. and the methods of this type are included in Table 4.9. A list of available relativistic effective potentials for various elements is given in Table 4.10.

The various "quasirelativistic", one-component approaches and perturbation ones are listed in Table 4.11. In Table 4.12. we give the 1/Z expansions and other similar calculations.

Relativistic calculations on nuclei fall outside the present review. For recent progress in this, active, field, see Chin (1977), Friar (1981), F. Gross (1982ab, 1984, 1985), Meyer (1983), Negele (1985) or Shepard et al. (1984, 1985).

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
Hartree (1928ab)	The Hartree Model.
Hartree (1929); Gaunt (1929b)	A Hartree (1928ab) model based on the Dirac equation.
Fock (1930)	Exchange.
Swirles (1935, 1936)	The DF equations.
Marvin (1947)	Spin-other-orbit and spin-spin energies.
Horie (1953)	Spin-spin and spin-otheer-orbit interactions.
Grant (1961, 1965, 1970, 1983b)	DF theory formulated using Racah algebra.
Cooper (1965ab)	Angular parts for electron-electron interaction.
Liberman et al. (1965)	The Dirac-Slater approach.
Braun and Labzovskii (1967)	Basic theory for relativistic atoms.
Malli (1968ab)	Evaluation of the Breit terms.
Braun et al. (1969); Labzovskii (1970a, 1978, 1983)	Basic theory for relativistic atoms.
Mayers (1970)	Open-shell DF.
Jones (1971)	Mutual spin-orbit and spin-spin interactions.
Mann and Johnson (1971)	Various forms of the Breit interaction.
Mittleman (1971, 1972, 1981)	Basic aspects of relativistic atomic calculations.
T.E.H. Walker (1971)	Orbit-orbit interactions.
Chang and Kelly (1972)	Continuum DF functions.
Mayers (1972)	A review on relativistic SCF calculations.
Merzbacher (1972)	A review on relativistic effects in atoms.
Odabasi (1972)	Combined CI and magnetic interactions.
Saxena et al. (1972)	Orbit-orbit interactions.
van der Eynde et al. (1972)	Matrix elements for the Breit-Pauli Hamiltonian.
Miller (1973)	Local representation of DF exchange.
Kichkin et al. (1974, 1975); Kichkin and Rudzikas (1974a-c); Rudzikas et al. (1976ab); Sivtsev et al. (1974, 1977); Sleptsov et al. (1975)	Matrix elements of the DF Hamiltonian.
Chang (1975)	Close-coupling equations for electron scattering.
Andriessen et al. (1976, 1977ab, 1978ab); Andriessen (1980)	Four component many-body techniques.
Grant et al. (1976)	The MCDF-AL ("average level") approach.

Table 4.1. (continued).

Larkins (1976)	Relativistic "LS multiplet energies".
Rudzikas et al. (1976ab); Rudzikas (1984); Rudzikas and Kaniauskas (1976)	Energy matrix elements for complex configurations.
Chang (1977ab)	R-matrix theory.
Dankwort (1977)	Orbit-orbit interaction.
Feneuille and Luc-Koenig (1977)	"Wave function" and operator" relativistic corrections not uniquely definied.
Koelling and Harmon (1977)	A spin-polarized QR LDF method.
Lin (1977b)	Gauge properties of HF and RPA approximations.
Huang (1978b)	Lagrangian multipliers for frozen-core calculations.
Calvert and Tuttle (1979)	jj-LS transformations for p^n, d^n, n>2.
Glass (1979b)	Spin-other-orbit and spin-spin interactions.
Huang (1979ab, 1980b); Huang and Starace (1978)	Graphical evaluation of matrix elemnets.
Driker and Ivanov (1980a)	Relativistic single-photon, two-photon and autoionization decay processes.
Grant and McKenzie (1980)	The transverse electron-electron interaction.
Sucher (1980-1985)	Foundations of relativistic atomic calculations.
Berry et al. (1981)	The foundations of relativistic atomic theory.
Eglais (1981)	Genealogical coefficients.
Pyper and Marketos (1981a, c); Pyper (1983a); Pyper et al. (1982a)	Fine structure splittings from MCDF and PT.
Dyall and Grant (1982)	Phase conventions, quasispin, and the jj-LS transformation coefficients.
Godefroid (1982)	Symmetry of mutual spin-orbit matrix elements.
Huang and Johnson (1982)	MC-RPA
Chang (1983)	Relativistic quantum defect theory. The close-coupling approximation.
Esser (1984ab)	Unitary-group approach to relativistic CI.
Fricke (1984)	A review.
Goldschmidt and Mallow (1984)	Magnetic interactions for $(nl)^N n'l'$ configurations.
Mitroy and Morrison (1984)	DF+large CI, using a Schmidt orthogonalized basis set.
Parpia (1984); Parpia and Johnson (1984)	The time-dependent local density approximation (TD LDA).
Simonis et al. (1984)	Isospin basis for relativistic calculations.
Dietz (1985)	The "g-Hartree" method.
Dyall (1985)	LS coupling using relativistic radial integrals.
Frye and Armstrong (1985)	"Liouville-Dirac-Fock Theory" for oscillator strengths and transition energies.

Table 4.1. (continued).

Grant (1985c)	Theory of many-electron atoms: a discussion summary.
Sucher (1985b)	"Healthy Hamiltonians" for many-electron atoms.
Zhao and Li (1985)	Configuration interaction theory. Excitation energies and radiative TP.

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 corrections are listed there.

Reference	Comments
Herman and Skillman (1963)	An HFS program with first-order Pauli corrections.
Klapisch (1971)	A parametric potential method.
Liberman et al. (1971)	A DS program.
Yates (1971)	Electron collisions with an arbitrary atomic potential. 2nd-order Dirac equation.
Grant (1972, 1973, 1976)	Angular-momentum coefficients for DF methods.
Chang (1974)	Reduced matrix elements of one-particle operators.
Eissner et al. (1974)	Breit-Pauli expectation values with numerical HF functions. Calculates radiative data.
Desclaux (1975, 1977)	A MCDF package.
Glass and Hibbert (1978)	Breit-Pauli operators in one-component calculations.
Pyper et al. (1978c)	Matrix elements of one-particle operators in jj-coupling.
Beatham et al. (1979b)	Angular coefficients for the Breit interaction.
Grant et al. (1980)	The Oxford MCDF package.
McKenzie et al. (1980)	The transverse Breit and QED corrections.
Bogdanovich (1982)	A DF program.
Dzuba et al. (1982b)	A DS/DF package, including a Sternheimer equation option.
Scott and Taylor (1982)	A Breit-Pauli model potential R-matrix program for atomic continuum processes.
Cook and Case (1983)	An $X\alpha$-program.
Liberman and Zangwill (1984)	Optical response with time-dependent LDF methods.
Cowan et al. (1985)	A combined MCDF and quasirelativistic HF package with automatic comparative output.
Pilipzuk and Pilipzuk (1985)	Electron scattering from atomic potentials with spin-orbit corrections.

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

Reference	Comments
Williams (1940)	A Dirac-Hartree approach for Cu^{+}.
Mayers (1957)	A Dirac-Hartree approach. Results for Hg.
Cohen (1960)	A Dirac-Hartree approach. Results for W, Pt, Hg, U.
Coulthard (1967ab)	A DF approach.
Smith and Johnson (1967)	A DF approach.
Mann (1969)	A DF approach.
Desclaux and Bessis (1970)	Spin-polarised DF calculations.
Desclaux et al. (1971a)	Numerical aspects of DF methods.
Desclaux et al. (1971b)	Implements the average-of-configuration DF method proposed by Mayers (1970).
Miller (1973)	A local representation of the DF potential for closed-shell approach.
Rosen (1973)	A DF approach.
Desclaux (1975, 1977)	MCDF calculations.
Grant et al. (1976)	The MCDF-AL ("average level") approach.
Johnson and Lin (1976-1979); Johnson et al. (1980);Shorer et al.(1977)	Relativistic random phase approximation.
Brattsev et al. (1977)	A DF approach.
Dzuba et al. (1982)	Semiclassical long-range behaviour of DF orbitals.
Huang and Johnson (1982)	MCRPA
Sasaki (1982)	An instruction manual for Desclaux (1975).
Desclaux (1983a)	A review of DF methods.
Grant (1983c)	Techniques for open-shell atoms.
Grant (1983d)	A review of DF methods.
Mayers and Turner (1984)	Evaluation of oscillatory wave functions on a logarithmic grid.
Mitroy and Morrison (1984)	A DF-CI approach, using single-particle states orthogonalised against the occupied DF ones.
Radojevic and Johnson (1985)	A multiconfiguration Tamm-Dancoff (MCTD) approximation.

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

Reference	Comments
Asaad (1960)	A variational fit of hydrogen-like functions for the $1s^2$ shell of Hg, using the Dirac Hamiltonian.
Synek (1964)	Formulates the DF-LCAO problem.
Kim (1967)	Closed-shell DF calculations.
Leclercq (1970)	The open-shell case formulated.
Kagawa (1975)	Open-shell atoms. Sc - Cu.
Picart (1975)	DF results, up to Kr.
Malli (1979)	Xe, using "spherical GTO" basis.
Rosicky and Mark (1979)	Minimal-basis STO DF with an approximate small component.
Datta (1980)	On avoiding variational collapse. Pb.
Kagawa (1980)	MCDF. O-like systems (Z = 8, 26, 80).
Ishikawa and Malli (1981a)	A recipe to avoid variational collapse.
Kulikova and Tupitsyn (1981)	He - Ar.
Kulikova et al. (1982)	U.
Lee and McLean (1982a); McLean and Lee (1982)	Ag^+, Au^+.
Matsuoka (1982)	Average-of-configuration results for He - Ne.
Solliec et al. (1982)	Ne, Ca.
Ishikawa et al. (1983, 1984)	Be.
Mukoyama and Kagawa (1983)	Momentum representation. Applications on Cu, Au.
Mukoyama and Kagawa(1983b)	Beta decay of W, Hg.
Trusov (1983)	Ground states of He-like systems, Z=2-8.
Esser (1984a)	DF + CI for ground and low-lying states of Hg and Pb.
Kutzelnigg (1984)	Review on methods to avoid the variational collapse.
Mukoyama and Kagawa (1984)	Radiative tansition rates. Applications on Cu - Au, W.
Wallmeier (1984)	He, Li, Be. DF using the squared Dirac operator.
Aerts and Nieuwpoort (1985b)	He, Be, C, Si, Ge, Sn. GTO.
Kagawa and Malli (1985)	Rare gases He - Rn.
Mark (1985)	Gaussian basis sets for H - Ne, and the H-, He- and Ne-like ions with Z = 50, 90.
Mark et al. (1985)	One-electron integrals over Gaussian lobes in a projected DF formalism.
Matsuoka et al. (1985)	"Kinetically balanced" calculations for Be, C, Ne, Ag, Hg.

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

Reference	Comments
Snow et al. (1964); Liberman et al (1965)	The DS approach.
Bhalla (1967-)	A DS approach.
Carlson et al. (1968-); Lu et al. (1971ab)	A DS approach.
Rosen and Lindgren (1968	A modified DS approach with a 3-parameter exchange potential.
Rozsnyai (1972)	Finite-temperature DS calculations.
Migdalek (1976a-e)	A Dirac-Hartree + partial statistical exchange scheme. Applications on oscillator strengths.
Chin (1977)	High-density matter.
Ellis (1977a)	A relativistic exchange potential.
Koelling and Harmon (1977)	Spin-polarized LDF theory.
Rajagopal (1978, 1985); Ramana (1981); Ramana and Rajagopal (1979-1983); Xu et al. (1984)	Relativistic inhomogeneous electron gas.
MacDonald and Vosko (1979); MacDonald (1983, 1984)	Relativistic LDF methods.
M.P. Das (1980-1983b); M.P. Das et al. (1980)	Applications of the relativistic exchange expression.
Migdalek and Baylis (1980, 1981b, 1984b)	Various LDF, applied to model-potential work.
Dreizler (1981); Dreizler and Gross (1983); Gross and Dreizler (1981, 1984, 1985)	Relativistic LDF methods.
Dietz et al. (1982ab) Dietz and Weymans (1984a-b); Connerade et al. (1984, 1985)	The "g-Hartree method" with a non-local exchange of parameterised strength.
Gollisch (1982, 1984)	An LDF model.
MacDonald (1983)	Spin-polarised electron gas.
Parpia and Johnson (1983ab) Parpia (1984), Parpia et al. (1984)	Time-dependent LD approximations.
Band et al. (1984)	Optimised for DS.
Liberman and Zangwill (1984)	A TD LDF program. Calculates static and dynamic polarisabilities and photoemission cross sections.
Mayol et al. (1984a)	A DS program.
Cortona et al. (1985); Doniach and Sommers (1981)	Spin-polarised LDF theory.
Eschrig et al. (1985)	Density functionals for QED terms.

Table 4.6. Thomas-Fermi calculations

Reference	Comments
Dirac (1930)	Exchange.
Vallarta and Rosen (1932)	The relativistic TF equations derived.
Jensen (1933)	The Vallarta-Rosen density is not normalizable for a point nucleus. Introduce a finite one.
Fermi and Amaldi (1934)	Solves the Dirac equation. Removes electron self-interaction. Important for anions.
Solomon (1934)	Discusses the difficulties near the origin.
Chandrasekhar (1935ab)	The relativistic TF equations derived from the KG one. See Plaskett (1953).
Kothari and Singh (1942)	Relativistic electron gas.
Gombas (1949)	Divergences near origin ascribed to quantum corrections. A Weizsaecker correction removes them.
Rudkjoebing (1952)	A TF model derived from the 2nd-order Dirac equation.
Scott (1952)	Introduces an empirical relativistic $Z^{9/2}$ correction to the energy.
Plaskett (1953)	A singularity-free (Z<137/2) version.
Gilvarry (1954)	Uses Rudkjoebing's density, proportional to $r^{-3/2}$.
Jancovici (1962)	Relativistic electron gas.
Tomishima (1969)	Introduces a modified Weizsaecker $(\nabla\rho)^2/\rho$ correction. The Darwin term is still missing.
Ashby and Holzman (1970)	The correct, Coulombic electron density near the nucleus used as TF boundary conditions.
Mueller and Rafelski (1975)	The charge in a superheavy collision system. Rediscover Vallarta-Rosen. $E_F=-2mc^2$.
Waber and Canfield (1975)	Numerical calculations using the Vallarta-Rosen or Gilvarry expressions.
Braun (1976)	Further variants.
Eletskii and Popov (1978)	The TF model for Z>137.
Rajagopal (1978, 1985); Ramana (1981); Ramana and Rajagopal (1979-1983)	Relativistic inhomogeneous electron gas.
Gross and Rafelski (1979, 1981)	Electromagnetic potentials.
Ferreirinho et al. (1980)	Rediscovers the Vallarta-Rosen model.
Mueller (1980)	Points out this.
Schwinger (1980)	Derives a relativistic correction δE/a.u.=-2.4 $10^{-6} Z^{9/2}$ from the sum of Dirac-Coulomb eigenvalues.

Table 4.6. (continued).

Dreizler (1981); Dreizler and Gross (1983), Gross and Dreizler (1981, 1984, 1985)	Relativistic density functionals of all kinds. Reviews earlier work.
Marconi and March (1981)	Scaling laws $E(Z, N, \alpha)$. Sums Dirac-Coulomb eigenvalues.
Ramana and Rajagopal(1981)	Role of the transverse photon-electron interaction.
Ruffini and Stella (1981)	Comments on Ferreirinho et al. (1980) and Mueller (1980)
Dmitrieva and Plindov (1982, 1983)	The leading relativistic correction terms.
Hill et al. (1984)	Variation of the chemical potential $\mu(Z, N_{el})$ studied and E_T compared with the DF one.
Boya et al. (1985)	Solution of the Vallarta-Rosen equations for a finite nucleus (Z=80).
Hill et al. (1985)	Extremely high magnetic fields.
March (1985)	Scaling properties of $E_T(Z, N)$ in d dimensions.
Senatore and March (1985)	Analytic properties of the relativistic TF equation.

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

Reference	Comments
Darewych et al. (1971)	An analytical potential for Z = 10, 20, ... 90.
Klapisch (1971); Klapisch et al. (1977)	A parametric potential method.
Gaspar and Erdos-Gyarmati (1972)	Introduces Pauli-level relativistic corrections to the "universal potential" of Gaspar. Li - Fr, He - Rn, C - Pb, Cu, Hg, U.
Koenig (1972); Luc-Koenig (1972-1980); Luc-Koenig and Bachelier (1978); Farrag et al. (1979-1982); Aymar and Luc-Koenig (1977); Bauche et al. (1982-1983)	A parametric potential method.
Gaspar and Erdos-Gyarmati (1976)	Dirac equation for the "universal potential" of Cu.
Driker and Ivanov (1978-); Driker et al. (1981-); Ivanov and Ivanova (1979)	A parametric potential method.
Nandi and Chatterjee (1978)	An analytically soluble, parametric potential for s, p and d electrons, Z = 20 ... 83.
Rogers (1981)	Effective potentials for Z<56.
Victor and Taylor (1983)	The Cu and Zn sequences, Z = 29-42.
Gurchumeliya et al. (1985)	Cu-like systems.
Ivanova et al. (1985)	Zn-like systems.

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

Definitions:	Concept	Definition
	Pseudopotential	Inner nodes in the wave function are omitted. May be local or non-local (different for different angular parts). A shape consistent or norm conserving pseudo wave function exactly reproduces the outer tail. First used by Fermi (1934).
	Model potential	An analytical approximation to an effective potential. First used by Heisenberg (1926).
Reviews	(Non-relativistic or empirical pseudopotentials):	
	Atoms:	Gombas (1967) Schwarz (1968); Chang et al. (1974) Bardsley (1974) Szasz (1985)
	Molecules:	Weeks et al. (1969) Kahn et al. (1976) Freed (1977) Barthelat and Durand (1978) Dixon and Robertson (1978) Szasz (1985) Topiol et al. (1981)
	Solids and Liquids:	Harrison (1966) Cohen and Heine (1970); Heine and Weaire (1970) Wiser and Greenfield (1971) Ziman (1971) Zunger (1979) M.L. Cohen (1982, 1984)
Summaries of relativistic pseudopotential work:		
		Y.S. Lee (1978) Bachelet et al. (1982) Hibbert (1982) Hay (1983) Ishikawa and Malli (1983) Pitzer (1983, 1984) Pyper (1983d) Kahn (1984) Krauss and Stevens (1984) Christiansen et al. (1985)

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
Fock et al. (1940)	The "strong orthogonality" condition (here required between core and valence functions).
Phillips and Kleinman (1959)	Theory for pseudopotentials.
Das and Wahl (1976)	Relativistic, non-local Phillips-Kleinman (1959) pseudopotentials derived from DF calculations.
Lee et al. (1977); Ermler et al. (1978); Lee (1978) Ermler et al. (1978)	Ditto.
Datta et al. (1978)	Ditto.
Hafner and Schwarz (1978a)	A relativistic pseudopotential fit to experimental data.
Kahn et al. (1978)	Non-local, quasirelativistic pseudo-potentials.
Christiansen et al. (1979)	(Non-relativistic) shape-consistent (="norm conserving") pseudopotentials. The Phillips-Kleinman ones shown to be inadequate for molecules. For a summary of earlier work on non-relativistic shape-consistent pseudopotentials by Durand and Barthelat in 1975, by Redondo, Goddard and McGill in 1977, by Hamann, Schlueter and Chiang in 1977 or by Zunger in 1979, see Kahn (1984, ch. 6 B).
Kleinman (1980)	Relativistic, norm conserving pseudo-potentials.
Pyper (1980a, 1981a, 1983d); Pyper and Marketos (1981b)	Analysis of the fundamentals of pseudo-potential methods.
Ermler et al. (1981); Stevens and Krauss (1982ab); Wadt (1982)	A non-local, $\|jm\rangle\langle jm\|$ pseudopotential for the spin-orbit splitting. See also the next reference.
Bachelet et al (1982); Bachelet and Schlueter (1982)	"Norm conserving" (="shape consistent") pseudopotentials for a local-density model. One-component average and a spin-orbit potential. Data given for Z =1-94.
Fuentealba (1982)	Introduce a radial, core-valence correlation potential, proportional to the electric dipole polarisability, α, of the core.
Jeung et al. (1982);	Ditto, with direction-dependent terms.

Table 4.9. (continued).

von Szentpaly et al. (1982)	For a detailed study of this (non-relativistic) problem, see W. Mueller and Meyer (1984), W. Mueller et al. (1984).
Victor and Taylor (1983)	Uses a DF core.
Ishikawa and Malli (1983)	A review on 4-component pseudo-potentials.
Andzelm et al. (1984)	Huzinaga-type one-component approach including nodes.

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

Z	Element	Approach	Reference	Remarks
Series:				
1-94	H - Pu	LD - SC	B82	SO
21-30	Sc - Zn	QR - SC	HW85a	Outermost spd shells
39-48	Y - Cd			
57, 72-80	La, Hf - Hg			
19-29	K - Cu	QR - SC	HW85b	Outermost core shells included
37-47	Rb - Ag			
55-57	Cs - La			
73-79	Hf - Au			
11-18	Na - Ar	QR - SC	WH85	Outermost sp shells.
19-20	K - Ca			
31-36	Ga - Kr			
37-38	Rb - Sr			
49-54	In - Xe			
55-56	Cs - Ba			
81-83	Tl - Bi			
3-18	Li - Ar	DF - SC	FC85	SO
4...56	Group 2.	E+DF+pol.	F85	
Individual elements:				
15	P	QR - SC	H84	
18	Ar	QR + SO	T83	
19	K	E	HS78, F83	
20	Ca	E	HS78	
		DF	IM81	A 4-component wave function.
26	Fe	QR	BP81	
29	Cu	E	HS78, F83	
		E + DF	S83	Includes a polarisability correction.
		QR	I85	
		QR - SC	B84	
30	Zn	E	HS78	

Table 4.10. (continued).

37	Rb	E	HS78, F83	
38	Sr	E	HS78	
		QR - SC	B85	
42	Mo	QR - SC	H83	Zn-like core.
46	Pd	DF	B80, B81	
		QR - SC	H81	
47	Ag	E	HS78, F83	
		QR	BP81	
		QR - SC	HM85	
		DF	K85	
		E + DF	S83	Includes a polarisability correction.
48	Cd	E	HS78	
49	In	QR + SO	BP81, T83	
50	Sn	QR	BP81	
51	Sb	QR	BP81	
53	I	QR	BP81	
54	Xe	QR	W78, A84	
		DF	E78	
		DF	L77	
55	Cs	E	HS78, F83	
		QR	LS81, J82	
		DF - SC	LWC83	5s5p6s valence space.
		DF	IM81	Four-components
56	Ba	E	HS78	
74	W	QR - SC	H84	
78	Pt	QR - SC	H81, NH82	
		DF	BT79, B80, BC83	
79	Au	QR	H78	
		E	HS78, F83	
		DF	L77, BT79, K85	
80	Hg	E	HS78	
		QR	H78	
		DF	BT779	
81	Tl	E	HS78	

Table 4.10. (continued).

		QR	BP81	
		DF	IM81	
82	Pb	QR	BP81	
83	Bi	QR	BP81	
		DF - SC	C84	5d6s5p valence space. SO.
88	Ra	E	HS78	
90	Th	QR - SC	W81	
92	U	QR	K78, H79	

References: A84 = Andzelm et al. (1984), B80 = Basch et al (1980), B81 = Basch (1981), B84 = Bagus et al. (1984), B85 = Bauschlicher et al. (1985a), BC83 = Basch and Cohen (1983), BP81 = Barthelat and Pelissier (1981), BT79 = Basch and Topiol (1979), C84 = Christiansen (1984), E78 = Ermler et al. (1978), F83 = Fuentealba et al. (1983), FC85 = Fernandez Pacios and Christiansen (1985), F85 = Fuentealba et al. (1985), H78 = Hay et al. (1978), H79 = Hay et al. (1979), H81 = Hay (1981), H83 = Hay, as quoted by Allison and Goddard (1983), H84 = Hay (1984), HM85 = Hay and Martin (1985), HW85ab = Hay and Wadt (1985ab), I85 = Illas et al. (1984, 1985), IM81 = Ishikawa and Malli (1981b), J82 + Jeung et al. (1982), K78 = Kahn et al. (1978), K85 = Krauss et al. (1985), L77 = Lee et al. (1977), LS81 = Laskowski and Stallcop (1981), LWC83 = Laskowski et al. (1983b), NH82 = Noell and Hay (1982, S83 = Stoll et al. (1983b), T83 = Teichteil et al. (1983), W78 = Wadt et al. (1978), W81 = Wadt (1981), WH85 = Wadt and Hay (1985).

Table 4.11. One-component and perturbation calculations.

Reference	Comments
Abragam and VanVleck (1953)	Atomic g_J factors.
Boys and Price (1954)	Mass-velocity and Darwin terms included variationally for Cl and S.
Froeman (1958, 1960)	Pauli approximation with HF functions.
Blume and Watson (1962, 1963); Blume et al. (1964)	Fine structure from a Breit-Pauli approximation with HF functions.
Herman and Skillman (1963); Herman et al. (1963)	PT for isolated atoms and for band structure.
Johnson et al. (1963)	PT for isolated atoms and for band structure.
Clementi (1964, 1965); Hartmann and Clementi (1964)	Pauli approximation with analytical HF functions.
Armstrong (1966)	Fine-structure matrix elements.
Condon and Odabasi (1966)	Excited-state fine structure with the Herman-Skillman approach.
Froese (1967)	Fine structure.
Malli (1968ab)	Spin-spin and spin-other-orbit interactions.
Thorhallsen et al. (1968)	Fine structure.
Beck (1969)	Valence electron CI with Breit-Pauli terms included using HFS radial functions.
Jones (1970, 1974, 1975)	Breit-Pauli approximation with HF functions.
Sharma and Bowtell (1970)	PT with a helium-like unperturbed solution.
Accad et al. (1971, 1975)	PT with Hylleraas-type functions.
Beck and Odabasi (1971)	One-to-three valence electron systems with Breit-Pauli terms included and HFS radial functions.
Fraga et al. (1971-1976)	PT with numerical HF functions.
Detrich (1972, 1975)	Pauli approximation with HF functions.
Saxena et al. (1972)	Orbit-orbit interaction.
Scherr (1972)	Criticizes Huzinaga and Arnau (1971).
van den Eynde et al. (1972)	Matrix elements of the Breit-Pauli operator.
Cowan and Griffin (1976); Wood and Boring (1978)	Proposes eq. (2.6) as a QR HF equation.
Holmgren et al. (1976)	Relativistic PT terms and n.r. MBPT explain the inverted alkali atom fine structure.
Glass (1978a-1982b); Glass and Hibbert (1978ab)	CI expansions incorporating Breit-Pauli term.
Snijders and Baerends (1978, 1982); Baerends et al. (1984)	A perturbative Hartree-Fock-Slater approach.

Table 4.11. (continued).

Takeda (1978)	A QR LDF approach using the Hedin-Lundqvist potential.
Warner and Blinder (1978)	Excited states of He.
Guimaraes and Ferreira (1979)	Deduces the $(\alpha Z)^2$ terms from a series expansion at the nucleus.
Marian (1981)	Evaluation of the Breit-Pauli matrix elements.
Pyper (1981a, 1983d)	Foundations of PT methods.
Pyper and Marketos (1981 a-c)	Fine structure.
Veseth (1981, 1983b)	Atomic fine structure.
Heully (1982)	Includes magnetic hyperfine and Zeeman effects in the QR approach.
Veseth (1983a)	Atomic g-factors.
Chandra and Buenker (1983ab)	Breit-Pauli matrix elements for Gaussian orbitals.
De Angelis et al. (1983)	Probabilistic solutions.
Weinert and Freeman (1983)	A spin-polarized QR LDF theory, applied on Pt.
Almloef et sl. (1984)	Comments on the methods of calculation of Breit-Pauli terms.
Heera et al. (1984)	A quasirelativistic $X\alpha$ model based on an averaged small component.
Selvaraj and Gopinathan (1984, 1985ab)	A quasirelativistic "ζ" method (DS, with the self-interaction removed.
Simas and Smith (1984)	Integrals over BP operators.
Farazdel et al. (1985)	Compare the usual $\langle h_T \rangle$ and a K-G-like kinetic energy. Z = 1-92, HF.
Matsushita et al. (1985)	An attempt to use the δ-function Darwin term self-consistently giving a relativistic E_T correction of wrong sign.
Veseth (1985)	Isotopic shifts in fine structure.

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

Reference	Comments
Christy and Keller (1942)	2p fine structure in many-electron atoms.
Dalgarno and Stewart (1960)	Ground-state energies of He-like systems.
Layzer and Bahcall (1962)	Z-expansions.
Collins (1964)	Identification of coronal emission lines.
Doyle (1969)	Review on Z-expansions.
McKibbin and Stewart (1969)	1sns $^{1,3}S$ states of He.
Safronova and Kharitonova (1970)	Fine structure of $1s^2 2s^i 2p^j$ configurations.
Klimchitskaya and Labzovskii (1971-)	Ground-state energy of two-electron ions.
Snyder (1971-1980)	Breit-Dirac energies for the He- and Li-like atoms.
Bowtell (1972)	Includes the Breit interaction. He-like systems.
Ermolaev and Jones (1973, 1974)	Z-expansions and other PT analyses.
Goldsmith (1974)	Li-like ions.
Jones (1974, 1975)	Uses the Breit-Pauli Hamiltonian.
Safronova et al. (1974)	He-like ions.
Ivanov et al. (1975)	He-like ions. QED effect included.
Safronova (1975)	O-like ions.
Safronova and Bolotin (1976-1977)	Expansion of DF + correlation energies and dipole matrix elements in 1/Z.
Shestakov (1976-1984)	Expansion of DF energies.
Safronova and Rudzikas (1976)	Basic theory for 1/Z expansions, including QED effects.
Feneuille and Luc-Koenig (1977)	Z expansions for $< r >$, $< r^{-1} >$.
Gurchumeliya and Safronova (1977)	Various coupling schemes.
Kononov (1977); Kononov and Safronova (1978)	Pictures of energy levels.
McEnnan et al. (1977)	Expansions in $Z^{1/3}$ for screened Coulomb potentials.
Safronova and Rudzikas (1977)	Basic theory for transition probabilities.
Braun and Labsovsky (1978)	A review.
Ivanov et al. (1978)	Level widths of autoionizing states pf two-electron atoms.
Vainshtein and Safronova (1978)	Wave lengths and transition probabilities of H- and He-like ions.
Bureeva and Safronova (1979)	Lifetimes for Ne-like systems.
Safronova and Lisina (1979)	Be-like ions.
Safronova and Urnov (1979)	Autoionizing states.
Knight and Sanders (1980)	Three-electron ions.

Table 4.12. (continued).

Safronova and Safronova (1980)	Transition probabilities for three-electron systems.
Snyder (1980)	Fine structure of 3p, $3p^{-1}\ ^2P$ and 3d, $3d^{-1}\ ^2D$ states, Z=11-27.
Wilson and Sharma (1980)	The expansion parameters 1/Z and $(\alpha Z)^2$ are not independent.
Davidson et al. (1981)	An α^2 expansion of the DF energies of rare gases.
De Serio et al. (1981)	2s-2p transitions of He-like systems, Z=4-26.
Safronova (1981)	He-like ions.
Drawin (1982)	Review on Z-expansions.
Knight (1982)	4-10 electron atoms.
Pokleba and Safronova (1982, 1984)	Line strengths for the Ne sequence.
Safronova and Senashenko (1982)	Transition probabilities for three-electron systems.
Bodashko and Safronova (1983)	Two-electron single-photon transitions for two-electron systems.
Drake (1983b)	Reviews QED terms.
Sanders and Knight (1983)	Two-electron ions.
Braun et al. (1984)	A book. See Ch. 7 for 1/Z-theory.
Cooper et al. (1984)	An α^2 expansion of the MCDF-EAL fine-structure energies of B - Cl.
Goldman (1984)	Two-electron systems (QED terms).
Vainshtein and Safronova (1984)	Two-electron satellites of Li-like ions.
Aglitskii and Safronova (1985)	Review on Z-expansions.
Safronova and Vainshtein (1985)	Dielectronic satellites of Be-like ions.
Vainshtein and Safronova (1985a)	Excitation cross sections for Be-like systems by electron scattering.
Viktorov and Safronova (1985)	Be- and O-like, Z < 101.
Zapryagaev et al. (1985)	Review on Z-expansions.

5. MULTIELECTRON ATOMS: RESULTS

In this chapter we summarize the available relativistic results for various properties of atoms with more than one electron. All relevant references in the Bibliography should appear in at least one table, and may be included in several ones.

Tabulations of atomic data are summarized in Table 5.1. Table 5.2. gives the papers on atomic energy levels (for papers, where QED corrections are the main issue, see Table 3.3.); papers on Auger effect and autoionization are given separately in Table 5.3 and papers on ionization potentials and electron affinities in Table 5.4.

The special case of supercritical ($Z>137$) collision systems is treated in Table 5.5. (For the lighter collision systems, see Ch. 7).

Transition probabilities are summarized in Table 5.6., polarisabilities and screening constants in Table 5.7., electric and magnetic hyperfine properties in Table 5.8., various $\langle r^n \rangle$ and magnetic moments (i.e. g-factors) in Table 5.9., Compton profiles or spin and momentum densities in Table 5.10., x-ray scattering factors in Table 5.11., electron scattering processes in Table 5.12., particle-atom collisions in Table 5.13, photon scattering in Table 5.14. and atom-atom collisions in Table 5.15. The corresponding stopping-power calculations are also included in the Tables 5.12 - 5.14. Nuclear processes, involving electrons (internal conversion, electron scattering etc.) are listed in Table 5.16. Parity-violation effcts are covered in Table 5.17.

The properties of atoms in crystal fields are discussed separately in Table 7.12.

Table 5.1. Tabulations of atomic ground-state properties.

Reference	Comments
Herman and Skillman (1963)	1st order, HFS+PT corrections for all shells, Z=2-102.
Mann and Waber (1970)	Search of DF ground states for Z=118-131.
Fraga et al. (1971)	HF atomic data of M^-, M, M^+-M^{4+} of He-Kr. 1st-order relativistic corrections included.
Fricke et al. (1971)	DS for Z=104-172.
Lu et al. (1971a)	DS properties for Z=2-126.
Desclaux (1973)	DF total and orbital energies, $\langle r^n \rangle$ for Z=1-120.
Mann and Waber (1973)	DF total and orbital energies, $\langle r^n \rangle$ for Z=57-70.
Fraga et al. (1976)	HF atomic data with 1st-order relativistic corrections. Z=2-102.
Huang et al. (1976)	DS electron binding energies, Z=2-106.
Fricke and Soff (1977)	DS for Z=100-173.

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

Reference	Comments
J.B. Green (1923)	Screening constants for x-ray transitions in Sommerfeld theory.
Lande (1924)	On the origin of fine structure in x-ray spectra.
Breit (1930b, 1932)	Helium fine structure.
Inglis (1938)	Transition from LS- to jj-coupling.
Williams (1940)	A Dirac-Hartree solution for Cu^+.
Sessler and Foley (1953)	Ground-state energy of He.
Schawlow and Townes (1955)	Effect of nuclear volume on x-ray fine structure.
Sucher and Foley (1955)	He-like atoms.
Bethe and Salpeter (1957)	Review on two-electron systems.
Kabir and Salpeter (1957)	Ground-state energy of He.
Mayers (1957)	Dirac-Hartree solutions for Hg^{2+} and Hg.
Froeman (1958, 1960)	Ground-state energies, up to Ne-like systems, Z=9-13. HF+BP.
Pekeris (1958)	Ground-state of two-electron atoms.

Table 5.2. (continued).

	Hylleraas+BP PT+QED. Z=1-10.
Sucher (1958)	Energy levels of two-electron atoms.
Araki et al. (1959)	The 2 ^{3}P levels of He.
Brown and Mayers (1959)	The K-shell in Hg.
Dalgarno and Stewart (1960ab)	The ground-state energies of the He sequence.
Blume and Watson (1962, 1963);Blume et al. (1964)	Calculations of s-o splittings using HF wave functions, for the 2p-4p, 3d-4d, 4f shells.
Knight and Scherr (1962)	E_T of He-like ions.
Herman et al. (1963)	HFS+PT valence p-shell corrections, Z=3-86.
Herman and Skillman (1963)	Dito for all shells, Z=2-102.
Clementi (1964)	Ground-state energies of 10-18 electron atoms with Z=11-36. PT with LCAO-HF, all BP terms.
Hartmann and Clementi (1964)	Ground-state energies of closed-shell atoms with 2, 4, 10, 12 or 18 electrons and Z=2-36. LCAO-HF, all BP terms.
Collins (1964)	Coronal emission lines.
Rajnak and Wyborne (1964)	Electrostatic corrections to s-o coupling.
Snow et al. (1964)	DS E_T for Z=2-101.
Clementi (1965)	Ground-state energies of Ca-Zn. LCAO-HF, all BP terms in PT.
Liberman et al. (1965)	DS x-ray spectra of Hg, U.
Schiff et al. (1965ab)	2 P - 4 P states of He and the 2 P one of Li^+.
Condon and Odabasi (1966)	Spin-orbit splittings. HFS+PT. Z=5-80.
Mande and Damle (1966)	Reproduces s-o splittings in x-ray spectra by a screening parameter.
Froese (1967)	S-o splittings.
Kim (1967)	DF-LCAO for He, Be, Ne ground states.
Smith and Johnson (1967)	DF for He, Be, Ne, Ar, Cu^+.
Carlson et al. (1968)	DS electron shake-off for Z=2-92.
Larson and Waber (1968)	N.r. HF valence configurations for Z=124-127: beginning of a 5g series.
Rosen and Lindgren (1968)	Modified DS binding energies for all shells of Cu, Kr, I, Eu, Hg, U.
Thorhallsson et al (1968)	S-o coupling in B-Kr and their ions. HF+BP PT.
Tucker et al. (1968)	Binding and x-ray energies for elements 114, 126, 140. DS.
Beck (1969)	Valence levels of Tl II.
Beck and Zare (1969)	Levels for two valence electrons.
Carlson et al. (1969)	DS K-N shell binding energies and K x-rays for Z=96-120.
Doyle (1969)	Review on Z-dependent corrections.
Griffin et al. (1969)	HFS+PT energies for many configurations of d-, f- and g-electron transition elements Z=2...126.
Mann (1969, 1975)	Stability of 8p electrons for Z=121-127. DF.

Table 5.2. (continued)

McKibbin and Stewart (1969)	1sns levels in the He series.
Waber (1969); Waber et al. (1969)	DS energies for many states of Z=104-132.
Bessis et al. (1970)	LS averages of relativistic states.
Grant (1970)	A review.
Jones (1970)	BP level corrections, including p- and d-level fine structure, for the F I, Na I and Mg I sequences, Z<29.
Lewis et al. (1970)	Actinoid ion s-o coupling constants.
Safronova (1970)	Relativistic corrections for two-electron atoms.
Safronova and Kharitonova (1970)	FS of $2s^m2p^n$ states as a series in 1/Z.
Schiff et al. (1970)	FS of the 2 P to 4 P states of Li^+.
Accad et al. (1971, 1975)	S and P states of He-like systems with Z=2-10.
Beck and Odabasi (1971)	Levels arising from one-electron, three-electron or one p-hole + two electron configurations.
Cowan and Mann (1971)	Energy levels and configurations of super-heavy elements.
Desclaux et al. (1971a)	Ground-state energies of He, Ar, Na, Br, Rn.
Desclaux et al. (1971b)	Excitation energies of Li- to F-like systems, Z=3-18.
Desiderio and Johnson(1971)	K-shell binding energies for Z=70-90.
Fricke et al. (1971)	DS ground states of the superheavy elements, up to Z=172.
Klimchitskaya and Labzovskii (1971)	Ground-state energies or two-electron ions Z=1-137.
Mann and Johnson (1971)	Various forms of the Breit interaction tested for Z=2...102.
Penneman et al. (1971)	Various IP_n and chemistry of element 164. DF.
Snyder (1971)	$2p_2$s-o splittings for the Li-, B-, F- and $1s^22p^5$ series, Z=3...20. 1/Z.
Varga et al. (1971)	DF and DS s-o splittings for all oxidation states of Th-No.
Verhaegen et al. (1971)	1s and 2s hole states of Ne. DF.
T.E.H. Walker (1971)	Orbit-orbit contributions for Be-Ar.
Bowtell (1972)	Ground-state energy of He-like systems, Z<21, including the magnetic interaction.
Daley et al. (1972)	Ground-state energy of He-like systems, Z<20. including the magnetic interaction.
Daley et al. (1972)	The 2 ^{3}P fine structure of He.
Desclaux (1972)	Fine structure of the group 14 (C-114) ground state.
Douglas (1972); Douglas and Kroll (1974)	Fine structure of He.
Freedman et al. (1972)	The 1s IP of Fm agrees with a DF calculation.

Table 5.2. (continued).

Fricke et al. (1972)	The K-, L- and M-shell IP of Fm agree with a DF calculation.
Fricke and Waber (1972b)	Influence of QED on the chemistry of element 184. DS.
Fricke and Waber (1972c)	Ground configurations of E159, E160. DS.
Hambro (1972)	Fine structure of He.
Snyder (1972)	S-o splittings for $1s^2 2s^a 2p^b$ from 1/Z theory.
van den Eynde et al.(1972)	Singlet-triplet mixing in the He sequence, Z=2-10.
Waber and Liberman (1972)	The DS problem solved for ions (Na^+, Cl^-, O^{2-}, S^{2-}) in a medium with dielectric constants of 20, 80.
Ermolaev (1973, 1975)	Lamb shifts and ^3P levels of two-electron ions.
Fricke and Waber (1973)	X-ray spectra of superheavy elements. DS.
Klimchitskaya and Labzovskii (1973a)	Transition energies in He-like ions.
Klimchitskaya and Labzovskii (1973bc)	Interpolation formulae for energy levels and spectra of isoelectronic ions, Z=1-137.
Maly and Hussonnois(1973ab)	DF total and binding energies for Z=1-120.
Mann and Waber (1973)	DF data for lanthanoid atoms.
Schiff et al. (1973)	Perturbations on the n $^3P_1$ of He-like systems.
Walker and Waber(1973b)	Hund rules for jj-coupling. Applications on Ln, An.
Andriessen et al. (1974)	d-levels of Mn^{2+}. MBPT.
Berkowitz et al. (1974)	Valence satellites of 5d PES for Hg.
Coulthard (1974)	Chemical shifts of x-ray energies.
Desclaux et al. (1974)	K- and L-shell x-rays of Tl.
Ermolaev and Jones (1974)	Ground, n $^{1,3}S$ and n $^{1,3}P$ states of two-electron ions, Z=11-20.
Fricke and Desclaux (1974)	Two-muonic atoms.
Goldsmith (1974)	1s-2p transitions in Li-like ions, Z=6-29. Z expansion.
Gurchumeliya and Safronova (1974)	Two-electron atoms.
Kovalevskii and Labzovskii (1974)	Vacuum polarization and inner levels in heavy atoms.
Lindgren and Rosen (1974)	DF binding energies of Ne, Ar, Cu, Hg.
Nugent et al.(1974)	The ground state of Lr from DF. See Desclaux and Fricke (1980).
Snyder (1974)	3p and 4p excited states of the He and Li sequences. 1/Z.
Trefftz (1974)	Mutual interaction of s-o and CI effects.
Wittel and Manne (1974)	Experimental s-o parameters for 19 elements.
Andriessen and van Ormondt (1975)	Atoms close to LS coupling. Mn^{2+}.
Detrich (1975)	Oxygen ^3P fine structure.
Foley and Sternheimer(1975)	The 3d inverted fine structure of Na explained as an exchange + s-o 2nd-order effect.

Table 5.2. (continued).

Fricke (1975); Fricke and McMinn (1976); Fricke and Soff (1977)	Ground states and properties of the superheavy elements Z=103-172,184.
Ivanov et al. (1975)	$1s^2$, 1s2s and 1s2p states of He-like systems, Z=10...100.
Kagawa (1975)	Total and orbital energies for Sc-Cu. DF-LCAO.
Karwowski et al (1975)	Fine structure of transition elements. HF+PT.
Safronova (1975)	$2s^2 2p^4$ - $2s2p^5$ - $2p^6$ wave lengths for O-like systems, Z=8-19.
Adachi et al. (1976)	DS calculation on U.
Bogdanovich et al. (1976)	The oxygen sequence.
Cheng and Johnson (1976)	Self energy corrections to K-electron binding. Z=50-160.
Desclaux (1976ab)	Review on relativistic effcts on inner-shell properties.
Fraga et al. (1976)	HF results for atomic ground states with 1st-order relativistic corrections.
Grant et al. (1976)	Low-lying levels of Hf III.
Holmgren et al. (1976)	p and d level fine structure of Na-like systems (Z=11-15).
Huang et al. (1976)	DS SCF IP for all shells, Z=2-106.
Larkins (1976)	The O I-like (Z=8,80) and Ar III-like ($2p^{-1}3p^{-1}$, Z=18,80) levels.
Luc-Koenig (1976b, 1980)	Doublet inversions of alkali metals.
Rajnak (1976)	QR HF levels for over 30 configurations of U I. S-o constants.
Safronova and Bolotin (1976)	The $2s^2 2p^3$, $2s2p^4$ and $2p^5$ levels of N-like systems, Z=7-30.
Safronova and Rudzikas (1976)	The $2s^2 2p$ - $2s2p^2$ - $2p^3$ levels for B-like ions, Z=7-29.
Shestakov (1976, 1977)	Approximate DF energies for Be...Hg using relativistic Coulomb Green functions.
Waber and Fricke (1976)	Ions of the superheavy elements in vacuum and in solution (a Debye-Huckel potential included in the Hamiltonian).
Bogdanovich et al. (1977, 1978a)	Si VII, Ca XII, XV, Fe XIX-XXI.
Carlson and Nestor (1977)	DF binding energies for the K to O shells and the K, L x-ray energies for Z=95-130.
Cheng and Johnson (1977b)	Mg sequence.
Dankwort (1977b)	Mg 3s3p ^3P fine structure.
Klapisch et al. (1977)	The 1s-3p x-ray spectrum of Fe IX-XVIII, XXIV-XXVI.
Kononov (1977)	A review on multicharged ions.
Kononov and Safronova (1977)	Graphical representations for Li- to F-like systems, Z=10-100.
Krause and Nestor (1977)	X-ray and binding energies for actinoids, Z=89-103.

Table 5.2. (continued).

Lee et al. (1977)	Valence levels of Xe, Xe^{+}, Au, Au^{+} as a test of a P-K PP.
Pyper and Grant (1977)	Interpretation of Hund's rules. Mostly valence-valence repulsion.
Schreckenbach et al.(1977)	K hypersatellites for Hg.
Shorer and Dalgarno (1977)	RRPA for the Zn sequence.
Sivtsev et al. (1977)	Energy spectra of the Fe XVII, Mo XXXIII. DF.
Zibert et al. (1977)	DS energies for highly ionized Xe.
Armstrong (1978)	Reyiew on hghly ionized atoms.
Bogdanovich et al. (1978b)	$2s^{2}2p^{5}3l$ - $2s2p^{6}3l$ transitions in Ne-like systems, Z=13...42. HF+BP.
Cheng et al. (1978)	Fine structure in the $1s2p^{2}$ ^{4}P and $1s2s2p$ ^{4}P Li-like atoms.
Cheng and Kim (1978)	Cu-like ions.
Driker and Ivanov (1978ab)	Zr XI-XV, Mo XIII-XVII.
Fricke (1978)	Review on inner shells.
Glass (1978a)	Fine structure of the $1s2p^{2}$ state of Li.
Glass (1978b)	Fine structure of the 1s2s2p state of Li.
Hafner and Schwarz (1978a)	Valence levels of Ca, Ba, Hg and Hg^{+} using PP-MCDF+CI.
Kichkin et al (1978)	$2p^{-1}3d$ configurations of highly ionized ions.
Lewis and Serafino (1978)	Second-order fine-structure of He.
Lundberg and Rosen (1978)	7s - 7p, 8p energies of Fr.
Mallow et al. (1978)	Binding and excitation energies of muons in muonic atoms (O...Pb).
Rajnak and Shore (1978)	s-electron binding energies in $s^{M}l^{N}$ configurations, as a function of N. QR HF.
Rashid (1978, 1980)	DS binding and excitation energies for highly ionized Cu, Zn, Ag and Sn.
Rose et al.(1978a)	Analysis of direct and indirect relativistic effcts on the valence electron of Lu, Au and Tl. Schroedinger or Dirac equations solved in HF or DF potentials.
Rose et al. (1978b)	Low-lying spectrum of Bi I. MCDF.
Rose et al. (1978c)	Low-lying even-parity spectrum of Ba I. MCDF.
Rudzikas (1978)	A review on the spectra of multicharged ions.
Sternheimer et al. (1978)	nd and nf fine structure of alkali atoms. Effect of the core.
Takeda (1978)	QR LDF for Yb.
Vainshtein and Safronova (1978)	Wavelengths of satellites to resonance lines of He-like ions. Z=4-34. 1/Z.
von Egidy and Desclaux (1978)	Electron screening for muonic p, d, f levels, n<31, s levels, n<13. Z=8-90. DF.
Warner and Blinder (1978)	Excited states of He, from 2 $^{1,3}P$ to 8 $^{1,3}K$.
Wood and Boring (1978)	A QR HF approach on U.
Bogdanovichene and Bogdanovich (1979)	CI+BP for $2s^{1}2p^{J}$ configurations of Z=24...28.
Braun et al. (1979)	Two-valence-electron atoms. Theory only.

Table 5.2. (continued).

Bureeva and Safronova(1979)	The Ne-like sequence.
Cheng and Kim (1979)	Ag-like ions. For Z>60 the ground state is 4f, not 5s.
Desclaux et al. (1979)	Levels of Fe XXI.
Drake (1979, (1982a)	$1s2p-1s^2$ transitions of He-like ions, Z=2-100. (Both ^3P and ^1P).
Fielder et al. (1979)	E1 and M2 transitions in the Ne sequence.
Froese Fischer and Hansen (1979)	$4s4d\ ^1D - 4p^2\ ^1D$ interaction in the Zn I isoelectronic sequence. MCDF.
Glass (1979a)	Highly ionized Be-like systems, up to Z=26.
Glass (1979c)	The $2s2p - 2s^2$ intercombination in Be-like Mg...Fe.
Guimaraes and Ferreira (1979)	An alternative HFS-PT approach, based on a power series at origin. Fine structure of O...Pb.
Ivanov and Ivanova (1979)	3s...6f states of Na-like ions, Z=25-80.
Johnson and Cheng (1979b)	Quantum defects for highly stripped ions. C IV, N V.
Karwowski and Szulkin (1979)	Excitation energies in the Li series using a rough pseudopotential.
Laughlin and Victor (1979)	$3s^2$-3s3p wavelengths; 3s3p, $3p^2$ fine structure for Z=12-18. Semiempirical model potentials.
MacDonald and Vosko (1979)	The tranverse interaction energy in the ground state tabulated for Z=2...102. LDF.
Shchornak et al. (1979)	DS calculations on U^{n+}.
Shestakov (1979)	Spectra of Li-like systems, Z=3-28.
Shorer (1979)	The 2p-3s and 2p-3d excitations in the Ne sequence. RRPA.
Anisimova and Semenov (1980)	$2p^5 3p$ and $2p^5 4p$ configurations of Ne. PT.
Band and Fomichev (1980); Band et al. (1981); Band (1981)	Two different DF solutions with the same nlj quantum numbers found for single-configuration models of La, $4f^1$, and Eu, $4f^7$.
Basch (1980); Basch et al. (1981)	Valence levels of Pt and Pd. DF.
Beatham et al. (1980)	MCDF ionization, Auger energies of rare gases and $K_{\alpha 1}$ hypersatellite energies of Hg.
Beatham et al (1980b)	5d core satellites of U V. MCDF.
Berry et al. (1980)	Comparison of theory and exp. for 2s-2p transitions in two-electron (Z = 2-22) and three-electron (Z = 3-45) systems.
Borchert et al. (1980)	K x-ray levels.
Braun and Gurchumeliya (1980)	PT for degenerate levels.
M.P. Das (1980)	Ground state energies of He...No using a relativistic LDF.

Table 5.2. (continued).

M.P. Das et al. (1980)	Total energies of Li-like ions and U, using a relativistic LDF.
Desclaux and Fricke (1980)	Ground state of Lr and the group 3 elements.
Driker and Ivanov (1980b)	S VII, Ca XI.
Feller and Davidson (1980)	The relativistic contribution to the carbon s^2p^2-sp^3 splitting and the splitting of CH_2.
Grant and McKenzie (1980)	Transverse electron-electron interaction. The E_T of closed-shell systems and the K_{α_1} and $K^h_{\alpha_1}$ energies of Hg.
Herbst (1980,1983ab,1984); Herbst and Wilkins (1982)	Inner-shell excitation energies of lanthanoids and actinoids, including solid-state effects.
Johnson et al. (1980a); Johnson (1983)	Reviews on RRPA work.
Kagawa (1980)	MCDF-LCAO term energies for O-like systems (Z=8, 26, 80).
Karwowski and Aniola(1980)	DF energies for several states of Li-like systems, Z=3-6.
Knight and Sanders (1980)	S, P, and D states of Li-like ions.
C.M. Lee and Johnson (1980)	1s excitations below the K threshold for the Be series.
McGilp and Weightman(1980)	Electron binding energies for Zn-Hg. DF+QED.
Merkelis et al. (1980)	Spectra of Fe XVIII-XXVI.
Nigam and Kathari (1980)	New K_α satellites for Fe. DF.
Pyper (1980a, 1983a)	Analysis of the Al ground-state fine structure.
Rose et al. (1980)	5p excitation of atomic Ba.
Sandner et al. (1980)	Spectrum of Pb between 37 and 105 eV.
Shorer and Dalgarno (1980)	Review on RRPA.
Snyder (1980)	Fine structure of 3p, $3p^{-1}$ ^2P and 3d, $3d^{-1}$ ^2D states of Na-Co. Z expansions.
Vainshtein and Safronova (1980)	Dielectronic satellite spectra of He-like ions, Z=6-33.
Wood and Pyper (1980ab)	The carbon s^2p^2 - sp^3 excitation energy and the singlet-triplet excitation energy in methylene.
Arndt et al. (1981)	K_{α_1} and K_{β_2} energies of highly stripped Pb. DS and DF.
Basch (1981)	Valence levels of Ag. DF.
Bhalla and Tunnell (1981)	1s2s2p states for Z=3-26.
Boring et al. (1981)	Satellites of the 5s and 5p PES of actinoids.
Chen et al. (1981e)	Inner-shell levels for Z=70-106.
Chen et al. (1981a)	Level shifts due to Auger continua.
M.P. Das (1981)	Binding energies of Fm, using a relativistic LDF.
Davidson et al. (1981)	Total energies of rare gases,He-Xe, expanded in α^2.
De Serio et al. (1981)	1s2s - 1s2p transitions of He-like Si, S and Cl.
Galan and Bunge (1981)	Core-excited states of 2- and 3-electron atoms.
Glass (1981)	Spin-forbidden $2p^2$ - 2s2p transitions in Be-like systems.

Table 5.2. (continued).

Herbst (1981)	3d levels of (metallic) Ba.
Karwowski and Szulkin (1981)	QR approach with different orbitals for different j. Valence transitions for alkali-like systems.
Key et al. (1981)	DS and DF binding energies for K 2p, Rb 3p Cs 3d, Mg 1s, Zn 2p and Cd 3d.
Klapisch et al. (1981b)	3d-4p x-ray transitions of the Mo XIV series, Z=39-47.
Kuchas and Karosene (1981)	Influence of the 5f electron collapse on $5d^{10}$ - $5d^{9}5f$ transition energies. HF+PT.
R.L. Martin and Hay (1981)	Relativistic (QR HF) contributions to valence excitations of 3d, 4d and 5d atoms
W.C. Martin (1981)	Series formulae for the He-like spectra of Z=11-18.
Mathews et al. (1981;1983)	3d PES of Cs, CsCl, CsI. DF.
Migdalek and Baylis (1981ab)	p-state fine structure in groups 1, 11, 13 (Rb; Ag, Au; In, Tl).
R.A. Moore et al. (1981)	Core-valence correlation potentials for alkalis. Relativistic PT only.
Neumann (1981)	Fine structure of He-like systems (a review, experimental).
Parente et al. (1981)	L x-ray satellite energies, Z=65-95. DS. E1 and E2 transitions in the presence of a M- or N-shell spectator hole.
Pyper and Grant (1981)	The 7p series of superheavy elements.
Pyper and Marketos(1981ac); Pyper et al. (1982)	Atomic fine structure analysed, DF or PP. Z=5...89. The inverted fine structure explained. Relativistic contributions to to E_{corr} defined, found important for Z>18.
Safronova (1981)	1s2s and 1s2p levels of He-like ions, Z= 10-42.
Sen et al. (1981)	DS TS s-o splitting for Ar-Xe, Ba, Hg, Pb.
Szulkin and Karwowski (1981)	np levels and their fine-structure for Li-Cs. QR HF with s-o terms and a core polarizability correction.
Vajed-Samii and MacDonald (1981)	E1 transitions of Cl-like ions, Z=26...82. MCDF.
Vajed-Samii et al. (1981a)	E1 and M1 transitions in the B sequence MCDF.
Veseth (1981, 1983b)	Fine structure of B...Cl. MBPT.
Vidolova-Angelova et al. (1981-1984)	Excited states of Tm, Yb, Lu and their ions.
Zapryagaev and Manakov (1981)	Correlation effects in multiply charged ions by a Green's function method.
Aberg and Suvanen (1982)	Review of x-ray-satellites.
Aglitskii et al. (1982)	K and K lines of Ti, Fe, Ni plasmas.
Banna et al. (1982)	Core binding energies of Li^{+} - Cs^{+}, F^{-}-I^{-}. DF with empirical correlation corrections.
Bauche et al. (1982, 1983)	LS-coupled energies with relativistic integrals. U IV, V.

Table 5.2. (continued).

Bauschlicher (1982)	Valence levels of Pd.
Bauschlicher et al. (1982)	Sc-Cu valence levels.
Beck and Nicolaides (1982)	Specific correlation effects in inner-shell-PES.
Berry et al. (1982)	Review on two-electron systems.
Bodashko et al. (1982)	Breit interactions for the He, Be, Ne-like series.
Braun et al. (1982)	Be- and B-like series, Z<101.
Burkhalter et al. (1982)	Nb XII-XVII. QR-HF.
Chen et al. (1982b)	Multiplet splittings of the $1s2p^2$ Li-like systems.
Chen et al. (1982c)	Effect of the Breit interaction on K x-ray hypersatellite spectra.
Cooper and Wilson (1982)	Fine-structure splittings for B - Ne^+ using PT and "even tempered" basis sets.
Cox (1982)	Dependence of U 4f binding energies on the valence configuration.
Curtis and Ramanujam (1982)	Semiclassical term energies of He I. High-lying D, F, G levels, n<12.
M.P. Das (1982)	Binding energies of Zn and Cd using a relativistic LDF.
Deslattes et al. (1982); Kessler et al. (1982)	Comparison of K-shell x-ray energies with experiment.
Detrich and Weiss (1982)	Inverted d-electron fine structure of alkali atoms explained.
Dietz et al. (1982b)	Total energies of He - Kr by the "g-Hartree" method.
Drake (1982a)	1s3d levels for the He series, Z=2-25.
Drake (1982b; 1983ab)	A review on two- and few-electron systems.
Drawin (1982)	Review on highly ionized atoms.
Driker et al. (1982)	2-2 transitions in O- and F-like ions.
Froese Fischer (1982)	The ^5F - ^3F separation in Ti.
Froese Fischer and Cheng (1982)	The 1s3d ^1D level of He.
Froese Fischer and Godefroid (1982)	"Plunging configurations" (n=3) in the Mg sequence.
Gagarin and Falkov (1982)	DS x-ray energies for Mo.
Glass (1982ab)	Spin-forbidden E1 lines for Be-like ions, Z=6-10.
Glass (1982b)	Ditto. The allowed $2s^2$ - 2s2p transitions. Z=26...74.
Hata and Grant(1982,1983cg)	Li-like series.
Huang et al. (1982)	Ground-state fine structure of B- and F-like ions.
Kessler et al. (1982)	Precision x-ray measurements for Z=47-92.
Kim and Huang (1982)	Ground-state fine structure of F-like systems, Z=9-56.
Lee and Freed (1982,1983)	Valence levels of Ti,V,Cr and their ions. N.r. MBPT+(DF-HF)corrections.
Li and Zhao (1982)	Dependence of L, M, N shell binding energies of lanthanoids on the valence state. DS.

Table 5.2. (continued).

Lindgren and Martensson (1982)	Fine structure of the nd states of Na-like systems, Z=11-42. N.r. MBPT+BP PT. Relationship to model-potential calculations analysed.
Perdew and Cole (1982)	An LDA for the Breit interaction. Transverse photon energies for Z=2...100.
Perera et al. (1982)	Core electron binding energies for group 2 atoms and ions (Ca-Ba). DF.
Ramana et al. (1982)	Correlation energy terms from the theory of relativistic electron gas used to evaluate K-shell x-ray energies, Z=10...100.
Rudzikas (1982)	A review on the theory of multicharged ions.
Safronova and Senashenko (1982)	Satellite structure due to CI for the $1s2s^22p^n - 1s^22p^{n+1}$ and $1s2p^n - 1s^22s^22p^{n-3}$ transitions, Z=12-14.
Slaughter et al. (1982)	The $3p_{3/2}$ level of Cs. DF+E_{corr} estimates.
Stevens and Krauss (1982)	np and (n+1)p fine structure of C and Si, and their ions, as a test of a spin-orbit effective potential.
Vidolova-Angelova et al. (1982)	Rydberg levels of Tm, Yb, Lu and their ions.
Weiss (1982)	Residual correlation corrections to MCDF calculations derived for $2s^22p^2$, $2s2p^3$ and $2p^4$ levels of Fe XXI from Pauli-level calculations.
Zapryagaev et al (1982)	Ground-state energies of He-like atoms using Coulomb Green functions.
Armstrong (1983)	A review.
Beck et al. (1983)	2p binding energies of P, As, Se.
Briand et al. (1983)	He-like Ar.
Bylander and Kleinman (1983)	Valence levels of Mo and W: d^4s^2 versus d^5s. LDF.
Cheng and Froese Fischer (1983)	Collapse of the 4f orbital for Xe-like systems.
M.P. Das (1983)	Core electron binding energies of heavy atoms using a relativistic LDF.
De Alti et al.(1983,1984); Decleva and Lisini (1985)	Shake-up levels in alkali-atom core-electron PES. Na-Fr.
Dobryshin et al. (1983)	DF assignment of Sm $4f^65d7p$ and $4f^65d8p$ autoionization states.
Dzuba et al. (1983ab)	Valence elctron levels (s-f) of Cs and Fr.
D.G. Ellis (1983)	$1s^22s2p$ levels of Ne VII - Fe XXIII. MCHF+Pauli.
Ermolaev and Swainson(1983)	Two-electron ions as a test of QED.
Fawcett (1983a)	E1 transitions within the ground complex of Al-like systems, Z=17...28.
Fawcett (1983b)	E1 transitions within the ground complex of Mg-like systems, Z=16...28.
Froese Fischer (1983)	The $2p_{3/2}$ - $2p_{1/2}$ transition in the B sequence, Z=5-54.
Froese Fischer and Saha (1983)	Forbidden transitions in the $2p^4$ series, Z=8-42.

Table 5.2. (continued).

Frye et al. (1983)	Fine structure in the B and F sequences. Z=5-39.
Glass (1983)	Closed-shell atomic systems.
Goldman and Drake (1983a)	Ground-state Lamb shift of two-electron ions.
Goldschmidt (1983)	Spin-dependent interactions in U V $5f^2$.
Hata and Grant (1983d)	Be-like series.
Hata et al. (1983); Hata and Grant (1984a)	F-like series.
Hata and Grant(1983g,1984a)	B- and C-like series.
Huang et al. (1983)	Cl-like systems, Z=17-92.
Johnson and Cheng (1983)	RRPA results on highly ionized atoms: a review.
Juncar et al. (1983)	Triplet levels of He I.
Kotochigova (1983); Kotochigova et al (1984, 1985)	VUV spectra of Eu I, Yb I. DF.
Mandelbaum et al. (1983)	X-ray spectra of Tm-Pt at 6-9 A.
Mathews et al. (1983)	3d PES of Cs. DF.
McClary and Byers (1983)	Heavy-quarkonium spectroscopy.
Pyper (1983a)	Analysis of the fine structure of B, N-F, Al, S. The importance of the correct n.r. limit is stressed. MCDF OL/EAL.
Rashid and Fricke (1983)	Binding and excitation energies for Na-like ions with fractional (quark) charges, Z=10...30.
Safronova et al. (1983)	Dielectronic satellites for C-like systems, Z=8...38.
Sanders and Knight (1983)	S, P and D states of two-electron ions.
Shestakov (1983)	Spectra of Na-like systems, Z=11-80. 3s-3p, 1/Z given.
Stevens and Krauss (1983a)	Valence levels of Hg^+, Hg as test of a PP.
Teichteil et al. (1983)	Low-lying levels of Ar, In as test of a PP
Theodosiou and Raftopoulos (1983)	DF energies for the Pm sequence.
Victor and Taylor (1983)	The Cu- and Zn-like sequences, Z=29-42. A model potential method.
Zilitis (1983b)	Rydberg levels of Li-like ions.
Zschornak (1983)	DF,DS agree on x-ray shifts upon ionization for Mo, Pb.
Aspromallis et al. (1984)	Doubly excited levels of He.
Au et al. (1984)	Retardation effects on He Rydberg states, n = 9-12, Z = 2...70.
Beck (1984)	K-shell binding energies of Mg, Ca.
Braun et al. (1984)	Book on the relativistic theory of atoms.
Briand et al. (1984)	He-like Fe.
Briand et al. (1984b)	He-like Kr.
Bruneau (1984)	MCDF calculation for ns^2-nsnp transitions of neutral atoms.
Cheng et al. (1984)	Interaction of fine and hyperfine structure of doubly excited quintet states of ^{7}Li
Chung (1984ab)	The 1s2s2p ^{4}P levels of He^-, Li - Mg X.
Chung and Davis (1984)	Quartet states of Be^+.
Connerade et al. (1984)	The critical double-well of Ba^+ by the "g-Hartree" method.

Table 5.2. (continued).

Cooper et al. (1984, 1985)	Fine structure splittings of B I to Cl I calculated by the MCDF-EAL method and expanded in powers of α^2.
Craseman et al. (1984)	Review on inner-shell processes.
B.P. Das et al. (1984)	Ground-state fine structure in the B sequence, Z=5-30. MCDF-EAL.
Davis and Chung (1984)	Total energies of the (1s2s2s) ^2S resonances for Z=2-5.
Desclaux and Freeman(1984)	Fine structure, PES of actinoid ions.
Dmitriev et al. (1984)	Book on the relativistic theory of atoms.
Esser (1984a)	Ground and low-lying levels of Hg and Pb. LCAO DF+CI.
Fawcett (1984a)	Allowed, n=2-3 transitions in Be-like ions, Z=8...28.
Fawcett (1984b)	Allowed, n=2,3 transitions in Be-like systems, Z=4-7.
Froese Fischer and Saha (1984)	Allowed $2s^22p^4$ - $2s2p^5$ transitions in O-like systems, Z=8-42.
Frye and Armstrong (1984)	The $2s^2$ - 2s2p transition in the Be-like sequence, Z=4-28. Comparison of MCDF and RRPA.
Gagarin et al. (1984)	4f s-o splitting of Pt for various 6s, 5d populations.
Gaspar et al. (1984)	DS IP of multiply charged ions.
Godefroid and Froese Fischer (1984)	FS of the N sequence.
Goldman (1984); Goldman and Drake (1984)	QED terms for $1s^2$, 1s2s and 1s2p levels of He-like systems, Z=2-26.
Grant (1984ab)	Reviews.
Hata (1984a-c): Hata and Grant (1982b, 1983ab,efg, 1984b)	High-precision calculations for He-like systems.
Hess et al. (1984)	Fine structure of Br. A QR calculation using the delta-function Darwin term and giving the wrong sign to the total energy correction.
Keski-Rahkonen et al.(1984)	The L-level x-ray absorption spectra of Ba and Hg.
Langhoff et al. (1984)	Lande interval rule in Mg - Ba.
Low and Goddard (1984)	Valence states of Pd and Pt, their chemical importance. QR PP.
Migdalek and Baylis(1984b)	Collapse of 4f and 5d orbitals in the Cs sequence. (The ground states are $6s^1$ for Cs, Ba^+, 5d for La^{2+} and $4f^1$ for Ce^{3+}, Pr^{4+}. Core-valence correlation essential to understand this).
Ohno (1984)	Dynamical relaxation shifts for M_{23} levels, Z = 42-97.
Rudzikas (1984)	A review on the spectra of atoms and ions with complex configurations.
Safronova and Senashenko (1984)	A treatise on the spectra of multicharged ions.

Table 5.2. (continued).

Spitsyn and Ionova (1984)	HF+PT $f^n s - f^{n+1}$ and $f^n s - f^{n-1} s^2$ energies for Ln^+, An^+. Trends for many other processes discussed.
Vainshtein and Safronova (1984)	Two-electron satellite spectra of Li-like ions.
Zilitis (1984)	Rydberg levels of Na-like ions.
Aglitskii and Safronova (1985)	Review of autoionization states.
Aspromallis et al. (1985)	Autoionization of Be^-.
Baluja and Hibbert (1985)	QR levels of Fe XV.
Bauschlicher et al (1985a)	Ca, Sr valence levels.
Berry (1985)	Review on 2- and 3-electron systems.
Bhattacharya et al. (1985)	Effect on additional vacancies on K-x-ray energies.
Chen et al. (1985a)	Electron binding energies: residual limitations.
Chung and Davis (1985)	He 2s2p ^1P.
Cogordan et al. (1985ab)	Ne-like ions, up to Fe XVII, $2p^5 3s$, -3p and -3d levels.
Cooper et al. (1985)	Fine structure of the B- and F-like series.
M.P. Das and Nayak (1985)	K- and L-shell binding energies, K hyper-satellite energies of Tm, Hg, Tl. LDF.
Desclaux (1985)	Energy levels of few-electron atoms: a review.
Deslattes (1985)	Review of single-electron and single-vacancy ions.
Drachman (1985)	Rydberg levels of He.
Drake (1985)	He-like U.
Drake (1985b)	QED and heavy atoms: a summary.
Drake and Byer (1985)	Fine structure of the 2s2p of one-muon, two-electron systems, Z=2-5.
Drake and Makowski (1985)	Two-electron QED corrections for He-like ions.
Ermolaev (1985)	Low-lying S-states of 2-electron atoms.
Fricke and Rashid (1985)	MCDF ground-state energies of two-electron atoms, Z=1-90.
Froese Fischer and Saha (1985)	The carbon sequence. Both $2s^2 2p^2$ and $2s2p^3$ levels. MCHF+BP. Z=6-30. For Z<20 better results than from other theories.
Frye and Armstrong (1985)	The $3p^6-3p^5 3d$ transition in Fe IX, Ti V, $3s^2 3p-3s3p^2$ in FeXIV using "Liouville DF" theory.
Gould (1985)	Review on very heavy few-electron atoms.
Grant (1985)	A review.
Gurchumeliya et al. (1985a)	Cu-like systems.
Gurchumeliya et al. (1985b)	Zn-like systems.
Hata et al. (1985); Cooper et al.(1984)	Additional terms from the anomalous electron g-factor to the Breit-Hamiltonian.
Hay and Wadt (1985a)	Valence levels of the 3d, 4d and 5d transition metals, as a test of the PP.
Huang (1985)	Fe XII-XIV.

Table 5.2. (continued).

Huang and Johnson (1985)	MC RRPA for ns^2 - nsnp of Mg- and Zn-like ions.
Ivanova et al. (1985)	4-4 transitions in the Zn sequence, Z=36-50. Also the 4lj and 5lj levels of the Cu sequence, Z=36-60.
Ivanova et al. (1985b)	Mg-like $3l_1 3l_2$ series, Ne-like $2p^{-1}3l$ and $2s^{-1}3l$ series using model potentials. Z=16...26.
Jankowski and Polasik(1985)	$3d^n$ and $3d^n4s^m$ configurations of Ni. QR HF+correlation.
Johnson and Cheng (1985)	A review on inner shells.
Kagawa and Malli (1985)	DF-LCAO on Kr, Xe, Hg, Rn.
Karwowski and Styszynski (1985)	Ground-state energies in the He, Be, Ne sequences. An estimate is found for the relativity-correlation cross term.
Kiyokawa et al.(1985)	X-ray spectra of Au^{n+}, n = 26-31. DS.
Kotochigova (1985)	VUV spectrum of Eu I. DF.
Koutecky et al. (1985)	Valence levels of Rh and Pd, as a test of QR PP.
Krauss et al. (1985)	Valence levels of Ag and Au, as a test of QR PP.
Kreuzer et al. (1985)	Properties of Fe^{2+}, Fe^{3+} as function of c.
Lawen and Klar (1985)	Fine structure in hyperspherical coordinates.
Matsushita et al. (1985)	S-o splitting of Se. The method gives a relativistic total-energy correction of wrong sign.
Mayo et al. (1985ab)	MCDF levels for Al VII, VIII.
McMichael Rohlfing and Hay (1985)	Valence levels of Ni, Pd, Pt as a test of QR PP.
Mohr (1985ab)	QED of high-Z few-electron atoms.
Pal'chikov (1985)	Correction energy of He-like systems.
Rohlfing and Martin (1985)	Valence levels of Ni. 4th order n.r. Moller-Plesset PT+QR corrections.
Rose (1985)	Line coincidences in He-like ions. MCDF.
Selvaraj and Gopinathan (1985a)	Electron binding energies for Na-Cs, Ne-Xe and Zn-Hg using an LDF method ("$R\Xi$").
Selvaraj and Gopinathan (1985b)	Shake-up energies using the $R\Xi$ method.
Stamp (1985)	1s2s - 1s2p ^3P transitions of He-like systems, Z=2-16.
Vainshtein and Safronova (1985b)	He-like (1snl) and Li-like ($1s^2nl$) series, n=2-5. Z<43. 1/Z.
Varade et al. (1985)	QR valence levels for alkali atoms.
Veseth (1985)	Isotope effect in atomic fine structure. C, Ne^+, Cl, Ar^+, Br. MBPT.
Viktorov and Safronova (1985)	2s-2p transitions for Be- and O-like systems, Z=4-100.
Wilson et al. (1985)	4d-shell PES of Sn.
Zapryagaev et al. (1985)	Theory of multicharged 1- and 2-electron ions. A book.

Table 5.3. Auger and autoionization processes.

Reference	Comments
Massey and Burhop (1935)	Relativistic theory of the Auger effect, based on Moller's (1932) electron-electron interaction, and using screened Dirac-Coulomb orbitals.
Asaad (1959); Asaad and Petrini (1976)	The K-LL Auger spectrum.
Listengarten (1961, 1962)	Auger probabilities for heavy elements.
Chattarji and Talukdar (1968)	The KLL Auger TP.
Bhalla (1970ab)	DS calculations of K-LM intensities.
Bhalla and Ramsdale(1970ab)	DS calculations of K-LL intensities.
Bhalla et al. (1970)	DS calculations of K-LM and K-MM intensities.
Manson (1971)	1s2s2p autoionization states of He^- and Li, including fine structure.
Safronova (1975b)	Autoionization states of two-electron systems.
Briancon and Desclaux(1976)	K-LL energies for Ne, Ar, U, Am. MCDF.
Chattarji (1976)	Theory of Auger transitions. A book.
Chen et al. (1977, 1979a-c, 1980a-c, 1981cd, 1983bd)	K, L and M shell Auger and Coster-Kronig energies and intensities.
Larkins (1977)	Semiempirical Auger energies, fit to DF, for Z=10-100.
Huang (1978)	Relativistic theory of radiationless transitions in atoms.
Safronova and Senashenko (1978)	Three-electron $1s^0$ systems, Z=2-10.
Safronova and Lisina (1979)	Autoionization states in the Be sequence, Z=6,8,10-42.
Tunnell et al. (1979)	The 1s2s3p4p (J = 5/2) state of Ar.
Johnson et al.(1980b);Johnson and LeDourneuf (1980)	Beutler-Faro autoionization resonances of rare gases.
Vainshtein and Safronova (1980, 1984)	Autoionization widths of two-electron satellites of He- and Li-like ions.
Darko et al. (1981)	The KLM Auger spectrum of Ar.
Lisina and Safronova(1981)	Autoionization of 2131' states of two-electron ions, Z=5-30.
Tulkki and Keski-Rahkonen (1981)	Coster-Kronig rates for metallic Zr, Rh, Ag. MCDF.
Vage et al. (1981)	Autoionization widths of ^1P states of He-like systems, Z=8-30.
Aberg and Howat (1982)	Theory of the Auger effect. A review.
Chen (1982)	Review on Auger intensities.
Weightman (1982)	X-ray excited Auger and photoelectron spectroscopy. A review.
Aksela and Aksela (1983ade)	$M_{4,5}N_{4,5}N_{4,5}$ of Cs and I in Cs and CsI.
Aksela and Aksela (1983b)	$N_{4,5}N_{6,7}X$ of Hg.
Aksela and Aksela (1983c)	$M_{4,5}N_{6,7}X$ of Yb.

Table 5.3. (continued).

Bruneau (1983)	MCDF calculation of Ar Auger processes.
Chen and Crasemann (1983)	Gauge dependence of Auger rates found small.
Chen et al. (1983a)	Auger rates for 1s2s2p states of Li-like systems, Z=6-10.
Chorkendorff et al. (1983)	The 4p and 4d Auger spectra of Yb.
Hedegard and Johansson (1983)	MNN Auger energy shifts in 5d transition metals.
Kotochigova and Tupitsyn (1983)	Influence of auto-ionization states on non-linear ionization.
Lisina and Safronova(1983)	Autoionization of 1s2l3l' states of three-electron ions.
Vidolova-Angelova et al. (1983)	Narrow, low-lying autoionization states of Yb^-.
Aksela et al. (1984a)	Open-shell configurations ns^1 of K, Ag, Au
Aksela et al. (1984b)	Several free atoms, Ne - Hg.
Aksela et al. (1984c)	$5s^0$ and $5s^1$ configurations of Xe.
Aksela et al. (1984d)	$4s^0$ and $4s^1$ configurations of Kr.
Aksela et al. (1984e)	NOO Auger spectra of Au.
Aksela et al. (1984f)	MNN Auger spectra of Pd.
Braun et al. (1984)	A book on relativistic theory of atoms, including autoionization processes.
Safronova (1984)	Autoionization widths of $1s2s^2$ and $1s2p^2$ states.
Safronova et al. (1984)	Autoionization states 1s2s2p in the Li-like series.
Safronova and Tsirekidze (1984)	Autoionization widths of 1s2s2p, $1s2s^2$ and $1s2p^2$ states, Z=6-30.
Trusov et al. (1984)	KLL Auger rates of Kr. MCDF.
Aglitskii and Safronova (1985)	A book on autoionization states.
Aksela and Aksela (1985a)	$L_{2,3}M_{4,5}M_{4,5}$ of Ga and Ge.
Aksela et al. (1985a)	$M_{4,5}N_{4,5}N_{4,5}$ of In and Sn.
Aspromallis et al. (1985)	Autoionization of Be^-.
Aymar (1985)	5dnd autoionization states of Ba.
Bhattacharya et al. (1985)	Effects of additional vacancies.
Chen (1985a)	Auger rates of Be-like systems.
Chen (1985b)	LMM Auger energies and rates Z=18-92.
Kellokumpu and Aksela(1985)	An anomalous MNN Auger spectrum of Ba.
Safronova and Vainshtein (1985)	Dielectronic satellites of Be-like ions, Z=6-42.
Selvaraj and Gopinathan (1985b)	Shake-up intensities using the $R\Xi$ method.

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
Sucher (1958)	The IP of He.
Keller et al. (1970)	DS IP of the groups 13 (Al-113) and 14 (Ge-114).
Penneman et al. (1971)	Various IP_n and the chemistry of element 164. DF.
Snyder (1971)	Relativistic contributions to the IP of the Li-, Be-, B- and F-like sequences, ionicity=0-9. 1/Z.
Keller et al. (1973)	DS IP1 - IP4 of group 11 (Cu-111).
De Sequeira and Connolly (1974)	DS TS IP1-4 of Th, IP1-6 of U.
Keller et al. (1974)	DF and DS IP1 - IP3 of group 15 (P-115).
Fraga et al. (1975)	HF IP with 1st-order relativistic corrections.
Baylis (1977)	DF IP from various shells of Hg, with a core-polarizability term appended.
Grant and Pyper (1977)	MCDF IP(1+2), IP(1-4) for groups 14 (Pb, 114) and 16 (Te-116), respectively.
Catlow (1978); Pyper and Grant (1978b)	IP1 - IP6 of U. MCDF+empirical correlation term.
Hafner and Schwarz (1978a)	EA of Li - Cs, Cu - Au using PP-MCDF+CI.
Pyper and Grant (1978a)	The relation between successive IP:s, $IP_n = n\ IP_1$, holds for s and p elements, not for d or f elements. Z=4...84...116.
Connerade et al. (1979)	Double ionization anomaly in Ba.
Sen et al. (1980, 1981)	DS calculation of the EA of lanthanoids an other heavy atoms.
Borovik et al. (1981)	DS calculation of IP_1 - IP_6 of Bi.
Martin and Hay (1981)	Relativistic (QR HF) contributions to the IP of 3d, 4d and 5d elements.
Cole and Perdew (1982)	QR-LDF EA for Z=2-86.
Jeung et al. (1982)	IP and EA of Cs, as a test of a QR PP including core-valence correlation.
Migdalek and Baylis(1982a)	The IP in the Cu-, Ag-, and Au-like sequences, Z=29-36, 47-53, 79-82.
Migdalek and Baylis(1982b)	EA for halogens, F-I.
Laskowski et al. (1983b)	IP of Cs as a test of the PP.
Nowak et al. (1983)	Relativistic contributions to the EA of alkali and halogen atoms from a HF-DF comparison.
Savin et al. (1983)	Influence of a LDF correlation correction on the DF IP of s^1 systems (K-Cs, Cu-Au, Ca^+-Ba^+, Zn^+-Hg^+).
Stoll et al. (1983, 1984)	EA of Cu, Ag as test of a PP.
Schwarz et al. (1983)	Relativistic contributions to IP analysed.

Table 5.4. (continued).

Baerends et al. (1984)	Perturbative HFS IP of Ne-Rn, Hg.
Bauschlicher et al.(1984a)	EA of Cu.
Chamizo (1984); Smith (1975)	The anomalous EA of Pb and IP of Bi attributed to relativity.
Migdalek and Bojara (1984)	IP of the Rb and Cs sequences (Z=37-42, 55-59).
Chen et al. (1985a)	Residual limitations of inner-electron binding energies.
Connerade et al. (1985)	Inner-shell IP of Ar...Hg by the "g-Hartree" method.
Fuentealba et al. (1985)	Group 2 IP_1 (Be-Ba). An accuracy of 0.02 eV claimed. PP-CI with a core polarizability correction.
Sen et al. (1985)	Relativistic LDF calculation of the "hardness" parameter (IP-EA)/2 for Z=5...15.
Wang (1985)	IP of Cu, as test of a PP.

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

Reference	Comments
Popov (1971)	On critical nuclear charges.
Zeldovich and Popov (1971)	"Superheavy atoms".
B. Mueller et al. (1972a)	A localised K-shell with a finite width found below Z=169. Positrons escape from K holes.
B. Mueller et al. (1972b, 1973b)	Electron shells in over-critical fields.
B. Mueller et al. (1973)	The two-centre Dirac equation.
Marinov et al. (1975)	Methods for solving the two-centre problem for R_{cr}.
B. Mueller et al. (1975)	Spectroscopy of superheavy two-centre orbitals.
Smith et al. (1975)	Dynamical theory of intermediate molecular phenomena.
Marinov and Popov (1976)	The "critical radius R_{cr}" for an electron in the field of two bare nuclei. Quotes earlier work.
Morovic et al. (1976)	M x-rays for Au+I.
B. Mueller (1976)	Review on positron creation.
B. Mueller and Greiner (1976)	Detailed, basis-set solution of the two-centre Dirac equation, Br-Br ... U-U.
Morovic et al. (1977)	L x-rays for Xe+Ag.
Popov (1977)	Superheavy (supercritical) atoms.
Reinhardt and Greiner(1977)	A review.
Morovic et al. (1978)	$Xe^{22+}+Ag^{19+}$.
Mur and Popov (1978); Popov et al. (1978, 1979); Eletskii et al. (1979)	Semiclassical approximation for the Dirac equation in strong fields.
Rafelski (1978); Rafelski et al. (1978)	Reviews. Fermions and bosons in arbitrarily strong external fields.
Soff et al. (1978)	Energies for one-electron Er-Er and Xe-Pb at R=100...1000 fm.
Soff et al. (1979)	Electrons in superheavy quasimolecules, using a basis from the two-centre Dirac equation. Bare nuclei only. A monopole (one-centre) approximation also considered Ionization, excitation and delta-electron emission considered.
Wietschorke et al. (1979)	The critical radius evaluated, for U+U etc., using a DS model within the monopole approximation.
Mur and Popov (1980)	Shifts of electronic levels due to finite nuclear sizes. Application on the critical radius.
Burnap et al. (1981)	A Dirac Hamiltonian for strong Coulomb fields.
Sepp et al. (1981)	DS for $(Pb\text{-}Pb)^{68+}$.

Table 5.5 (continued).

Soff et al. (1981)	Spin-polarization for a superheavy collision system, $Z_1+Z_2=178$, in a strong magnetic field, $B < 10^{16}$ G.
Greiner and Scheid(1982)	A review.
M. Mann et al. (1982)	S-o effects cause novel couplings around Z=165.
Morovic et al. (1982)	$2p\pi$ - $2p\delta$ crossings for homonuclear systems, Z_1=18...82.
U. Mueller et al. (1982, 1983)	Theory of positron creation.
Soffel et al. (1982)	Stability and decay of the Dirac vacuum in external gauge fields. A review.
Kobe and Kennedy (1983)	Gauge invariance in heavy-ion collisions.
Krause and Kleber (1983, 1985)	Time-dependent Dirac equation solved for inner-shell ionization and positron production.
Soff et al. (1983)	Electron excitation processes and QED in high-Z systems: a review.
de Reus et al. (1984)	The influence of electron-electron interaction on K-hole, delta-electron and positron production.
Baer and Soff (1985)	Relativistic wave packets and delta-electron emission.
Bottcher and Strayer (1985ab)	Numerical solution of the time-dependent Dirac equation for U+U, U+Cm.
Greenberg (1985)	A session summary on superheavy collision systems.
Greiner et al. (1985)	A review.
Mehler et al.(1985)	Delta electron emission for Z>137.
Mehler et al. (1985b)	Coupled-state analysis of electron excitations in asymmetric collision systems.
Schlueter et al. (1985)	Bound electrons in critical magnetic fields.
Soff et al. (1985)	Ionization and positron emission in giant quasiatoms.

Table 5.6. Electromagnetic transition probabilities.

Reference	Comments
Levinger and Rustgi(1956); Levinger et al. (1957); Payne and Levinger (1956)	Relativistic corrections to the dipole sum rule. K shell, Coulomb wave functions. See Grant (1957).
Taylor and Payne (1960)	Retardation and K x-ray relative intensities.
Babushkin (1962b,1964, 1965)	Relativistic treatment of radiative transitions (E and M, various multipolarities). K shells.
Cromer (1965a)	DS oscillator strengths and dispersion terms for Z=10-98.
S.H. Lin (1966)	TP for the $^5S_2(2s2p^3)$ $^3P_2$ transitions of C.
Anderson et al. (1967)	DS calculations for the 6p electron of Tl.
Dogliani and Bailey (1969)	Relativistic corrections to the Thomas-Reiche-Kuhn sum rule.
Scofield (1969)	Radiative TP of K- and L-shell vacancies. DS.
Bhalla (1970c)	DS TP of Tl.
Rosner and Bhalla (1970)	DS x-ray TP for Z=21-93.
Drake (1971)	M1 lifetime of the $2\ ^3S$ state of He-like ions.
Feinberg and Sucher (1971)	$2\ ^3S_1 - 1\ ^3S_0$ TP in He.
Feneuille (1971)	Relativistic theory of TP in atoms.
Lu et al. (1971b)	K x-ray intensities for Z=92-126. DS.
Drake (1972)	Relativistic corrections to radiative TP.
Koenig (1972)	The np-6s TP of Cs using a model potential
Bhalla (1973)	DS TP of In, Ga.
Drake (1973)	Radiative decay of metastable states of the H and He sequences.
Kim and Bagus (1973)	The resonance (ns^2-nsnp) transitions of Mg-Ba. MCDF.
Luc-Koenig et al. (1973)	The $P_{1/2}$-$P_{3/2}$ TP of np^5 Br and I.
Sinanoglu and Luken (1973, 1976)	The B-like series, $2s^22p$-$2s2p^2$ TP.
Cheng et al. (1974)	M2 TP of ^4P Li-like ions for Z=3-26. DF.
Garpman et al. (1974)	$np^3(n+1)s$ - np^4 TP of Se I and Te I.
Grant (1974); Grant and Starace (1975)	Gauge invariance and radiative transitions.
Holmgren and Garpman(1974)	$np(n+1)s$-np^2 transitions of group 14(Si-Pb).
Johnson and C.-P.Lin(1974)	1s2s - $1s^2$ TP in the He sequence.
Kaniauskas et al. (1974, 1979)	Theory of EM multipole transitions.
Luc-Koenig (1974)	$^{1,3}P_1$ - $^1S_0$ TP for groups 2 and 12 (Ca-Ba, Zn-Hg).
Safronova et al. (1974)	1s-2s and 1s-2p TP for He-like ions, Z=9...22.
Scofield (1974a)	Exchange-induced nonorthogonality corrections to K x-ray TP.
Scofield (1974b)	DS TP for K- and L-shell x-rays.
Scofield (1974c)	DF values of L x-ray TP.

Table 5.6. (continued).

Desclaux and Kim (1975)	MCDF for the 6p-6s transitions of Au, Hg.
Feinberg and Sucher (1975)	M1 transitions in charmonium.
Friar and Fallieros (1975)	Thomas-Reiche-Kuhn sum rules for a particle in a potential.
Klimchitskaya et al.(1975)	TP for two-electron multicharged ions.
Safronova (1975)	$2s^2 2p^4$ - $2s2p^5$ - $2p^6$ TP for O-like systems, Z=8-19.
Younger and Weiss (1975)	Hydrogen-like relativistic correction factors for E1 TP.
Armstrong et al. (1976)	E1 TP of the Li and Be sequences in MCDF. Two gauges tested.
Bogdanovich et al. (1976)	The oxygen-like sequence.
Drake (1976)	Spin-forbidden E1 transitions.
Garpman and Spector (1976)	The $5p^4 6p$ - $5p^4 6s$ transitions of Xe II.
Johnson and Lin (1976)	RPA TP for the E1, M1 and M2 TP for the $1s^2$ - 1s2p, 1s2s transitions of He-like systems, Z=2-100.
Kim and Desclaux (1976)	Resonance transitions of Li- and Be-like systems, Z=3-90.
Migdalek (1976ab)	Al I - Tl I and Al III - Tl III "sharp", "principal" and "diffuse" series.
Migdalek (1976c)	The Au I series, Z=79-83.
Migdalek (1976d)	Group 14 (Si II - Pb II).
Migdalek (1976e)	Group 15 (P III - Br III).
Muehlethaler and Nussbaumer (1976)	E1,M1,E2,M2 TP within $2s^2$-2s2p-$2p^2$ in the Be I sequence, Z=4-28.
Safronova and Bolotin (1976)	The $2s^2 2p^3$ - $2s2p^4$ - $2p^5$ TP of N-like systems, Z=7-30.
Aymar and Luc-Koenig(1977)	TP in the Mg sequence.
Bogdanovich et al. (1977, 1978)	Si VII, Ca XIII, XV, Fe XIX-XXI.
Cheng and Johnson (1977ab)	TP in the Be, Mg sequences.
Dankwort (1977b)	TP of the Mg 3s3p $^3P_1$ - $3s^2$ ^1S intercombination line.
Hodge (1977)	Two-electron,one-photon x-ray transitions.
Kagawa (1977)	Two-electron,one-photon x-ray transitions. Z=10...29.
C.D. Lin et al. (1977)	n=2 states of He-like ions.
D.L. Lin (1977a)	Transition operators for two-electron systems.
D.L. Lin (1977b)	Gauge properties of DF and RPA.
D.L.Lin et al. (1977)	E1 TP in the Ar sequence.
Safronova and Rudzikas (1977)	The 1s-2p TP for He-like systems, Z=2... 100.
Shorer et al. (1977)	$3s^2$ - 3snp TP in the Mg sequence, Z=12-92. RRPA.
Shorer and Dalgarno(1977)	RRPA for the Zn sequence.
Soff and Mueller (1977)	K-, L- and M-shell TP for the superheavies Z=114,...173. DS.
Weiss (1977)	E1 TP of the Li-, Na- and Cu-like series. HF+BP energies, hydrogenic correction factors for TP. (See Younger and Weiss (1975)).
Braun (1978, 1984)	PT for TP of two-electron systems.
Braun and Labsowski (1978)	A review.

Table 5.6. (continued).

Cheng and Kim (1978)	Cu-like ions.
Flambaum and Sushkov(1978)	6p-ns TP of Tl, Pb, Bi using a model pot.
Glass and Hibbert (1978b)	Influence of the Breit interaction on the $2s2p\ ^3P_1 - 2s^2\ ^1S_0$ transition of Be-like systems, Z=4-10, 14.
Hafner and Schwarz (1978b)	Valence-shell E1 TP for groups 1 (Cs), 2 (Ca^+, Ba^+, Ca, Ba), 11 (Cu-Au) and 12 (Zn-Hg). PP-MCDF+CI.
Ivanov et al. (1978)	Level widths of 2-electron $2s^2$, $2p^2$, 2s2p levels, Z=10...60.
Kim and Cheng (1978)	The 3s-3p and 3s-4p TP of Na-like ions, Z=11...90.
D.L. Lin et al. (1978)	M2 transitions in the Be sequence.
Luc-Koenig and Bachelier (1978)	The principal series of Rb.
Marrus and Mohr (1978)	Review on forbidden transitions of two-electron systems.
Migdalek (1978a)	Group 11 (Cu I - Au I).
Migdalek (1978b)	Group 13.
Migdalek and Baylis (1978, 1979a,c)	ns-np and np-nd TP in group 11 (Cu-Au).
Nussbaumer and Storey(1978)	The E2,M1,M2 TP for $2s^2$-2s2p of C III.
Shorer (1978)	Effect of 3d shells on the 4s-4p resonance TP in the Zn sequence. RRPA.
Sucher (1978)	Theory of M1 transitions.
Sushkov et al. (1978)	Theory of M1 transitions: 6s-7s of Cs, 6p-np of Tl using a model potential.
Vainshtein and Safronova (1978)	TP of satellites to resonance lines of He-like ions, Z=4-34. 1/Z.
Weinberger and Rosicky (1978)	L and M x-ray TP for V and Nb.
Bureeva and Safronova(1979)	The Ne sequence.
Cheng and Kim (1979)	The Ag sequence.
Cheng et al. (1979)	E1, E2 and M1 TP of Li-like systems, Z=3-9.
Desclaux (1979)	Review of relativistic effects on TP.
Drake (1979)	$1s2p - 1s^2$ transitions of He-like ions, Z=2-100. (Both ^3P and ^1P)
Farrag et al. (1979, 1980)	E1 transitions within the ground complex of B-like systems, Z=5-93.
Gruzdev and Sherstyuk (1979)	The 3p-3d and 4p-4d E1 TP for Na-like systems, Z=11-42, using "effective orbital quantum numbers".
Gurchumeliya and Safronova (1979, 1980)	Radiative and non-radiative linewidths. Application on the $2p_{1/2}\ 3p_{3/2}$ levels of two-electron ions, Z=5-45.
Hansen and Persson (1979)	The $5s5p^6$ state of Xe II.
Laughlin and Victor (1979)	The Mg I $3s^2$-3s3p TP for Z=12-18.
Migdalek (1979)	Group 14 (Sn I, Pb I) np^2-np(n+1)s transitions.
Migdalek and Baylis (1979b,e)	s-p transitions of the Rb I and Cs I sequences.
Migdalek and Baylis (1979d)	p-s and p-d transitions in group 13 (Ga I-Tl I).

Table 5.6. (continued).

Nussbaumer and Storey(1979)	$2s^2$ - 2s2p TP for Be-like Ca...Mo.
Shorer (1979)	RRPA for the 2p-3s and 2p-3d TP in the Ne sequence.
Tunnell and Bhalla (1979)	M1 TP in the Be sequence, Z=4...92.
Zapryagaev et al. (1979)	The 2 ^3S - 1 ^1S TP of He-like systems, using Coulomb Green functions.
Bardsley and Norcross(1980)	Tl, using a semiempirical potential.
Driker and Ivanov (1980b)	Fe X hole-state E1, M1 and autoionization TP.
Johnson et al. (1980a); Johnson (1983)	Reviews RPA work.
Klimchitskaya (1980)	2s-1s TP for a hydrogenic atom in a strong homogeneous E.
Migdalek (1980)	Yb II - Hf IV. Lowest s-p transitions.
Roshchupkin and Inopin (1980)	Relativistic corrections to multipole sum rules and the f-sum rule (nuclear ones).
Safronova and Safronova (1980)	The 2s-2p and 1s-2p TP for Li-like ions, Z=10-100.
Vainshtein and Safronova (1980)	Dielectronic satellite TP for He-like ions, Z=6-33.
Anderson and Anderson (1981ab, 1983)	E1-E3, M1, M2 transitions of Be, Mg and Zn-like systems. MCDF.
Bhalla and Tunnell (1981)	DF TP for 1s2s2p states of the Li series, Z=3-26.
Chen et al. (1981b)	Widths and fluorescence yields of L-shell vacancy states.
Farrag et al. (1981, 1982)	E1 transitions within the ground complex of Al-like systems, Z=13-93.
Gabriel et al. (1981)	Analytic expressions for L - K TP in a screened Coulomb potential. Retardation and all multipoles included.
Glass (1981)	Spin-forbidden $2p^2$-2s2p transitions in Be-like systems.
Karwowski and Szulkin (1981);Szulkin and Karwowski (1981)	A QR approach with different orbitals for different j. Valence transitions for alkali-like systems.
Shorer (1981)	The 6s-6p resonance TP of Hg.
Vajed-Samii and MacDonald (1981)	E1 TP of Cl-like ions, Z=26...82. MCDF.
Vajed-Samii et al. (1981a)	E1 and M1 TP in the B sequence. MCDF.
Braun et al. (1982)	Be- and B-like atoms, Z<101.
Chen (1982)	Review on inner-shell TP.
Chen et al. (1982b)	The $1s2p^2$ states of Li-like systems.
Drawin (1982)	Review on highly ionized atoms.
Edlabadkar and Mande(1982)	E1, M1 K and L shell TP, Z=57-82. LDF.
Glass (1982ab)	Spin-forbidden E1 lines for Be-like ions, Z=6-10.
Glass (1982b)	Ditto. The allowed $2s^2$-2s2p transition. Z = 26...74.
Goldman and Drake (1982)	Relativistic sum rules.
Hardekopf and Sucher (1982)	Dipole decay in quarkonium.
Huang (1982)	Relativistic MBPT of atomic transitions. The relativistic equation-of-motion approach.
Johnson and Huang (1982)	$2s^2$-2s2p TP for Be-like systems, Z=4-28.

Table 5.6. (continued)

Judd and Pooler (1982)	A two-photon process involving a $4f^6 5d$ state explains the anomalously high $^8S_{7/2}$ - $^6P_{7/2}$ TP of Gd^{3+}.
Mendoza and Zeippen (1982)	Forbidden lines in the $3p^2$ configuration.
Migdalek (1982ab)	One-electron spectra of Yb^+, Lu^{2+}.
Parpia and Johnson (1982)	2E1 and M1 decay of 2s states of hydrogenic atoms, Z = 1-92.
Pokleba and Safronova (1982,1984)	2-2 and 3-3 transitions in the Ne series, Z=14...42.
Arndt and Hartmann (1983)	Fluorescence yields of highly stripped atoms.
Aspromallis et al. (1983)	Processes needed for Li lasers.
Biemont and Bromage (1983)	Forbidden lines for the $3p^2$ sequence, S^{2+} - Sn^{36+}. QR.
Bodashko and Safronova (1983)	Two-electron single-photon transitions for two-electron atoms.
Chen and Crasemann (1983)	Gauge-dependence of inner-shell transitions.
Chen et al. (1983a)	The 1s2s2p states of Li-like systems, Z=6-10.
Dyall (1983)	Excited-state populations following 1s ionization of Ar.
D.G. Ellis (1983)	$1s^2 2s2p$ lifetimes for Ne VII - Fe XXIII. MCHF+Pauli.
Fawcett (1983a)	E1 transitions within the ground complex of Al-like systems, Z=17...28.
Fawcett (1983b)	E1 transitions within the ground complex of Mg-like systems, Z=16...28.
Froese Fischer (1983)	M1 and E2 TP for the $2p_{1/2}$-$2p_{3/2}$ transition in the B sequence, Z=5-54.
Froese Fischer and Saha (1983)	M1 and E2 TP in the $2p^4$ series, Z=8-42.
Gurchumeliya et al.(1983)	Doubly excited states of multicharged ions
Huang et al. (1983)	Cl-like systems, Z=17-92. E1, E2 and M1.
Migdalek (1983)	Some ions with ns^2np (n=4-6) configurations.
Rudzikas et al. (1983)	2s-2p TP of the Be sequence, Z=6...92.
Victor and Taylor (1983)	The Cu- and Zn-like sequences, Z=29-42. A model potential method.
Zilitis (1983a)	E1 TP for Li-like ions.
Bauschlicher et al.(1984b, 1985ab)	Ca - Ba.
Braun et al. (1984)	Book on the relativistic theory of atoms.
Bruneau (1984)	ns^2-nsnp TP in neutral atoms. MCDF.
Chen and Crasemann (1984)	M x-ray emission rates. DF.
Crossley (1984)	Review of TP.
Dmitriev et al. (1984)	Book on the relativistic theory of atoms.
Fawcett (1984)	Allowed n=2-3 transitions in Be-like ions, Z=8...28.
Fawcett (1984b)	Allowed n=2,3 transitions in Be-like systems, Z=4-7.
Feldman and Fulton (1984)	Gauge invariant theory of radiative transitions.
Froese Fischer and Saha (1984)	E1 TP for $2s^2 2p^4$ - $2s2p^5$ in the O series, Z=8-42. MCHF + BP.

Table 5.6. (continued).

Godefroid and Froese Fischer (1984)	E2 and M1 TP for the N sequence, Z=7...30.
Grant (1984ab)	Reviews.
Huang (1984)	E1, E2 and M1 TP of P-like ions, Z=16-92.
Langhoff et al. (1984)	The ^1P, $^3P_1$ TP of Mg - Sr.
Migdalek (1984)	$4f^n6s^2$ - $4f^n6p^1$ TP of Eu II, Tb II, Ho II.
Migdalek and Baylis(1984a)	Hg $6s^2$-6s6p, with a new, combined correlation approach.
Mukoyama and Adachi(1984ab)	DS x-ray TP for Z=58-92.
Mukoyama and Kagawa (1984)	TP for a K-shell vacancy in Cu, Ag, W, Au. DF-LCAO.
Vainshtein and Safronova (1984)	TP for two-electron satellite spectra of Li-like ions.
Baluja and Hibbert (1985)	Fe XV.
Braun and Parera (1985)	TP for weakly relativistic atoms using an effective potential.
Chen (1985a)	X-ray emission rates of Be-like systems.
Chen (1985c)	Review.
Drake (1985)	E1M1 TP for He-like U.
Froese Fischer and Saha (1985)	E1, E2 and M1 TP between $2s^22p^2$, $2s2p^3$ levels in the C series, Z=6-30.
Frye and Armstrong (1985)	The $3p^6$-$3p^53d$ transition in Fe IX, Ti V, $3s^23p$-$3s3p^2$ in Fe XIV using "Liouville" DF theory.
Godefroid and Froese Fisher (1985)	TP of the 3s4p ^3P levels of Mg-like S and Cl.
Grant (1985)	A review.
Huang (1985)	Fe XII - Fe XIV.
Huang and Johnson (1985)	MCRRPA for Mg- and Zn-like ions, ns^2 - nsnp.
Migdalek and Baylis(1985a)	$6s^2$-6s6p TP in the Hg sequence, Z=80-86.
Schmitt and Arenhoevel (1985)	Integrated photoabsorption strength and sum rules for a bound Dirac particle (for nuclei).
Viktorov and Safronova (1985)	2s-2p TP for Be- and O-like systems, Z=4-100.
Zapryagaev et al. (1985)	A book on multicharged 1- and 2-electron ions.
Zilitis (1985a)	Fundamental series of Na-like ions.

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

Reference	Comments
Johnson and Feiock (1968)	DS E1, E2, M1 and M3 polarisabilities and shielding factors for Z=2-92 neutral atoms
Flambaum and Sushkov(1978)	α_1 of Tl, Pb, Bi using a model potential.
Skovpen and Flambaum (1978)	$\underline{\underline{\alpha}}^1$ tensor for Tl.
Konowalow et al. (1979)	α_1 of Zn-Hg using relativistic PP.
Basch et al. (1980)	PP-DF α_1 of Xe, Pb.
Pal'chikov (1980)	$\alpha_1(\omega)$ for He-like ions.
Rosenkrantz et al. (1980)	$\underline{\underline{\alpha}}_1$ tensors for the lowest S and P states of group 12 $(Zn - Hg)_2$ PP.
Desclaux et al. (1981)	DF α_1 for ns^1 and ns^2 atoms, He-Hg.
Sin Fai Lam (1981)	Relativistic effects on α_1 of s^2 and p^6 atoms investigated, using an approximation by Pople and Schofield.
Christiansen and Pitzer (1982)	PP-DF α_1 of Rb, Cs.
Kolb et al. (1982)	Formulates the RRPA theory of electric and magnetic susceptibilities and shielding factors. He-Rn, Be-Ba, Zn-Hg.
Fuentealba (1982); Fuentealba et al. (1983)	α_1 of ns^1 atoms using empirical PP.
Krauss et al. (1982)	Polarisabilities of Xe, Xe^+ as a test of QR PP.
Pal'chikov (1982)	χ_1 for He-like systems, Z=2-100.
Weinhold (1982)	Mass-polarisation and BP corrections for the α_1 of He.
Johnson et al. (1983)	RRPA susceptibilities α_1, α_2, χ_1 and shielding factors γ_1, γ_2, σ_1 for the He, Ne, Ar, Cu^+, Kr, Pd and Xe sequences.
Parpia and Johnson (1983, 1984)	TD LDA α_1 for Kr-Xe, Sr-Ba, Cd-Hg.
Pyper (1983bc)	Relativistic contributions to σ_1.
Stevens and Krauss (1983a)	$\underline{\underline{\alpha}}_1$ of Xe, Lu, Hg^+, Hg, Tl, At from PP. Shape-consistent ones superior.
Stoll et al. (1983)	α_1 of Cu, Ag as test of a PP.
Childs and Cheng (1984)	Sternheimer factors for 4f and 5d shells, Z=63-79.
Gollisch (1984)	LDF α_1 for 2nd and 3rd row atoms (Li-Ar) and group 11 ones (Cu-Au).
Liberman and Zangwill (1984)	An LDF program for calculating static and dynamic polarisabilities.
Fuentealba et al. (1985)	α_1 of group 2 (Be-Ba). PP-DF.
Zapryagaev et al. (1985)	χ_1 of He-like atoms (see p. 129).

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
Hargreaves (1929, 1930ab)	Theory of M1 hfs.
Breit (1930a)	Observability of M1 hfs in x-ray spectra.
Fermi (1930)	Derives the "Fermi contact" formula for n.r. M1 hfs of s-states from the Dirac equation.
Breit (1931ab)	M1 hfs of heavy atoms.
Racah (1931ab, 1932)	Relativistic corrections for M1 hfs.
Breit (1932b); Rosenthal and Breit (1932)	Isotope shift in M1 hfs.
Breit and Wills (1933)	M1 hfs in intermediate coupling,
Casimir (1936)	A review of E2 and M1 hfs.
Broch (1945)	Theory of the volume isotope shift in M1 hfs.
Smorodinskii (1947)	Theory of (M1) isotope shift.
Crawford and Schawlow(1949)	Nuclear-structure corrections to M1 hfs.
Bohr and Weisskopf (1950); Bohr(1951)	Nuclear-structure corrections to M1 hfs.
Bodmer (1953)	Introduces finite-nucleus relativistic corrections for isotope shifts.
Schawlow and Townes (1955)	Effect of nuclear volume on x-ray fine structure.
Schwartz (1955,1957)	Theory of M1, M3, E2 and E4 hfs. Radial integrals from a solution of Dirac's equation for a TF potential. Relativistic corrections discussed.
Sessler and Foley (1955)	M1 hfs of $^3He^+$ and ^3He.
Wertheim and Igo (1955)	Isotope shifts in x-ray spectra.
Inokuti and Usui (1957)	Hydrogen-like relativistic corrections for M1 hfs of s-states.
Breit (1958)	Theory of (E0) isotope shifts.
Kopfermann (1958)	Tables of Racah's (1931ab, 1932) relativistic correction factors.
Bodmer (1959)	Theory of isotope shift.
Greenberg and Foley (1960)	Hyperfine anomalies for deuterium, tritium, ^3He.
Stroke et al. (1961)	M1 hfs integrals evaluated for a Hofstadter nuclear model.
Babushkin (1962a, 1963)	Finite nuclear size and the (E0) isotope shift. An $(\alpha Z)^2$ expansion.
Shirley (1964)	Relativistic correction factors for the Moessbauer isomer shift.
Evans et al. (1965)	The relativistic E2 hfs in d^5 Mn.
Sandars and Beck (1965)	A formulation of the relativistic theory of M1 and E2 hfs using LS-coupling.
Coulthard (1967a)	DF M1 and E2 hfs of Mn and Eu.
Hafemeister (1967)	DS Moessbauer isomer shifts, Z=9...55.

Table 5.8. (continued).

Labzovskii (1968)	Three-particle forces and the 1s2s state M1 hfs of ^{3}He.
Tterlikkis et al. (1968)	Restricted DF for alkali atoms.
Bessis et al. (1969)	"Unrestricted HF" calculations of M1 for $(4p)^N$ atoms. Relativistic effects from DS.
Rosen (1969)	Hfs of the Sm ground multiplet. DS.
Seltzer (1969)	K x-ray isotope shifts.
Tucker et al. (1969)	E0 and M1 hfs integrals for Au. DS with Wigner-Seitz boundary conditions.
Desclaux and Bessis (1970)	Both restricted and unrestricted DF for M1 and E2 hfs of Sc, Cu, Ga, Br.
Lurio and Landman (1970)	Hfs evidence for jj-coupling in $6p^2$ Pb.
Sandars (1970)	E2 hfs of the "spherical" N atom. See Raghunathan (1980)
Amoruso and Johnson (1971)	M1, M3 and E2 of Li-Cs, F-I. DS.
Armstrong (1971)	Theory.
Broch (1971)	Theory of E0 isotope shifts.
Childs (1971)	$5p^2$ $^3P_2$ - $^1D_2$ mixing and the M1 hfs of Sn.
Dunlap (1971)	Relativistic effects on hfs (especially of Moessbauer lines).
Labzovskii (1971)	M1 hfs of ^{3}He and $^3He^+$.
Lindhard and Winther(1971)	Enhanced, transient hfs for heavy ions in magnetic materials.
Pyykkoe and Pajanne (1971)	Hydrogen-like relativistic corrections for M1 hfs of s-states. Shown to work for many-electron atoms.
Desclaux (1972)	M1 and E2 hfs of Li-Fr. Core-polarization included in DF for both M1 and E2.
Koenig (1972)	M1 and E2 hfs of Cs valence levels using a model potential.
Luc-Koenig (1972)	M1 and E2 hfs of lowest levels of Xe I.
Rosen (1972)	Hfs of the Bi ground state.
Rosen and Lindgren (1972)	M1 hfs of ns and np state alkali atoms.
Rosenberg and Stroke (1972)	Finite-nucleus effects on M1 hfs.
Coulthard (1973a)	DF isotope shifts of Eu.
Coulthard (1973b)	DF M1 and E2 hfs of lanthanoid atoms and ions.
Feneuille and Armstrong (1973)	Additive nature of relativity and correlation in M1 hfs.
J.Lindgren and Rosen(1973)	Hydrogen-like relativistic corrections for d and f electron M1 and E2 hfs.
Pyykkoe et al. (1973)	Tables of hydrogen-like relativistic corrections for M1 hfs of s and p, and E2 hfs of p orbitals.
Rosen (1973)	Restricted DF for the M1 of $3d^N4s^2$ atoms.
Rosen and J.Lindgren(1973)	Hydrogen-like relativistic corrections for M1 and E2 hfs of p electrons.
Holmgren and Rosen (1974)	M1 and E2 hfs of Bi^+.
Kalvius and Shenoy (1974)	A table of DS isomer shifts (E0).
Lindgren and Rosen (1974)	A review on M1, M3, E2 and E4 hfs of many-electron atoms. The various $\langle r^{-3}\rangle_{ij}$ integrals tabulated for many elements, Z=5...75.
Mahanti et al. (1974)	A comment on relativistic core-polarization and M1 hfs.

Table 5.8. (continued).

Fujita and Arima (1975)	The M1 hyperfine anomaly of electronic and muonic atoms. A new, l=2 core-polarization term.
Trautwein et al. (1975)	Moessbauer shifts of Fe.
de Vries et al. (1975)	DS E0 and E2 parameters for Fe and Sn.
Andriessen et al. (1976)	M1 of Mn. MBPT.
Bauche and Champeau (1976)	Theory of isotope shifts.
Kichkin et al. (1976)	Theory of the hfs in many-electron atoms.
Mallow et al. (1976)	(E0) isomer shifts for 3d, 4d and 5d ions.
Andriessen et al. (1977a)	M1 in Eu. MBPT.
Andriessen et al. (1977b)	Relativistic effects on core polarization. Mn, Fe, Eu, Gd^{3+}.
Desclaux et al. (1977)	Unrestricted DF for transition metals.
Rajnak and Fred (1977)	Isotope shifts (E0) for actinoids. QR HF.
Andriessen et al. (1978a)	A review.
Andriessen et al. (1978b)	M1 in Gd^{3+}. MBPT.
Dunlap and Kalvius (1978)	Theory of Moessbauer isomer shifts (E0).
Glass (1978a)	Hfs of the $1s2p^2$ state of Li.
Glass (1978b)	Hfs of the 1s2s2p state of Li.
Sushkov et al. (1978a)	M1 hfs of Tl, Pb, Bi ground states and np states of Tl, using a model potential.
Wilson (1978a)	QR E0 isotope shifts for Ba II.
Wilson (1978b)	Ditto for Ce II.
Arcimovicz and Dembczynski (1979)	Relativistic effects on M1 and E2 of $6s^2 6p^2$ Bi II.
Band and Fomichev (1979)	(E0) Moessbauer isomer shifts for 25<Z<96. DF.
Gustavsson et al. (1979)	M1, E2 hfs of the 6s5d state of Ba. DF.
Andriessen (1980)	Reviews relativistic MBPT. M1 of Rb, Tl.
Bauche (1980, 1981)	Theory of isotope shifts.
Freeman et al. (1980)	The muonic hyperfine anomalies of Pd, Rh.
Grant (1980)	Many-electron effects in the theory of the (E0) isotope shift.
Raghunathan et al. (1980); Raghunathan (1980)	Explanation of the E2 hfs in the "spherical" nitrogen ground state.
Vajed-Samii (1980); Vajed-Samii et al. (1979, 1981b, 1982ab)	M1 hfs of ground and excited states of the alkali atoms. MBPT.
Antoncik (1981); Antoncik and Gu (1982)	Moessbauer isomer shifts. Ge. DS.
Buettgenbach and Traeber (1981)	CI effects on the hfs of 4d-shell atoms.
Mallow et al. (1981)	The muonic hyperfine anomaly.
Pyykkoe and Wiesenfeld (1981)	Table of DF M1 hfs integrals (s and p) for the main-group elements, Z=1-83.
Ahmad et al. (1982)	M1 of Ba^+. MBPT.
Asada and Terakura (1982, 1983)	Influence of relativity on M1-induced nuclear spin-lattice relaxation in metals (Sc-Tc).
Buettgenbach (1982)	Review of the hfs of 4d- and 5d-shell atoms.

Table 5.8. (continued).

Gabriel and Pratt (1982)	Inner-shell vacancy M1 hfs in a screened Coulomb potential.
Heully (1982); Heully and Salomonsson (1982)	Incorporates M1 hfs in a QR treatment. Various shells of Rb.
Huang and Hughes (1982)	Hfs of muonic He.
Olsson and Rosen (1982a)	M1 and E2 hfs of the 3d elements. DF integrals given.
Olsson and Rosen (1982b)	Ditto for the 4d and 5d elements.
Olsson and Salomonsson (1982)	4s4p state of Ca.
Van Puymbroeck et al.(1982)	M1 hfs of Ga and In atoms. MBPT.
Wilson (1982)	Isotope shifts of Eu.
Ahmad et al. (1983)	M1 of Mg^+. MBPT.
Andriessen (1983)	Reviews relativistic MBPT. M1 of Li-Fr,Tl.
Fricke et al. (1983)	Isotope shifts of Ba I and Ba II.
Grundevik et al. (1983)	Low-lying states of Sr I.
Heully and Martensson-Pendrill (1983ab)	Alkali atoms, up to Fr.
Page et al. (1983)	Volume dependence of the electron density at the nucleus for Z=3-95.
Starchenko and Faustov (1983)	Contribution from weak interactions to the hfs of hydrogen-like atoms.
Ahmad (1984)	E0 and M1 of Au. MBPT.
Blundell et al. (1984)	Isotope shifts related to M1 hfs.
Buettgenbach (1984)	Magnetic hyperfine anomalies.
Cheng et al. (1984)	Interaction of fine and hyperfine structure of doubly excited quintet states of $^7Li^-$.
Chermette (1984)	Spin-polarized QR LDF M1 hfs of Li-Cs.
Desclaux and Freeman (1984)	DF E0, E2 and M1 hfs integrals for actinoid ions.
Dzuba et al. (1984b)	Hfs of Cs and Fr. MBPT.
Olsson et al. (1984)	d^4s^2 and d^5p M1 and E2 hfs of Mo I.
Rosen et al. (1984)	Isotope shifts (E0) for low-lying transitions of Au I.
Zimmermann (1984)	(E0) isotope shifts. Finds a normalization error in Babushkin (1963).
Blundell et al. (1985)	Evaluation of s-electron isotope shifts for 9<Z<96.
Cheng and Childs (1985)	MCDF M1 and E2 hfs of $4f^N6s^2$ states of neutral Pr-Tm.
Dzuba et al. (1985b)	M1 hfs of Ra^+.
Gould (1985)	Review on very heavy few-electron atoms.
Heully and Martensson-Pendrill (1985)	M1 and E2 hfs of s, p and d states of Be^+-Ra^+.
King and Wilson (1985)	QR-HF isotope shifts for Ba I-II.
Shabaev (1985)	Review on E0 and M1 hfs in relativistic atomic theory.
Torbohm et al. (1985)	E0 hfs of low-lying states for groups 2 and 12, and Yb. MCDF.

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

Reference	Comments
Breit (1928)	The g-factor of a hydrogen-like atom.
Margenau (1940)	Relativistic corrections to g-factors.
Lamb (1941)	Relativistic corrections to g-factors.
Phillips (1952)	S-o perturbations on atomic g-values.
Abragam and Van Vleck (1953)	Relativistic effects on the g_J of oxygen.
Perl (1953)	Relativistic effects on the g_J of many-electron atoms.
Judd and Lindgren (1961)	g_J of lanthanoids, including relativistic corrections.
Kneubuehl (1962)	Anisotropic s-o coupling in ESR.
Boyd et al. (1963)	Discovers the relativistic destabilization and expansion of the 5f shell of U.
A.J. Stone (1963)	Gauge invariance of the g-tensor.
Waber and Cromer (1965)	DS r_{max} for atoms and ions, Z=2-102.
Wybourne (1966)	Relativistic contributions to the Gd^{3+} g_J.
Bessis et al. (1969)	g_J of Ga-Br from DS calculations.
Brodsky and Primack (1970)	Foundations of the Zeeman effect.
Grotch (1970)	g-factors of hydrogen-like atoms. (1s states).
Lewis et al. (1970)	DS and DF $\langle r^n \rangle$ for actinoid ions.
Lewis (1971)	DS $\langle r^{-3} \rangle$ and $\langle r^{+n} \rangle$ for crystal field theory.
Fricke and Waber (1972a)	DS atomic and ionic radii (from r_{max}) for Z=104-120, 156-172.
Grotch and Hegstrom (1973 ab); Hegstrom (1975a)	Relativistic and radiative corrections to g-factors of many-electron atoms. He, Li.
Rosen and Waber (1974)	DS and DF $\langle r^n \rangle$ of Gd^{3+}, Er^{3+}.
Bagus et al. (1975)	The "lanthanoid contraction" studied by n.r. HF on "pseudo" 6th row atoms without a 4f shell.
Gilbert et al. (1975)	Charge radii and softness for closed-shell systems from DF densities.
Lewis and Hughes (1975)	Higher-order relativistic corrections to g_J of triplet states for He-like systems, Z=2-10.
R.A. Moore (1975ab)	g-factors for metals.
Cowan and Griffin (1976)	U $\langle r^n \rangle$, n=-2,2, as a test of the QR approach.
Luc-Koenig (1976a)	g_J for 5s5p of Cd, 6s6p of Hg. The Breit-Margenau operator shown to be insufficient for coupling, deviating from jj.
Singh et al. (1976)	Theory of g_J.
Castner and Tan (1978)	The Breit-Margenau correction to g_J calculated with HFS orbitals and potentials. Mn^{2+}, Gd^{3+}.
Desclaux and Freeman (1978, 1984); Freeman et al.(1976)	DF $\langle r^n \rangle$ for actinoid ions.
Harriman (1978)	Theory of ESR parameters.
Sushkov et al. (1978ab); Flambaum et al. (1978)	g_J of heavy atoms. Cs and Tl 6p states using a model potential.

Table 5.9. (continued).

Pyykkoe (1979d)	"Secondary periodicity" in group 16 (O-Po) analysed by DF on "pseudo-Se"(no 3d shell, Z=24) and "pseudo-Po" (no 4f shell, Z=70).
Sham et al. (1980)	DF $\langle r^{-3} \rangle$ for various states of Au atoms, with Wigner-Seitz boundary conditions. Used for Moessbauer E2 hfs.
Anikin and Zhogin (1981)	Relativistic corrections to g factors of alkali atoms.
Heully (1982)	Incorporates magnetic fields in a QR treatment. g_J for various states of Rb.
Huet and Luc-Koenig (1982)	g-factors for the 5s5p and 5s5d levels of Cd I using a model-potential method.
Veseth (1983a)	g_J of Li...Cl from MBPT.
Dupont-Roc and Cohen-Tannoudji (1984)	Effective Hamiltonian theory of g-2.
Pyykkoe and Laaksonen(1984)	Double-zeta STO fits for DF on the actinoids Th-Am.
Cheng and Childs (1985)	MCDF g_J of $4f^N6s^2$ states of Pr-Tm.
Cortona et al. (1985)	Various $\langle r^n \rangle$ for Ce^{3+}-Gd^{3+}.
Dzuba et al. (1985c)	g-factors for Cs, Au, Hg^+ and Fr.
Fournier and Manes (1985)	Reviews the sizes etc. of the lanthanoids and actinoids.
Gould (1985)	g_J of U^{91+}.
Hess (1985)	BP $\langle r^n \rangle$ using Sucher's projection operators in a two-component model.

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

Reference	Comments
Freeman and Desclaux(1972)	Neutron magnetic form factor of Gd^{3+}. DF.
Lander et al. (1973)	Neutron magnetic form factor of Tb^{3+}. DF.
Mendelsohn et al. (1973, 1974)	DF Compton profiles for U, Ar-Xe, Pb.
Eisenberger and Reed (1974)	Relationship between the Compton cross section and the electron velocity distribution.
Manninen et al. (1974)	Relativistic theory of the Compton effect.
Biggs et al. (1975)	DF Compton profiles for the elements.
Ribberfors (1975ab)	Relativistic theory of the Compton effect.
Freeman et al. (1976)	Neutron magnetic form factors of U ions, U^{3+} - U^{5+}.
Lander et al. (1976)	Neutron magnetic form factor of U^{4+}.
Stassis et al. (1977)	Neutron magnetic form factors for Ln^{3+}.
Desclaux and Freeman (1978, 1984)	Neutron magnetic form factors of actinoid ions. DF.
Freeman and Desclaux (1979)	Neutron magnetic form factors for lanthanoids. DF.
Pattison and Schneider (1979)	1s Compton profiles of Au and Pb.
Mitroy and Fuss (1982)	Momentum distribution of Hg from (e,2e) scattering.
Grotch et al. (1983)	Spin-dependent Compton scattering.
Cook et al. (1984)	DF calculation and observation of 5p momentum distributions in Xe.
Cortona et al. (1985)	Spin-polarised relativistic LDF calcula- of various spin moment densities and magnetic form factors for Ce^{3+}-Pr^{3+}.

Table 5.11. X-ray scattering factors.

Reference	Comments
Levinger (1952)	Analytical Dirac-Coulomb scattering factors for 1s electrons: The "Bethe-Levinger" correction factors.
Cromer (1965b); Cromer and Waber (1965)	DS x-ray scattering factors for atoms and ions with Z=1-102.
Doyle and Turner (1967, 1968)	DF x-ray scattering factors for 76 atoms or ions.
Cromer and Liberman (1970)	DS anomalous x-ray scattering factors for Z=3-98.
Øverbø (1977)	Form factors for large momentum transfers. DF. Z=20...92.
Hubbell and Øverbø (1979)	Relativistic x-ray form factors, Z=1-100. DF.
Jensen (1980)	Anomalous x-ray scattering factors beyond the dipole approximation.
Cromer and Liberman (1981)	Explains the deviation of some experiments from the anomalous x-ray scattering factor of Cromer and Liberman (1970)

Table 5.12. Electron and positron scattering.

Reference	Comments
Mott (1929, 1932)	Polarization of electrons by double scattering from atomic potentials.
Moeller (1932)	Stopping power for fast electrons.
Bethe and Heitler (1934)	Solve the Bremsstrahlung problem in the Born approximation.
Massey and Mohr (1941)	Polarization of electrons by double scattering.
Bethe and Maximon (1948)	Theory of Bremsstrahlung and pair production. Reviews earlier work. Uses the 2nd-order approximate Dirac equation of Sommerfeld and Maue (1935) or Furry (1934).
Khuri and Treiman (1958)	Dispersion relations for Dirac potential scattering.
Johnson et al. (1964)	Single-quantum annihilation of positrons.
Bunyan and Schonfelder (1965)	Polarization of 100 to 2000 eV electrons by Hg.
Mott and Massey (1965)	Atomic collisions.
Browne and Bauer (1966)	Relativistic effects in the scattering of slow electrons.
Schonfelder (1966)	Electron scattering for Hg, Au, Bi from Dirac-Hartree.
Dawson (1967)	Relativistic effects in the scattering of slow electrons.
Doyle and Turner (1967, (1968)	DF electron form factors for 76 atoms or ions.
D.W. Walker (1969, 1970, 1975)	Elastic e-Hg scattering. DF.
D.W. Walker (1971)	Relativistic effects in low-energy electron-atom scattering. A review.
Jones (1974, 1975)	Relativistic effects in electron-atom scattering.
D.W. Walker (1974)	Electron impact excitation of hydrogenic ions.
Chang (1975)	Close-coupling equations for electron-atom scattering. DF results for Cs.
Davidovic and Moiseiwitsch (1975)	K-shell ionization cross sections for Z=29-79.
Fano et al. (1976)	Influence of relativistic corrections on phase shifts.
Chang (1977b)	R-matrix calculation of electron scattering by Ne^+.
Pratt et al. (1977)	DS electron Bremsstrahlung spectra for 1 keV-2MeV electrons and neutral atoms, Z=2-92.
Almaliev and Batkin (1978)	Electron Bremsstrahlung in a screened Coulomb potential.
Oh and Macek (1978)	A rough estimate for relativistic effects in electron excitation.

Table 5.12. (continued).

Callaway et al. (1979)	Electron-impact excitation of the $2p_{1/2}$, $2p_{3/2}$ states of C^{3+}-W^{71+}. DF.
Ndefru (1979); Ndefru et al. (1980); Ndefru and Malik(1980,1982)	Inner-shell ionization of heavy elements by slow and fast electrons.
Pindzola and Carter (1980)	Electron-impact excitation of Fe XXV and Kr XXXV.
Scott and Burke (1980)	Electron induced $2s^2$-2s2p of Fe XXIII. Formulates the BP-level theory, using a R-matrix approach.
Sin Fai Lam (1980); Sin Fai Lam and Baylis(1981)	Elastic electron scattering by Hg.
Staunton et al. (1980)	Application of electron scattering on the theory of random metallic alloys.
Klapisch et al. (1981)	Bely's approximation for exchange in electron-atom collisions.
Norrington and Grant(1981)	Electron scattering from Ne II, using a relativistic R-matrix method.
Fuss et al. (1982)	Theory of relativistic (e,2e) reactions.
Genz (1982)	Inner-shell ionization by relativistic electron impact: a review.
Gevers and David (1982)	Theory of electron and positron diffraction at high and low energies.
Keller and Combet Farnoux (1982)	Relativistic effects and photoionization of d and f electrons in Hg.
Majumdar et al. (1982)	Electron-atom scattering at intermediate energies.
Mitroy and Fuss (1982)	Momentum distribution for Hg from (e,2e) scattering.
Scott and Taylor (1982)	A model-potential R-matrix program at the BP PT level.
Sin Fai Lam (1982)	Elastic electron scattering by Kr-Rn.
Soh et al. (1982)	Born cross sections for Li-like C and W.
Awe et al. (1983)	Elastic scattering of slow electrons from Xe.
Bartschat and Scott (1983)	A program for electron scattering amplitudes.
Chang (1983)	Relativistic quantum-defect theory.
Dufton et al. (1983)	Electron excitation of Ca XVII.
Feng et al. (1983)	"Gaunt factors" for electron Bremsstrahlung in hot dense plasmas. DS.
Kim (1983)	Theory of electron-atom collisions: a review.
Kissel et al. (1983)	Tables of atomic-field Bremsstrahlung from 1-500 keV electrons for Z=1-92.
Leung et al. (1983)	Stopping power of K electrons for relativistic incident electrons.
Mann (1983)	QR HF excitation collision strengths for Fe X...XXVI.
Scott et al. (1983)	The $6s6p^2$ resonances in e-Hg scattering.
Bartschat and Scott (1984); Bartschat et al. (1984b)	Low-energy electron scattering by Hg and Tl.
Bartschat et al. (1984a)	Stokes' parameters for inelastic e-Hg scattering.

Table 5.12. (continued).

Choi et al. (1984)	Born cross sections for the boron sequence
Genz (1984)	A review on inner-shell ionization by relativistic electron impact.
Kemper et al. (1984)	Elastic electron scattering from He and Ne: a two-channel DF theory.
Strange et al. (1984)	Electron scattering from a site in a solid: s-o coupling and spin polarization treated on equal footing.
Scott et al. (1984ab)	Low-energy e-Cs scattering.
Bartschat (1985)	R-matrix calculations for Pb. $0<E<7$ eV.
Chakraborty (1985)	K-shell ionization by electrons. A TF potential used, major relativistic effects for the ejected electron included.
Jaskolski (1985)	Relativistic effcts in elastic scattering of slow positrons by heavy atoms.
Keller and Combet Farnoux (1985)	Spin polarization of 5d, 5p and 4f photoelectrons of Hg.
L. Kim et al. (1985)	Bremsstrahlung spectra of Al, Cs, Au plasmas.
Pilipczuk and Pilipczuk (1985)	Electron scattering amplitudes on an atomic potential.
Pratt and Feng (1985)	Review on electron-atom Bremsstrahlung.
Roshchupkin (1985)	Bremsstrahlung of a relativistic electron scattered by a nucleus in a strong EM wave field.
Vainshtein and Safronova (1985a)	Excitation cross-sections for Be-like systems ($2s^2$-2s2p-$2p^2$) using 1/Z PT. Only target relativistic.

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

Reference	Comments
Mott and Massey (1965)	Atomic collisions.
Amundsen and Kocbach 1975); Amundsen et al. (1976)	K-shell ionization by protons.
Stassis and Deckman (1976)	Magnetic scattering of neutrons by a relativistic atom: the theory.
Davidovic et al. (1978)	K-shell ionization of Ag, Au by relativistic protons.
Pauli et al. (1978)	Electronic relativistic effects in K-shell ionization.
Amundsen and Aashamar(1981)	K-shell ionization by relativistic ions.
Komarov and Novikov (1981)	Inner-shell ionization by heavy charged particles.
Ahlen (1982)	Relativistic corrections to stopping power
Avaldi et al. (1982)	K-shell ionization by protons.
Chen et al. (1982a, 1983c)	L- and M-shell ionization by protons.
Gundersen et al. (1982)	Proton and deuteron deflection using hydrogenic wave functions.
Leung (1982, 1983)	Relativistic effects on energy losses.
Yudin (1982)	Semiclassical theory of 1s-2s and 1s-2p excitation due to charged particles. Dirac-Coulomb wave functions used.
Demkov et al. (1983)	1s - 1s charge transfer for proton collisions with Z=10,20.
Leung and Rustgi (1983)	Ionization of heavy atoms by polarized relativistic protons.
Mukoyama (1984); Mukoyama and Sarkadi(1981ab,1982ab, 1983)	K- and L-shell ionization by charged particles.
Chen (1984)	L- and M-shell ionization by protons. DS versus HFS.
Humphries and Moiseiwitsch (1984, 1985ab)	Electron capture between bare nuclei, Z_1 and Z_2.
Jakob et al. (1984)	Wave function effects in inner-shell ionization by light ions.
Komarov (1984)	Inner-shell ionization cross sections for binary collisions.
Sheth (1984a)	K-shell ionization by protons.
V.E. Anderson et al. 1985)	Relativistic corrections to stopping power
Anholt (1985a)	X-ray studies of heavy-ion - atom collisions.
Anholt and Eichler (1985)	Electron capture by relativistic projectiles.
Becker et al. (1985)	K-shell ionization cross sections for 4.88 GeV protons or 670 MeV/amu Ne projectiles.
Chen and Craseman (1985)	K- and L-shell ionization by protons. DS.
Hansteen et al. (1985)	K-shell ionization cross sections at very low projectile energies.

Table 5.13. (continued).

Jakubassa-Amundsen and Amundsen (1985)	Exact relativistic 2nd Born approximation for electron capture.
Meyerhof et al. (1985)	Electron capture from Be to Au by high-energy Xe^{n+}, n = 52-54.
Moiseiwitsch (1985)	Scattering of atomic particles at relativistic energies.
Mukoyama (1985)	1s-2s excitation by heavy charged particles.
Mukoyama (1985b)	Review on electronic relativistic effects in ion-atom collisions.
Rosenberg (1985)	Relativistic Coulomb Bremsstrahlung in soft-photon approximation.
Sokhi and Crumpton (1985)	L-shell ionization by protons. Dy-U.

Table 5.14. Photon scattering and photoionization.

Reference	Comments
Nishina (1928, 1929)	Polarization of Compton scattering.
Klein and Nishina (1929)	Photon scattering by free electrons.
Roess (1931)	K-shell photon absorption. Two non-interacting Dirac electrons in a Coulomb field.
Sauter (1931b)	K-shell photoeffect.
Brenner et al. (1954)	Scattering of x-rays by the K-shell of Hg.
Brown et al. (1954)	X-ray scattering by K-shell: the method.
Brown and Mayers (1956)	Coherent gamma-ray scattering from K electrons of Hg.
Nagel (1960)	Relativistic photoeffect in the K-shell.
Alling and Johnson (1965)	K- and L-shell photoeffect.
Matese and Johnson (1965)	Photoionization with screened Coulomb fields and, for Hg, with a Dirac-Hartree approach.
Brysk and Zerby (1968)	Photoelectric cross sections in the keV range.
Johnson and Feiock (1968)	Rayleigh scattering and frequency-dependent susceptibilities of rare gases. DS.
Brodsky and Primack (1969)	Foundations of the Compton effect.
Storm and Israel (1970)	Photon cross sections from 1 keV to 100 MeV for Z=1-100.
Chang and Kelly (1972)	Photoionization cross sections and spin orientation for K-Cs.
Pratt et al. (1973)	Atomic photoionization above 10 keV.
Walker and Waber (1973a,c, 1974)	Angular distribution of photoelectrons. DS for Zn-Hg, Xe.
Eisenberger and Reed (1974)	Relativistic theory of the Compton effect.
Manninen et al. (1974)	Relativistic theory of the Compton effect.
Ribberfors (1975ab)	Relativistic theory of the Compton effect.
Drukarev and Karpeshin (1976)	Relativistic double (two-electron) photoeffect.
Scofield (1976)	DS photoionization cross sections at 1254 and 1487 eV.
Chang (1977a)	R-matrix theory of photoionization. Application to Ne.
Johnson and Lin (1977	RPA theory of photoionization. He, Be.
Owen (1977)	Compton scattering for electrons in bound states.
Cherepkov (1978)	Angular distribution and spin polarization of Xe 5s photoelectrons.
Johnson and Cheng (1978, 1979)	Photoionization of outer shells for Ne-Xe.
Johnson and Radojevic(1978)	Photoelectron branching rates for the 4d shell of Xe.
Kissel and Pratt (1978, 1979)	Rayleigh scattering by neutral atoms. DS data for Hg, Pb.
Ong and Manson (1978,1979a)	Photoelectron angular distribution of outer s shell of noble gases.
Ong and Manson(1978b,1979b)	Ditto for alkali metal valence electrons.
Band et al. (1979)	Influence of the DS hole and exchange terms on cross sections.

Table 5.14. (continued).

Band et al. (1979b)	Cross sections and angular distributions for x-rays. 1<Z<101.
Beatham et al. (1979a)	PES intensities of lanthanoid 4f electrons.
Huang et al. (1979, 1980, 1981)	Spin polarization of photoelectrons from noble gases.
Huang and Starace (1979, 1980b)	Cross-section, angular distribution and spin polarization of 6s photoionization in Cs.
Hubbel and Overbo (1979)	Coherent photon scattering cross sections, Z=1-100. DF.
Johnson and Cheng (1979)	Ne - Xe. RRPA.
Johnson and Lin (1979)	Multichannel RPA approach to photoionization.
Lin and Johnson (1979)	RRPA for photoionization of He-and Be-like ions.
Ong et al. (1979)	Photoionization cross sections of highly stripped ions: almost independent of ionicity. Ca, Th. DS.
Huang (1980a)	Theory of angular distribution and spin polarization of photoelectrons.
Huang and Starace (1980a)	Photoionization of 5s electrons in Xe.
Johnson (1980, 1983); Johnson et al. (1980a)	Reviews on photoionization. RRPA.
Ong and Manson (1980)	Branching ratios and angular distributions for outer p shells of noble gases.
Shorer and Dalgarno(1980)	Photoionization cross sections in the Mg and Zn sequences.
Tulkki and Aberg (1980)	Relativistic theory of inelastic photon scattering by oriented atoms.
Borstel et al. (1981,1982)	Necessity of relativistic dipole selection rules in photoemission.
de Barros et al (1981)	Rayleigh scattering by different atoms.DS.
Y.S. Kim et al. (1981b, 1980)	Photoeffect subshell branching ratios at high energies.
Y.S. Kim et al. (1981c)	Cooper minima and shape resonances in photoionization.
Y.S. Kim et al. (1981a)	Relativistic shifts and splittings of Cooper minima.
Parker et al. (1981)	Rayleigh scattering at x-ray energies: a review.
Pindzola (1981)	Photoionization of excited-state Xe. HF-DF
Pindzola et al. (1981)	Two-photon excitation of Xe.
Ron et al. (1981)	Subshell branching ratios for partial photoionization cross sections. DS. Sn, U.
Rullhusen et al. (1981)	Vacuum polarization from Delbrueck scattering. DS on Na.
Stroscio (1981)	Relativistic corrections to multiple-photon ionization in intensive laser fields.
Tambe et al. (1981)	Branching ratios of Cd 4d and Hg 5d. DF.
Theodosiou et al. (1981)	Photoionization of the 4d shell of Cd. DF.
Whittingham (1981)	Compton scattering of 279.1 and 661.6 keV photons by K-shell electrons. Hydrogenic functions for Z=62...92 used.
Aymar and Crance (1982)	Two-photon cross sections of Cs near the 7p resonance.

Table 5.14. (continued).

Elci and Rogovin (1982)	Two-photon induced spin-orbit transitions. One photon is resonant, the other much smaller.
Johnson and Radojevic (1982)	Cross sections, branching ratios and angular distributions for the 5p, 5d and 4f shells of Hg. RPA.
Johnson et al. (1982a)	Photoionization of the outer ns and (n-1)d shells of Zn-Hg.
Manson and Starace (1982)	Photoelectron angular distributions for s shells.
Pratt (1982)	Relativistic effects in inner-shell photoeffect: a review.
Ribberfors and Berggren (1982); Ribberfors (1983)	Theory of incoherent x-ray scattering.
Roy and Pratt (1982)	Validity of nonrelativistic dipole approximation for forward Rayleigh scattering.
Zilitis (1982)	Photoionization cross sections for the Li sequence. DF.
Benbow and Smith (1983)	Photoemission from d-band metals.
Cheng and Johnson (1983)	Orbital collapse and the 4d photoionization for Xe-La^{3+}.
Cherepkov (1983)	Review on spin polarization of photoelectrons.
Deshmukh and Johnson (1983)	Photoionization of Ca. RRPA.
Deshmukh and Manson (1983)	Photoionization of Mg. RRPA.
Johnson (1983b); Huang et al. (1983); Johnson and Soff (1983)	Photoionization especially of alkali atoms.
Manson et al. (1983)	6p photoionization for Z=82-100. DS. Relativistic Cooper minima.
Parpia and Johnson (1983b)	Photoionization of Hg. TD LDA.
Radojevic and Johnson(1983)	Photoionization of Pd 4d. RRPA. MQDT.
Radojevic and Johnson (1983b)	Photoionization of 3d and 3p of Hg. RRPA.
Reineking et al. (1983)	Cross sections for Compton scattering of Cu, Sn, Pb. DS.
Roy et al. (1983)	Elastic photon scattering at small momentum transfer. Validity of form-factor theories.
Schaupp et al.(1983, 1984)	Rayleigh-scattering form factors for gamma rays. DS.
Trautmann et al. (1983ab, 1985)	Inner-shell ionization form factors in momentum space and coordinate space.
Grelland (1984b, 1985)	Relativistic kinematic scattering of x-rays.
Liberman and Zangwill (1984)	An RRPA (TD LDA) program. Calculates photoemission cross sections.
Parpia et al. (1984)	Photoionization of the outer shell of Ne-Xe, TD LDA.
Salzmann et al. (1984); Salzmann and Pratt (1984)	Photoionization of excited atoms. (3p of K or 5s and 6s of Ba).
Tambe and Manson (1984)	Photoionization of 5d and 4f subshells of high-Z elements. DS.
Thoerner and Borstel(1984)	Theory of photoemission from solids.

Table 5.14. (continued).

Wang and Pratt (1984)	Photoeffect from outer-shell and Rydberg states of high-Z elements. E1 and E2 matrix elements considered. DS on U.
Zangwill and Liberman (1984)	3d photoabsorption of Xe: interplay between dielectric screening and core-hole relaxation.
Aberg and Tulkki (1985)	Inelastic x-ray scattering, including resonances.
Bartschat and Scott(1985ab)	Photoinization of Hg: electron polarization.
J. Braun et al. (1985)	Theory of photoemission from solids.
Deshmukh and Manson (1985)	Photoionization of Xe. RRPA.
Kissel and Pratt (1985)	A review of elastic photon (Rayleigh) scattering.
Radojevic and Johnson(1985)	Photoionization of the outer shell of Be and Mg.
Tulkki (1985)	Near-edge K photoabsorption of Xe, Rn. DF.
Tulkki and Aberg (1985)	Ditto for Ar.
Weñskus et al. (1985)	Compton scattering cross sections using "form factors" or "impulse" approximations and DS wave functions. C, Cu, Pb, all shells.
Wong and Yeh (1985)	Use of the Dirac-Coulomb Green function in Rayleigh scattering.
Yin and Pratt (1985)	Ionic Cooper minima.
Zilitis (1985b)	Photoionization cross sections for Na-like ions. DF.

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

Reference	Comments
Mott and Massey (1965)	Atomic collisions.
Pyper et al. (1977)	The Hg-Hg potential.
Bister et al. (1979)	Stopping powers of heavy ions using DF atomic densities.
Cohen (1979)	Collisions of U^+ with U, U^+ or U^{2+} with Gordon-Kim.
Cohen et al. (1979)	Inelastic collisions of O (^1D) with Ar, Kr, Xe.
Moiseiwitsch (1980)	Relativistic effects in atomic collision theory.
Moiseiwitsch and Stockmann (1980);Moiseiwitsch (1982)	Electron capture between two high-Z nuclei.
Stiebing et al. (1981)	K-shell ionization of Pb by Cl projectiles.
Wood and Pyper (1981b)	Electron-gas predictions of interatomic potentials. Na^+-Cl^-, Ag^+F^-, Tl^+Cl^-, Rn-Rn using DF densities.
Dul'yan and Kotsinyan (1983)	Transition probabilities for exotic hydrogen-like atoms (positronium, $\pi\mu$, πe), colliding with Al or W.
Easa and Shukla (1983)	Long-range interactions between H, He, Li.
Kobe and Kennedy (1983)	Gauge-invariance in heavy-ion collisions.
Krause and Kleber (1983)	Time-dependent study of inner-shell excitation during an atomic collision.
Leung (1983)	Relativistic effects in energy losses and other atomic scattering processes.
Anholt (1985b)	X-rays from quasimolecules.
Anholt (1985c)	Light-ion charge states in collisions with relativistic heavy ions.
Krause and Kleber (1985)	Time-dependent study of positron production during ion-atom collisions.
McCann (1985)	Electron capture between highly charged atoms with relativistic velocities.

Table 5.16. Nuclear processes involving electronic wave functions.

Reference	Comments
Hoyle (1938)	Beta transitions using Coulomb wave functions.
Reitz (1950)	Effect of screening on beta-ray spectra and internal conversion. Dirac eq. solved in a TF potential.
Rose et al. (1952)	Angular correlations in internal conversion.
Bodmer (1953)	Finite-nucleus relativistic corrections for electron scattering.
Fogel (1954)	K-shell internal conversion.
Brysk and Rose (1958)	Theory of orbital captures.
Feynman and Gell-Mann(1958)	Theory of the Fermi interaction.
Martin and Glauber (1958)	Radiative orbital electron capture from K- and L-shells.
Weiner and Iusim (1960)	Effect of nuclear quadrupole moment on beta-decay.
Holzwarth and Meister (1964)	Elastic electron scattering by screened Au, Hg nuclei.
Bhalla (1967)	DS calculations of internal conversion.
Band et al. (1970, 1978)	Internal conversion coefficients.
Bergkvist (1975)	Influence of nuclear quadrupole moments on beta decay.
Bambynek et al. (1977)	Review on electron capture.
Roesel et al. (1978)	Internal conversion coefficients for all atomic shells. Z=30-104.
Band et al. (1979)	Influence of the DS hole and exchange terms on internal conversion.
Anderson et al. (1980)	Dependence of internal conversion on atomic state.
Bunaciu et al. (1980,1981)	Internal-conversion coefficients for screened-Coulomb potentials.
Batkin et al. (1981)	Internal Bremsstrahlung accompanying beta-decay.
Dragoun et al. (1981)	DS calculations for M1, E2, E3, M4 internal conversion for Z=47-80.
Zilitis et al. (1981)	Effect of exchange on internal conversion. Applications on Fe.
Anholt and Amundsen (1982)	K-shell ionization during alpha-decay.
Batkin et al. (1982a)	K-shell ionization during beta=decay.
Batkin et al. (1982b)	Internal Compton effect.
Behrens and Buhring (1982)	Electronic wave functions for beta-decay.
Law (1982)	Shakeoff accompanying beta-decay: a review of the relativistic theory.
Ichimaru and Utsumi (1983)	Enhancement of thermonuclear reaction rates due to screening by relativistic electron gas.
Mukoyama and Kagawa(1983b)	K-shell ionization in beta-decay. LCAO-DF for W, Hg.
de Forest (1984)	Coulomb sum rule for electron scattering from nuclei.

Table 5.16. (continued).

Harston and Pyper (1984)	Chemical effects on beta decay. Each of the three factors analysed changes the decay of ^{63}Ni by one part in 10^5.
Mayol et al. (1984b)	DS internal conversion coefficients for Z=13...79.
Shepard et al. (1984)	Inelastic electron scattering by nuclei.

Table 5.17. Parity-violation effects in atoms and molecules.

Reference	Comments
Sandars (1966)	Electric dipole moment of Li-Fr. Introduces a relativistic correction factor.
Sandars (1968)	Electric dipole moment of a 1s hydrogenic system.
Bouchiat and Bouchiat (1974)	Basic theory, including relativistic effects.
Gorshkov and Labzovskii (1974)	Parity-nonconservation in heavy ions.
Khriplovich (1975)	Cs 6s-7s M1 transition.
Brinicombe et al. (1976)	Bi. Dirac's equation in a model potential.
Sushkov et al. (1976, 1978c); Sushkov and Flambaum (1978a)	M1 transitions of Tl, Pb, Bi.
Gorshkov et al. (1977)	Electron-electron weak interaction in atoms and ions.
Gorshkov et al. (1977b)	Parity-nonconservation effects on spectra of multicharged ions.
Henley et al. (1977)	Bi. Effect of CI.
Sandars (1977, 1980)	Theory of parity-nonconservation in atoms.
Neuffer and Commins (1977ab)	Cs, Tl.
Hiller et al. (1978,1980)	Relativistic theory of parity-violation in many-electron atoms.
Sushkov and Flambaum (1978b)	Diatomic molecules.
Carter and Kelly (1979); Kelly and Carter (1980)	Optical rotation of Bi.
Khriplovich (1980)	Theory.
Martensson (1980); Martensson et al. (1981)	Bi.
Das B.P. (1981)	MBPT of parity-violation in atoms.
Khriplovich (1981)	Book on parity non-conservation in atoms.
Das B.P. et al. (1982)	Tl.
Gorshkov et al. (1982)	Parity-nonconservation effects on hfs of stereoisomeric molecules.
Khriplovich and Zhizhimov (1982)	P-odd van der Waals forces.
Bouchiat et al. (1983)	Cs, using a model potential.
Melibaev (1983)	Parity-nonconservation in x-ray spectra of heavy atoms.
Starchenko and Faustov (1983)	Contribution of a weak interaction to the hfs of hydrogen-like atoms.
Dzuba et al. (1984a, 1985)	Parity violation in Cs.
Johnson (1985)	P- and CP-violation in heavy atoms.
Johnson et al. (1985)	C and CP violation in Rb, Cs, Au, Tl using various potentials and DF.
Khriplovich (1985)	P-odd difference of hfs constants in optical isomer molecules.
Martensson-Pendrill (1985)	P- and T-nonconservation in Xe and Hg.

Table 5.17. (continued).

Martensson-Pendrill (1985b)	Cs. MBPT.
Plummer and Grant (1985)	MCDF results for Tl, Pb, Bi.
Schaefer et al. (1985)	The parity-violating E1 matrix element for 6s-7s of Cs. DF.

6. SYMMETRY

The molecular orbitals, spanned by jj-coupled basis functions, are classified using double-group theory. The general theory is summarized in Table 6.1. and the available tabulations are listed in Table 6.2. Time-reversal symmetry aspects are discussed separately in Table 6.3.

Table 6.1. Theory of double groups and related aspects.

Reference	Comments
Bethe (1929)	First application of double groups in crystal field theory.
Mulliken (1930)	Diatomic molecules.
Opechowski (1940)	Foundations of double-group theory.
Herzberg (1950)	Diatomic molecules.
Koster (1957)	Review on space groups.
Rose (1957)	Rotation operators.
Wigner (1959)	Book on group theory.
Griffith (1960)	A book on transition metals. Ch.6: groups.
Heine (1960)	Book on group theory.
Nikitin (1961)	Diatomic molecules.
Griffith (1962)	Irreducible tensors for molecular symmetry groups.
Hamermesh (1962)	Book on group theory.
Messiah (1962)	Definition of rotation operators.
Koster et al. (1963)	Properties of the 32 point groups.
Tinkham (1964)	Book on group theory.
Herzberg (1966)	Character tables, irrep multiplication tables for most double groups.
Hurley (1966, 1983)	Ray representations of double groups.
Jansen and Boon (1967)	Book on group theory.
Loewdin (1967)	Applications of group algebras and convolution algebras in QM.
Wolf (1969)	Rotation operators.
Brown (1970)	Derives ray representations.
Cotton (1971)	Book on group theory.
Bradley and Cracknell (1972)	A treatise on symmetry in solids. Extensive bibliography.
Backhouse (1973)	Projective character tables.
Koenig and Kremer (1974)	Coupling constants and time-reversal symmetry.
Oreg and Malli (1974, 1976ab)	General formulae for the C_n^*, D_n^* and T^* symmetry orbitals.

Table 6.1. (continued).

Mizushima (1975)	Diatomic molecules.
Varshalovich et al.(1975)	Rotation operators and irreducible tensors.
Chisholm (1976)	Book on group theory.
Silver (1976)	Rotation operators and irreducible tensors.
Harter and dos Santos (1978)	Educational. Describes a slide-rule for adding rotations.
Altmann (1979); Altmann and Palacio(1979); Altmann and Herzig (1982)	"Ray" or "projective" representations as an alternative to double groups.
Desmier and Sharp (1972); Patera et al. (1978)	Polynomial tensors for double point groups.
Kibler (1979, 1984)	Theory of coupling coefficients.
Snijders (1979)	Ch. 4, pp. 36-89 on double-group theory, construction of symmetry orbitals. Gives general formulae for C_n^*, D_n^*, T^*, O^*, I^*.
Hafner (1980)	Time-reversal symmetry and various, particular point groups.
Cartan (1981)	Theory of spinors.
Couture and Le Paillier-Malecot (1982)	Character tables for D_8^*, C_{8v}^*, D_{4d}^* with "Tisza isomorphism".
Damhus et al. (1984)	Phase-fixed double-group 3-Γ symbols.
Aerts (1984)	Two-electron integrals in DF-LCAO calculations.
Altmann and Dirl (1984)	Symmetrization of MO:s using projective representations.
Damhus (1984)	Double groups as symmetry group of h_{so}. Traces their history to F. Klein (1884), C. Jordan (1878) and further back.
Ellis and Goodman (1984)	Automatic construction of basis functions.
Caride and Zanette (1985)	An alternative definition for double groups.

Table 6.2. Available data for double groups.

Reference	Comments
McLellan (1961)	Basis functions for C_{3v}^*, I_h^*, $j=(1/2)-(15/2)$.
Koster et al. (1963)	Gives character tables, irrep multiplication tables, coupling coefficients and compatibility tables for the 32 crystallographic point groups.
Kovalev (1965)	Representation matrices for the 230 space groups.
Onodera and Okazaki(1966b)	Basis functions and representation matrices for C_{2v}^*, C_{3v}^*, D_{3d}^*, C_{4v}^*, D_{4h}^*, T_d^*, O^* and O_h^*.
Telemann and Glodeanu(1967)	Basis functions for D_{3h}^*, O_h^*.
Leushin (1968)	Basis functions for the 32 double groups, $J<19/2$. Influence of orbital quantum number, l, not considered.
Golding (1971)	Coupling coefficients for O^*.
Bradley and Cracknell (1972)	Representation matrices for the 32 point groups. Basis functions $\|lm_l m_s\rangle$.
Dobosh (1972)	Coupling coefficients for O^*.
Golding (1973)	Coupling coefficients for the icosahedral group.
Harnung (1973)	Irreducible tensors for O^*.
Koenig and Kremer (1973)	Standardization of phases.
Oreg and Malli (1974, 1976ab)	General formulae for the symmetry orbitals of $C_{\infty v}^*$, $D_{\infty h}^*$, C_n^*, D_n^*, C_{nv}^*, C_{nh}^*, D_{nv}^*, D_{nh}^*, S_{2n}^*.
Golding and Newmarch (1977)	Coupling coefficients for C_n^*, D_n^*, T^*.
Toivonen and Pyykkoe (1977)	Central-atom- and ligand-based symmetry orbitals for D_{3h}^*.
Pyykkoe and Desclaux (1978)	Basis functions and ligand field coefficients for T_d^*, O_h^*.
Rosen (1978b)	Central-atom- and ligand-based symmetry orbitals for C_{2v}^*, $C_{\infty v}^*$, $D_{\infty h}^*$ and O_h^*. sl (rather than ls) coupling.
Oreg and Malli (1979)	Use of molecular symmetry in DF calculations.
Tang et al. (1980)	SO(3) and O^*.
Couture and Le Paillier-Malecot (1982)	Character tables for D_8^*, C_{8v}^*, D_{4d}^*, with "Tisza isomorphism".
Pyykkoe and Toivonen (1983)	Representation and rotation matrices and basis functions for 38 double groups (including the 5-fold ones) with the influence of the l-quantum number included
Ellis and Goodman (1984)	Automatic construction of basis functions.
Dirl et al. (1985)	Relativistic cubic harmonics.

Table 6.3. Time-reversal symmetry and related questions.

Reference	Comments
Kramers (1930)	The "Kramers degeneracy".
Wigner (1932)	Theory of time-reversal symmetry.
Johnston (1958)	Time reversal for a Dirac electron in a crystal field.
Koenig and Kremer (1974)	Coupling constants and time-reversal symmetry.
Hafner and Schwarz (1979);	Time-reversal symmetry and the HF approach.
Hafner (1980)	For a final solution, see Roesch (1983a).
Esser et al. (1981); Esser (1984b)	Use of time-reversal symmetry in relativistic CI calculations.
Newmarch and Golding (1981ab, 1983)	Racah algebra for groups with time reversal symmetry.
Roesch (1983a)	Use of time-reversal symmetry to simplify diagonalization: theory.
Roesch (1983b)	Fortran implementation of the method.
Dongarra et al. (1984ab)	Use of time-reversal symmetry to simplify diagonalization.
Eschrig (1984)	Use of time-reversal symmetry to simplify diagonalization.

7. MOLECULAR CALCULATIONS

In this chapter we review the relativistic calculations on molecules. One-electron molecules form a rather special case, discussed in Table 7.1. The other tables are classified by the method of calculation. The LCAO - DF calculations on molecules are listed in Table 7.2. and the one-centre expansions (OCE) (mostly DF, with one DS calculation) in Table 7.3. The four-component DS "Discrete Variational Method" (DVM) calculations are given in Table 7.4. and the DS "Multiple Scattering" (MS) $X\alpha$ ones in Table 7.5. The "quasirelativistic" or one-component approximation to the DS MS $X\alpha$ method is discussed separately in Table 7.6. Molecular pseudopotential calculations are summarized in Table 7.7. (for the available pseudopotentials, see the Tables 4.8.-4.10). The perturbative Hartree-Fock-Slater (P-HFS) method, including both 1st- and 2nd-order contributions, is covered by Table 7.8.

A selection of the 1st-order perturbation theory calculations of relativistic energy terms in molecules is given in Table 7.9. (For a more complete summary of spin-orbit effects in molecules, see the book by Richards et al. (1980)). Various density-functional calculations using relativistic atomic densities are collected into Table 7.10. The "semiempirical", Extended-Hueckel-type calculations are discussed in Table 7.11 and the relativistic crystal-field theory for transition-metal ions in Table 7.12. For certain properties the theoretical framework itself needs modification in the relativistic case. Such theories are discussed in Table 7.13.

Early reviews of the relativistic methods for molecules were presented by Pyykkoe (1978) or Bersuker and Ogurtsov (1979).

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

Reference	Comments
Roberts et al. (1962)	Fine and hyperfine structure of H_2^+.
Coulson and Joseph (1967b)	Show, at the Pauli level, that the relativistic two-centre problem is inseparable.
Pavlik and Blinder (1967)	PT using simple trial functions.
Luke et al. (1969)	PT. Finds a relativistic contraction and stabilization of the bond.
B. Mueller et al. (1973); B. Mueller and Greiner (1976)	Solution of the one-electron two-centre Dirac equation in a basis of exp(-x/2) L(x)P(η), x=(ξ-1)/a, (ξ,η) elliptical coordinates.
Marinov et al. (1975); Marinov and Popov (1976)	The two-centre Dirac equation, especially near the critical radius.
Bishop (1976, 1977); Bishop and Cheung (1978b, 1980, 1981b)	PT calculations of relativistic and radiative corrections for H_2^+ and its isotopic species, for a large number of R and v or J.
Kaufmann and Wille (1976)	H_2^+ and high-Z collision systems at the BP level.
Lyul'ka (1976)	Series expansions in ξ^{-n}, $\xi=(r_1+r_2)/R$, for the Dirac equation at large ξ.
Mukherjee and Chandel (1978)	Relativistic electron scattering from a two-centre potential.
Gonsalves and Moss (1979)	No problems with diverging integrals for Pauli-level H_2^+.
Hegstrom (1979)	g-factors and other magnetic properties of H_2^+.
Bakalov (1980)	Mu-mesic molecules.
Mark et al. (1980)	An attempt to solve the H_2^+ problem in a Gaussian basis.
Wolniewicz and Poll (1980)	Rovibrational energies of HD^+.
Wallmeier (1981); Wallmeier and Kutzelnigg (1981)	H_2^+ using a squared Dirac operator.
Mark and Schwarz (1982)	H_2^+ using a new representation of the kinetic-energy operator and LCAO.
Becker et al. (1983)	Time-dependent Dirac eq. solved for a head-on collision system $(Ca-U)^{111+}$.
Daubechies and Lieb (1983); Daubechies (1984)	Analytic properties of the discrete spectrum.
Schluter et al. (1983); Wietschorke et al. (1983)	The Dirac equation in orthogonal coordinate systems. Inseparability proven.
Wallmeier and Kutzelnigg (1983)	H_2^+ using a "forth-back free-particle FW transformation".
Laaksonen and Grant (1984)	A two-dimensional, fully numerical solution of the 2nd-order Dirac equation for H_2^+ and HeH^{2+}. The same method is extended to a DF treatment of H_2 and HeH^+ by Laaksonen and Grant (1984b).

Table 7.1. (continued).

Bakalov et al. (1985)	Fine and hyperfine splittings of weakly-bound levels of ddμ and dtμ.
Berinde et al. (1985)	N-Au, S-Au one-electron levels and coupling matrix elements.
Bottcher and Strayer (1985ab)	Numerical (1D), time-dependent studies of high-energy head-on collision systems. For comments, see Grant (1985d)
Greiner et al. (1985)	A review (see ch. 11.2).
Schlueter (1985)	Methods of solution.

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

Reference	Comments
Malli and Oreg (1975)	Formulation of the closed-shell DF problem.
Oreg and Malli (1979)	Symmetries of the matrix elements.
Aoyama et al. (1980)	H_2, LiH, Li_2, HF, F_2, H_2CO. GTO basis. Spurious s-o splittings.
Desclaux and Pyykkoe (1980)	Points out that some DF-LCAO calculations are inadequate.
Ishikawa and Schwarz (1980)	MCDF formalism.
Malli (1980)	Formulation of the open-shell problem.
Malli and Oreg (1980)	Li_2 and Be_2. Confuses basis-set and relativistic effects.
Mark and Rosicky (1980)	Formulation of the problem using separate basis sets for the four components. Application on H_2.
Mark et al. (1980)	Ditto. H_2^+.
Matsuoka et al. (1980)	H_2, LiH using an STO basis.
Roszak and Chojnacki (1980)	Formulation of the problem.
Ishikawa and Malli (1981a)	Proposes a Lagrangian multipler technique for avoiding variational collapse.
Malli (1981)	Molecular integrals for Hulthen-type functions.
Wallmeier (1981); Wallmeier and Kutzelnigg (1981)	H_2^+ and H_2 using the squared Dirac operator.
Datta and Ewig (1982)	Be_2. Expands the atomic basis spinors in Gaussians.
Lee and McLean (1982); McLean and Lee (1982)	AgH and AuH using a large, "kinetically balanced" STO basis. Reports R_e, D_e.
Mark and Schwarz (1982)	A new representation of the kinetic-energy operator. Application on H_2^+.
Rosicky (1982)	Proposal for avoiding variational collapse
Rosicky (1982b)	Formalism for the Breit terms.
Schwarz and Wallmeier (1982); Schwarz and Wechsel-Trakowski (1982)	Considers ways of avoiding the variational collapse.
Solliec et al. (1982)	Proposes a small-component basis related to the large-component one.
Esser (1983, 1984ab)	Formulates a relativistic MRCI approach.
Schwarz et al. (1983)	H_2^+ using a <u>small</u> c (> 5 a.u.).
Wallmeier and Kutzelnigg (1983)	H_2^+ using a "forth-back free-particle FW transformation".
Aerts (1984)	Use of molecular symmetry to simplify two-electron integrals.
Datta and Jagannathan (1984)	The constrained-component variation.
Kutzelnigg (1984)	Reviews various ways to avoid the variational collapse.
Malli (1984)	Matrix elements for Dirac-Coulomb basis functions.

Table 7.2. (continued).

Mark et al. (1984)	The fine structure of F_2 and F_2^+.
Simas and Smith (1984)	Integrals over the BP operators.
Stanton and Havriliak (1984)	"Kinetically balanced basis sets".
Wallmeier (1984)	H_2 and LiH using the squared Dirac operator.
Aerts and Nieuwpoort (1985b)	H_2, CH_4, SiH_4, GeH_4. GTO.

Table 7.3. Molecules treated by the DF-OCE method. For reviews on non-relativistic OCE calculations, see Bishop (1967) or Hayes and Parr (1967).

Reference	Comments
Mackrodt (1970)	CH_4 to SnH_4,... HF to HI. Relativistic contributions to total energies discussed; conclusions invalidated by numerical inaccuracies.
Desclaux and Pyykkoe (1974)	CH_4 to PbH_4. Relativistic bond length contraction; relativistic increase of the force constant.
Desclaux and Pyykkoe (1976)	CuH, AgH, AuH. Relativistic increase of dissociation energy D_e; chemical difference between Ag and Au "mainly a relativistic effect".
Pyykkoe and Desclaux (1976)	BH to TlH. Relativistic decrease of D_e for TlH; $p_{1/2}$ bonding, monovalency of Tl partially due to 6p spin-orbit splitting.
Pyykkoe and Desclaux (1977)	TiH_4 to $(104)H_4$. Chemically similarity of Zr and Hf attributed to cancellation of relativistic effects; a small relativistic bond-length expansion for TiH_4 and ZrH_4. See Pyykkoe et al. (1981) for another explanation.
Pyykkoe and Desclaux (1978; 1979a)	CeH_4, ThH_4; CrH_6 to $(106)H_6$; UH_6. Relativistic effects explain why W-H bonds are stronger but not longer than Mo-H bonds, relativistic effects move W 5d density to bonding region thus explaining its higher valency; the lanthanoid contraction is mainly a non-relativistic effect; the actinoid contraction is about 30 pm; further evidence for 5f participation in U-H bonds.
Hotokka and Pyykkoe (1979)	TiH_4. Compares the OCE and LCAO densities.
Pyykkoe (1979b)	MH^+ and MH_2 with M = Be to Ra, Zn to Hg, Yb or No. Strong d contributions to the bonds of Ca to Ra; relativistic effects make them smaller for Ra than for Ba; small or even negative bond-length contractions; Ra-H bonds longer than Ba-H bonds; Yb-H and No-H bond lengths are comparable; linear two-coordination of Hg attributed to relativistic effects; anomalously small 3p character for Mg.
Pyykkoe (1979c)	$^1\Sigma$ states of ScH to AcH; TmH, LuH, LrH. SCF lanthanoid expansion of the 5d shell from La to Lu; trends in group IIIa; Lu-H

Table 7.3. (continued).

	and Lr-H bond lengths comparable.
Snijders and Pyykkoe (1980)	AuH and TlH. Confirms that the relativistic bond-length contraction is not an orbital-contraction effect.
Pyykkoe et al. (1981)	BaH^+, RaH^+, ZrH_4, MoH_6, WH_6. The relativistic bond-length contractions and expansions reproduced in 1st-order perturbation theory.
Aguilar-Ancono et al. (1983)	CH_4 to PbH_4. A QR HFS approximation gives semiquantitative agreement with Desclaux and Pyykkoe (1974).
Desclaux (1983b)	A review.

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

References	Comments
Ellis and Painter (1970)	The DVM in band theory.
Rosén and Ellis (1974)	XeF_2. Correct ordering of energy levels with nearly quantitative agreement with expt.; reasonable π-level spin-orbit splitting.
Rosén and Ellis (1975)	H_2X (X = O - Te); InX (X = F - I); MCl (M = B - Tl). The central article on the method. Agreement with experiment as above.
Ellis et al. (1975)	UO_2^{++}. Population analysis yields a relativistic decrease from $5f^{3.1}$ to $5f^{2.8}$ only.
Fricke et al. (1976);	Collision system AuI^{76+}.
Morovic et al. (1976)	X-ray emission spectrum obtained.
Koelling et al. (1976)	UF_6, NpF_6, PuF_6. Detailed interpretation of the UV and optical spectra and ionization energies. The 5f populations resemble the free-atom ones. The nature of bonding and the AO character of the various MO:s are discussed. The deficiencies of an one-electron model become evident for the "f^2 system" PuF_6.
Walch and Ellis (1976)	UO_2^{++} in a crystal field. Effect of secondary ligands simulated by a crystal field, yielding a considerable improvement for the "$6p_{3/2}$ splitting".
Adachi (1977)	LiF, CsF, UF. Describes the DS-DVM, gives orbital energies (R and NR).
Adachi et al. (1977)	CsX (X = F - I). Experimental photoelectron spectra interpreted.
Ellis (1977ab)	FeO. Attempt to use different functions for different $\lvert m_j \rvert$.
Ellis and Rosén (1977)	MF_6 (M = W, Re, Os, Ir, Pt). A relativistic reduction of the "crystal-field splitting" between 5d t_{2g} and e_g levels, in agreement with experiment. The spin-orbit splitting of the t_{2g} level also successfully interpreted. Strong covalency of the bonds is found. Difficulties with term splittings of $(t_{2g})^n$ for n > 1. For a summary of experimental energy levels, see McDiarmid (1980).
Gubanov et al. (1977)	UO_6^{10-}. Relativistic effets claimed to be small for the orbital energies of the 2p- and 5f-like levels.

Table 7.4. (continued).

B.-I. Kim et al. (1977)	UF_6. Orbital energies and the optical absorption spectrum calculated. A relativistic population decrease from $5f^{3.35}$ to $5f^{1.76}$.
Morovic et al. (1977)	Collision systems.
Rosén (1978)	UF_6. A non-relativistic HFS-DVM reference calculation. A relativistic population decrease from $5f^{3.20}$ to $5f^{2.75}$, Smaller relativistic 5f-level expansions than those of Kim et al.
Rosén et al. (1978)	$(110)F_6$. One-electron levels.
Ellis et al. (1979); Gubanov et al (1979)	ThO_6^{10-}, UO_6^{10-}. Small relativistic effects found for the valence levels, large ones for the 6p levels. Evidence for 5f - 6p hybridization in the bonds. Orbital composition given.
Rosén and Fricke (1979)	UF_5. Energy levels and optical spectrum for an assumed C_{4v} structure.
Rosén et al. (1979)	MF_6 (M = Mo, W, 106). Energy levels and ionisation energies.
Berkowitz et al. (1980)	AgX (X = Cl - I). Ionisation potentials and orbital composition given at the transition state level.
Euler et al. (1980)	XF_2 (X = Ne - Xe). Potential energy curves. D_e much larger than exp. (for X = Kr, Xe), decreases due to relativity.
Grundevik et al. (1980)	XF_6 (X = S - Po). Energy levels given.
Rosén et al. (1980)	IrCO. Energy levels given as function of the Ir-C distance.
Fricke et al. (1981)	Pb - Pb
Sepp et al. (1981)	$(Pb-Pb)^{68+}$ collision system. Important electronic screening effects found on all energy levels.
Ellis (1982)	Review on actinoid compounds.
Ellis et al. (1982)	AcF_4 (Ac = Th, U, Np, Pu), $(UO_4)^Q$,(Q=2-, 3-). Photoelectron spectra, low-lying optical transitions and bonding discussed.
Hartung et al. (1982); Hartung and Fricke (1983)	Collision systems.
Morovic et al. (1982)	Ar-Ar,...,Pb...Pb. Level structure of the $2p_\pi$- $2p_\sigma$ crossing studied.
Ruscic et al. (1983); Ellis and Goodman (1984)	LnX_3 (Ln = La, Ce, Nd, Gd, Er, Lu; X = F, Cl, Br, I). PES adequately interpreted, except for 4f-level multiplet structures. The von Barth-Hedin correlation potential used. Bonding discussed. Moment polarization introduced by lifting the Kramers degeneracy. Includes a review.

Table 7.4. (continued).

Ellis and Goodman (1984)	AnO_8^{12-} An = U - Cm. Cluster models for the dioxides AnO_2. Embedded in a crystal field. Ionicity almost independent of actinoid.
Fricke et al. (1984)	$ArCl^{10+}$. The 2pπ - 1sσ transition energy interpreted using a correlation diagram. The method of Sepp et al. (1984) was used.
Fricke and Rosén (1984)	A review on collision systems.
Guo and Ellis (1984)	TmS_n. Energy levels for Tm-activated ZnS phosphors.
Larsson et al. (1984a)	$PdCl_4^{2-}$, $PtCl_4^{2-}$. The d - d and d - p optical transitions assigned.
Sepp et al. (1984)	N_2. A new method is tested, in which the orbitals are still solved by the DVM but the Poisson equation for V_c and the integrals are solved using fully numerical methods. Then the potential energy curves can be calculated with a satisfactory accuracy.
Hartung et al. (1985)	Quasimolecular structure in elastic ion-atom scattering.
Sepp and Fricke (1985)	Connection of the method with positive-energy projection operators.

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

Reference	Comments
Cartling and Whitmore (1975, 1976)	Theoretical formalism.
Yang and Rabii (1975)	Theoretical formalism.
Neto and Ferreira (1976)	Theoretical formalism.
Rosicky et al. (1976)	Theoretical formalism.
Yang (1976ab)	C_2, I_2. Experimental ionisation potentials of I_2 interpreted.
Yang and Rabii (1976)	$(PbSe)_n$ (n=1, 2, 4, 6). Vacancies and hydrogen atoms also included. PES of solid PbSe interpreted. Relativistic effects decrease the energy gap from 2.74 to 0.90 eV (exp. 0.29 eV). Atomic hydrogen is shown to occupy a Pb vacancy.
Messmer et al. (1977)	M_4 and M_4H, (M = Ni, Pd, Pt). Hydrogen-metal bonding dominated by d AO:s for Pd and Pt and by s AO:s for Ni, consistent with PES. Explanations suggested for variations of hydrogen solubility among these metals. Non-relativistic energy levels for Pd and Pt are similar, relativistic ones not. The relativistic SCF expansion of the d shell is missing.
Yang (1978)	Theory: normalization and symmetrization.
Yang et al. (1978)	UO_2^{++}. The XPS spectrum successfully interpreted, despite of a non-relativistic potential.
Yang and Rabii (1978)	PbS, PbSe. Optical spectra discussed. Later calculations by Lee et al. (1980) and the experiments give much more strongly bound levels.
Case and Yang (1980)	UF_6. The quasirelativistic MS Xα potential of Boring and Wood (1979a) is used. Semiquantitative agreement of energy levels with those from DS-DVM, QR-Xα and pseudopotential methods. The merits of the four methods are compared.
Case and Yang (1980b)	Algorithms.
Gagarin and Kovtun (1980)	AlO_4^{5-}, NiF_6^{4-}. A hybrid method with a n.r. valence part and a relativistic core.
Yang and Case (1981); Yang et al. (1981)	Pt_nCO (n = 1, 2, 5) SCF. Bonding of CO to Pt discussed.
Balazs and Johnson (1982)	Pt_{10}, $Pt(PH_3)_4$. The main relativistic effect is to widen the d-band. The "dangling-bond" MO:s of catalytic importance are largely unaltered.
Case (1982)	A review.
Lopez et al. (1982)	$[Pt(CN)_4]_3^{6-}$. The character of the valence MO:s discussed

Table 7.5. (continued).

	for Pt-Pt bond lengths, corresponding to insulators and to conductors. Relativistic effects decrease the Pt 6s+5d character and increase the ligand character.
Arratia-Perez and Case (1983)	XeF, CsO. Magnetic hyperfine properties calculated. Four-component plots of the spin-density reported.
Yang (1983)	Pd, Pt, Ag, Au clusters.
Arratia-Perez and Case (1984)	$W_2Cl_8^{4-}$. Energy levels and orbital composition discussed.
Case (1984)	4H-pyran-4-thione, C_5H_4OS. A method for calculating zero-field splittings in triplets is outlined. It yields the splitting in first-order PT for cases, dominated by spin-orbit (rather than spin-spin) effects.
Case and Lopez (1984)	YbF_6^{3-}, YbF_8^{5-}. Simulates Yb^{3+} sites in $KMgF_3$ and CaF_2 lattices, respectively. Crystal field splittings and hyperfine interactions (both ^{171}Yb and ^{19}F) compared with experiment. Isotropic fluorine HFS of YbF_6^{3-} found to arise from $2p_{1/2}$ rather than 2s AO:s.
Lopez and Case (1984)	$IrCl_6^{2-}$, $IrBr_6^{2-}$. Energy levels, magnetic properties (g, A) and excitation energies calculated.
Rabii and Yang. (1984)	Ag_2, Au_2. Ionization potentials for the various levels calculated. A large s-d hybridization found for Au_2.
Yang et al. (1984a)	$W(CO)_6$. Ionization and transition energies calculated. The 59 % W $5d_{5/2}$ e_g HOMO suffers a slight relativistic destabilisation while the orbitals with a large W 6s character are stabilised by up to 0.6 eV.
Yang and Case (1984)	XeF, I_2, $Pt(CN)_4^{2-}$. Hyperfine tensors interpreted for XeF. Ionization potentials calculated for I_2. (A review article).
Arratia-Perez and Yang (1985)	$M(CO)_6$, M = Cr - W. Bonding analysed. In addition to the CO 5σ donation and $2\pi^*$ back donation mechanisms, the "$\sigma+\pi$" t_{1u} one, where the metal p AO:s mix the σ MO:s of one CO with the π AO:s of another CO, is shown to be important. Relativistic effects are found to be small.
Case (1985)	NpF_6. Hyperfine and g-tensors. Spin polarisation from a QR treatment.
Soldatov (1985)	UF_6. Orbital energies and populations.

Table 7.6. Molecules treated by the quasirelativistic DS-MS $X\alpha$ or "$RX\alpha$" approach. See Table 2.2. for the QR 1-electron equation.

Reference	Comments
Hemstreet (1975)	Cluster models for solid PbS.
Hemstreet (1975b)	M_xTe_{13} (M = Sn, Pb; x = 13, 14) Electronic character of cation and anion vacancies studied.
Machado and Ferreira (1976)	Theoretical formulation.
Rosicky et al. (1976)	Theoretical formalism.
Boring and Wood (1979a)	UF_6. Relativity raises the 5f levels about 1 eV and diminishes the 5f population from 3.3 to 2.3. Energy levels in the RX -SO approximation are in reasonable agreement with experiment and with DS-DVM.
Boring and Wood (1979b)	UF_6, UO_2^{++}. Importance of the indirect relativistic effects is emphasised. An analysis of the relativistic change of the potential given for both molecules.
Michels et al. (1979a)	Hg_2^+. The ground state is stable with D_e = 0.67 eV. Considerable relativistic shortening and strengthening of the bond occurs. Photoabsorption of Hg_2^+ is not an important loss mechanism in excimer lasers. See also Celestino and Ermler (1984).
Thornton et al. (1979)	UCl_6. Assignment of the experimental PE spectra without spin-orbit coupling.
Bursten et al. (1980ab)	Re_3Cl_9, Re_3Br_9, $Re_3Cl_{12}^{3-}$. Energy levels and their AO character discussed. Transition-state ionisation potential for Re_3Cl_9. Relativistic rehybridization effects found. The 5d-type levels expand by up to 0.4 eV, the 6s-type levels contract by up to 0.8 eV.
Cotton (1980)	$Re_2Cl_8^{2-}$. Energy levels and optical spectrum discussed.
Thornton et al. (1980)	PaX_6^{2-}, UX_6^-, NpF_6 (X = F - I). No spin-orbit effects included. Fair agreement between transition-state 5f-5f excitation energies from the HOMO, and experiment. Trends in bonding discussed.
Wood et al. (1981)	UO_2^{n+} (n = 0, 1, 2). Excitation energies calculated. The electronic coupling is discussed. All species have about three 5f electrons, of which 1, 2 and 3 are bonding ones for n = 0, 1 and 2, respectively.

Table 7.6. (continued).

Balazs and Johnson (1982)	$Pt(PH_3)_4$, Pt_{10}. Relativistic effects on properties of catalytic importance found to be small.
Chermette et al. (1982)	WO_6^{6-}. Relativistic effects give the right order of W 4f and 5p levels.
Cotton et al. (1982)	$M_2Cl_4(PH_3)_4$, M = Mo. W. PES interpreted and bonding discussed.
Goursot and Chermette (1982)	$IrCl_6^{3-}$. UV and PES interpreted.
Le Beuze et al. (1982)	Mo_6, $Mo_6S_8^{2-}$. Energy levels and bonding discussed.
Sontum and Case (1982)	Cu, Ag, Au porphines. Hyperfine data interpreted.
Arratia-Perez and Case (1983)	XeF, CsO. Magnetic hyperfine properties compared to full four-component DS-MS $X\alpha$ results.
Bursten et al. (1983)	$Re_2Cl_4(PH_3)_4^{n+}$ n = 0, 1. The (two or one) electrons in excess of a $\sigma^2\pi^4\delta^2$ quadruple bond reside in the δ^* Re-Re antibonding MO. Nevertheless, the IR spectra suggest stronger bonding than in $Re_2Cl_8^{2-}$.
Bursten et al. (1983b)	$Re_2Cl_8^{2-}$. UV spectra reassigned.
Bursten and Fang (1983)	$(C_5H_5)_2UX_2$, X = Cl, Me. PES interpreted. U 5f and 6d AO:s interact with the C_5H_5 e_π MO.
Chermette et al. (1983)	$IrCl_6^{n-}$ (n = 2, 3), WO_6^{6-}. PES interpreted.
Cook and Case (1983)	The program.
Goursot et al. (1983)	$PtCl_6^{2-}$. Bonding compared with that of $IrCl_6^{2-}$. Larger covalency found for Pt (a more covalent 5d bond and a more polar Cl σ bond for Pt; metal charge comparable, 1.02 and 0.96 for Ir and Pt, respectively). Photoelectron and optical spectra interpreted.
Heera et al. (1983a,b)	UO_8^{n-} (n = 10, 12), UC_6^{6-}. Simulates UO_2, α-UO_3 and UC. Energy levels, atomic charges and Moessbauer isomer shifts given.
Pedrini and Chermette (1983)	$AgCl_6^{5-}$. Simulates Ag^+ in NaCl. Relativistic effects on Ag-Cl bond lengths and breathing force constants discussed.
Roesch and Streitwieser (1983); Roesch (1984)	$M(C_8H_8)_2$ M = Ce, Th, U. Relativistic effects improve the agreement with experimental optical and photoelectron spectra. The 6d populations of uranocene and thorocene are comparable (0.20 and 0.21) while the 5f populations are 0.33 and 0.20 respectively. This explains the

Table 7.6. (continued).

	smaller $e_{2u}(\pi)$-$e_{2g}(\pi)$ splitting of uranocene ($e_{2g} < e_{2u}$). The success of earlier non-relativistic calculations is explained by a cancellation between increased ligand-U(5f) overlap and weakened ε(COT)-ε(5f) resonance in the relativistic case.
Topol' and Kovba (1983)	$MoCl_5$. Optical and photoelectron spectra assigned.
Chermette and Goursot (1984)	A review.
Ginsberg et al. (1984)	$[Pt(NH_3)_2(C_5H_4NO)]_4(NO_3)_5$. Pt-Pt bonding mainly due to δ overlap between Ptd_{z^2}-s hybrids. Redox chemistry and optical properties interpreted.
Goursot et al. (1984)	$IrCl_6^{2-}$. Photoelectron, optical and electron spin resonance spectra interpreted. A spin-polarised calculation; spin-orbit effects included as a perturbation.
Goursot et al. (1984b)	$PtCl_6^{3-}$, $PtCl_5^{2-}$, $PtCl_4^{-}$. Energy spectra for various short-lived Pt(III) complexes involved in pulse radiolysis or flash photolysis of $Pt^{IV}Cl_6^{2-}$.
Heera et al. (1984a)	C_2, I_2. A modified quasirelativistic method, using an "averaged small component" in a two-component formalism. Eigenvalues compared to the average of a four-component calculation.
Seifert et al. (1984)	M_4, M_6, M_6H (M = Pd, Pt). Energy levels and charge distributions discussed. A dominantly covalent metal-hydrogen bond found. The lesser stability of the Pt-H bond is explained as a relativistic effect, caused by the increased Pt 6s character, with weaker directional properties, in the $1a_{1g}$ bonding MO.
Topol' and Zhilinskii (1984)	UF_4. Energy levels and charge distributions, photoelectron and UV spectra and electron affinity calculated assuming T_d geometry. Various approximations to the spin-orbit splitting included.
Topol' et al. (1984)	$MoCl_5$. Optical and photoelectron spectra assigned, now using the experimental C_{4v} geometry. Largest relativistic changes 0.1 - 0.2 eV.
Braydich et al. (1985)	$W_2(O_2CH)_4$, $W_2(O_2CH)_4(CH_3)_2$. The coexistence of strong axial W-C bonds and a strong W-W bond is explained.
Bursten et al. (1985)	$An(C_5H_5)$, An = Th, U. Photoelectron spectrum assigned. Both 6d and 5f shells are shown to contribute to the bonding.

Table 7.6. (continued).

Bursten and Fang (1985)	UCl_4, $UCl_2(cp)_2$, $U(cp)_4$, cp = C_5H_5. The η^5-C_5H_5 ligand is shown to be a better donor to U^{4+} than Cl^-.
Case (1985)	NpF_6. Hyperfine constants at Np and F nuclei. The QR spin-polarization term is added to the full DS A(Np) and A(F).
Gagarin et al. (1985)	NiO_6^{10-}. Spin-polarised treatment of 2p, 3s and 3p levels. A model for NiO, including a Watson sphere.
Goursot et al. (1985)	$PtCl_5^{2-}$, $PtCl_4O^{3-}$, $PtCl_4O_2^{5-}$. The nature of the possible Pt(III) complexes involved in pulse radiolysis of $PtCl_4^{2-}$ studied. Charge-transfer spectra calculated.
Goursot and Chermette (1985)	$PtCl_4^{2-}$. High-intensity bands assigned as Pt 5d - 6p ones.
Streitwieser et al. (1985)	$Ce(C_8H_8)_2$. Transition-state ionization energies (cp. Roesch and Streitwieser (1983)).

Table 7.7. Molecules treated by pseudopotential methods.

Reference	Comments
Das and Wahl (1976)	HgH. "Inner core" up to 3d handled with pseudopotentials. Orthogonality of valence AO:s (5s - 6s) to "outer core" (4s - 4f) handled explicitly. Fair agreement with agreement with experiment for R_e and other spectroscopic constants of the X $^2\Sigma$ and $^2\Pi$ states.
Hyde and Peel (1976, 1977)	XX', SnX_4, SbX_3; X = halogen. A n.r. PP scheme, with s-o terms added.
Das and Wahl (1978)	I_2. Potential energy curves obtained for several low-lying states. Spectroscopic constants in good agreemeent with experiment.
Datta et al. (1978)	PbO. Only a slight relativistic bond-length contraction of 1 pm found.
Ermler et al. (1978)	Xe_2, Xe_2^+. Potential energy curves for nine states of Xe_2 and four states of Xe_2^+. Transition moments calculated. Effects of the mass-velocity and Darwin terms found unimportant in this case. Experimental spin-orbit splittings used.
Hay et al. (1978)	AuH, HgH, $HgCl_2$, AuCl. MC-SCF-CI or GVB. Multiconfiguration wave functions used for correct dissociation. Relativistic contraction and strengthening of the Au-H bond confirmed. Relativity shortens and weakens the Au-Cl and Hg-Cl bonds. The relativistic contraction of the Hg-Cl bond by 12 pm is needed for agreement with experiment. Ionisation energies of $HgCl_2$ interpreted. Potential energy curves obtained for the lowest states of HgH.
Wadt et al. (1978)	XeF, Xe_2, Xe_2^+. Apart from spin-orbit effects (extrapolated from the free atoms), relativistic effects found negligible. The pseudopotential approach gives a too small Xe-Xe repulsion for small R. Excellent agreement between the present quasirelativistic pseudopotential and the averaged DF pseudopotential of Ermler et al. (1978).
Basch and Topiol (1979)	$HgCl_2$, AuCl, PtH. Relativity shortens and weakens the bonds of $HgCl_2$ and AuCl; shortens and streng-

Table 7.7. (continued).

	thens PtH. The relativistic expansion of the Pt 5d AO increases its participation in bonding and gives a $^2\Delta$ ground state for PtH instead of the non-relativistic $^2\Sigma$.
Ermler et al. (1979)	Au_2. Ground state and excited states by MC-SCF-CI.
Hay et al. (1979a)	UF_6, UF_6^-, UF_6^+. CI included. The bonding in the ground state is discussed. The U-F distance calculated to be 196 pm (exp. 200 pm). PES of UF_6 and the optical spectrum of UF_6^- interpreted.
Hay et al. (1979b)	A review on molecular lasers.
Lee et al. (1979)	Au_2. Ground state only. MC-SCF. Relativity contracts R_e by about 35 pm and increases D_e by about 1 eV. Only a small relativistic expansion for the orbital energies of the 5d-type MO:s in the molecule.
Wadt (1979)	HgCl, HgBr. CI. Spectroscopic constants for the lowest states in good agreement with available experiments. Spin-orbit interaction decreases the D_e (X $^2\Sigma$) of HgBr by 0.15 eV by lowering the covalent asymptote.
Wadt and Hay (1979)	UF_5. SCF. The relative energies of the C_{4v} and D_{3h} structures calculated to be very close, leading to fluxional behaviour. The same U charge of +2.4 and a comparable U-F bond length found as in UF_6. The f-f transition energies and oscillator strengths calculated.
Basch (1980)	Ag_2, Au_2, AgAu. CI. Calculated bond lengths for Cu_2, Ag_2 and Au_2 about 12 pm above experiment. The ECP - AE (all electron) difference accounts for about 5 pm of it. A R/NR comparison for Ag_2.
Basch et al. (1980a)	Pd_2, Pt_2, PdH, PtH. MC-SCF. Earlier resultss for PtH improved. The correct $^2\Sigma$ ground state and an R_e in agreement with experiment obtained for PdH. The odd-electron MO has an AO character in agreement with EPR hyperfine constants. Bonds of Pt stronger than those of Pd. The bond of Pd_2 is essentially a 5s-5s one but the bond of Pt_2 has a substantial 5d contribution.
Basch et al. (1980b)	PbHe, $PbHe^+$, PbXe, $PbXe^+$. CI. Energy curves and transition moments determined for estimating collision-induced absorption cross sections.

Table 7.7. (continued).

Christiansen and Pitzer (1980)	TlH. MC-SCF using ω - ω coupling. A five-configuration function gives 85 % of the experimental D_e. Principally a σ bond with $Tl^{0.3}H^{-0.3}$. $N(6p^*)/N(6p) = 0.66$.
Forstmann and Ossicini (1980)	Cu, Ag, Au in rare-gas matrices. The observed blue shift of the P ← S absorption line interpreted.
Julienne et al. (1980)	HgCl. Transition moments and energies calculated for the X-A bound-to-continuum transition.
Kleier and Wadt (1980)	HgF, Hg_2F_2, Hg_2Cl_2. GVB. The covalent Hg-Hg interactions dominate, giving a linear X-Hg-Hg-X structure with Hg-Hg bond lengths in good agreement with solid-state experiments. Excited electronic states also calculated.
Lee et al. (1980)	TlH, Au_2^+, PbS,PbSe. SCF. Satisfactory R_e and ω_e obtained. Ionisation energies for PbS and PbSe in fair agreement with experiment.
Pélissier (1980)	Cu_2; MH, MH_3 (M = In, Tl); MH_2, MH_4 (M = Sn, Pb).
Wadt (1980)	$HgCl_2$, $HgBr_2$. Potential curves for the lowest states. Excited states are bent. Excitation energies and oscillator strengths given. CI.
Basch (1981)	Ag_n^-, Ag_n, Ag_n^+ (n = 1-3). CI. Geometries, ionization potentials and electron affinities determined.
Basch et al. (1981)	PbO ($X\ ^1\Sigma^+$). MCSCF. Dipole moment function.
Christiansen et al. (1981)	X_2, X_2^+ (X = Kr, Xe). Potential energy curves using ω -ω-coupled SCF or CI. Explicit inclusion of ω - ω - coupling gives nearly the same results as a semiempirical s-o term. "Shape-consistent" pseudopotentials give potential curves much closer to all-electron ones than the V^{PK}.
Christiansen and Pitzer (1981)	Tl_2, Tl_2^+. CI. Weak bonding found for Tl_2, rather stronger one for Tl_2^+. Weakness attributed to spin-orbit effects.
Hafner et al. (1981)	Au_2^+, Tl_2, Pb_2, $HgCl_2$, $PbCl_2$, PbH_2. SCF. The influence of spin-orbit effects on bond energies, bond angles and bending force constants discussed. As the Pb_2 molecule is s-o stabilized by 1.5 eV, but the Pb atoms by 2.5 eV, s-o effects decrease D_e by 1 eV at the SCF level. $PbCl_2$ is destabilized and $HgCl_2$ stabilized by relativity.

Table 7.7. (continued).

Hay (1981)	$MCl_3(C_2H_4)^-$, (M = Pd, Pt). Barriers for ethene rotation calculated. Stronger bonding to Pt than for Pd. Bonding analysed.
Kitaura et al. (1981a,b)	$Pt(PH_3)_2$, $Pt(H)_2(PH_3)_2$. An energy gradient technique introduced for geometry optimisation. Pseudopotential for Pt from Basch and Topiol (1979). Geometries fully optimized for <u>cis</u>- and <u>trans</u>-$Pt(H)_2(PH_3)_2$. Transition state found.
Laskowski et al. (1981)	NaXe. Potential energy curves for the lowest electronic states.
Laskowski and Stallcop (1981)	CsH. Potential curves, dipole moment curves and the transition moment curves for the X $^1\Sigma^+$ and A $^1\Sigma^+$ states calculated.
Pitzer and Christiansen (1981)	TlH. The "orthogonal triplet bond" contribution to bonding (Pyper 1980b) is shown to be very small.
Wadt (1981)	ThO_2, UO_2^{++}. UO_2^{++} is linear while ThO_2 is bent because 5f bonding dominates over 6d bonding in the former but not in the latter molecule.
Christiansen et al. (1982)	TlH. CI+SO with the ab initio s-o potential of Ermler et al. (1981) gives improved D_e.
Hay (1982)	$Re_2Cl_8^{2-}$. The spin-orbit operator diagonalized over CI wave functions. Metal-metal bonding and optical spectrum discussed.
Jeung et al. (1982)	Cs_2^+, Cs_2, CsH. Inclusion of a core-valence polarisation potential improves D_e, R_e.
Krauss et al. (1982)	XeF, XeF^-. S-o and dispersion energy effects on the energy curves examined. Rapid variation of S-o splitting with R found. Dispersion and charge-transfer effects found comparable.
Laskowski and Langhoff (1982)	Cs_2. Role of 5p-6s core-valence correlation in getting a good potential curve demonstrated.
Noell and Hay (1982a)	$Pt(PH_3)_2XY$, (X,Y = H, Cl). The <u>trans</u> isomers found to be more stable than the <u>cis</u> ones. Diffuse valence s and p AO:s on Pt found important.
Noell and Hay (1982b)	$Pt(PH_3)_2 + H_2$, $Pt(P(CH_3)_3)_2 + H_2$. MCSCF+CI. Activation barriers and exothermicities for the oxidative addition process examined.
Pitzer and Balasubramanian (1982)	Pb_2. S-o included at the CI step. Good agreement with experiment for T_e, ω_e and D_e. Spin-

Table 7.7. (continued).

	orbit effects weaken the X 0_g^+ D_e to half of that for the LS coupled $X^3\Sigma_g^-$.
Rosenkrantz et al. (1982)	Ca_2. Potential energy curves and transition moments for the three lowest $^1\Sigma_u^+$ states.
Stevens and Krauss (1982b)	CH, OH, SiH, CO^+, CO, SiO. The ab initio effective spin-orbit operators applied on molecular s-o splittings.
von Szentpaly et al. (1982)	MM'^+, MH^+, (M = Li - Cs). Empirical pseudopotentials and a direction-dependent core-valence polarisability correction yield accurate spectroscopic constants.
Allison and Goddard (1983)	MoN. The $^4\Sigma^-$ ground state is found to be a triply bonded $d\sigma^2 d\pi^4 d\delta^1 d'\delta^1 5s\sigma^1$ one. The first excited, $^4\Pi$ state corresponds to a 5s-to- 5pπ excitation. The calculated R_e (160 pm), ω_e and E(Σ-Π) agree well with experiment (R_e = 163 pm). Non-monotonic changes in the dipole moment as function of R are observed.
Balasubramanian and Pitzer (1983)	Sn_2, Pb_2. S-O effects included at the CI stage. Ten low-lying states considered. D_e (calc.) is 1.86 and 0.88 eV compared to D_e (exp.) of 2.04(10) and 0.86(1) eV for Sn_2 and Pb_2, respectively. Effect of the calculated excited levels on the experimental, "third-law" D_e calculated.
Balasubramanian and Pitzer (1983b)	SnO. Potential energy curves calculated for seven low-lying states.
Balasubramanian and Pitzer (1983c)	PbO Potential energy curves for eleven low-lying states, including s-o and CI. Chemiluminescent emission bands assigned. Relativity influences the excited states with occupied π^* MO, mainly at Pb. R_e(X) 202 pm (exp. 192 pm).
Basch and Cohen (1983)	PtCO. Bonding discussed. A $^1\Sigma^+$ ground state predicted.
Bernholc and Holzwarth (1983)	Cr_2, Mo_2. "Short" bond lengths obtained in agreement with experiment.
Christiansen (1983)	Tl_2. Nine low-lying states considered. An X 0_u^- D_e of 0.16 eV found.
Fuentealba et al. (1983)	K_2^+. Empirical pseudopotentials, fitted to the Hartree-Fock or the Dirac-Fock valence s orbital energy, with the core-valence

Table 7.7. (continued).

	correlation coupled off, were used to study the relativistic effects on R_e, D_e and ω_e.
Hay (1983)	$PtCl_4^{2-}$. Energy levels at the CI+SO level given.
Hay (1983b)	UF_6. Energy levels at the CI+SO level given, including multiplet effects arising from electron-electron repulsion. The major electron impact peaks in the 3-10 eV energy range are assigned.
Jeung et al. (1983)	CsH, Cs_2. Potential curves for the ground and excited states.
Kato et al. (1983)	$Hg(^3P)$ + CO. Potential energy surfaces and the energy transfer to CO vibration discussed.
Klobukowski (1983)	AgH, Ag_2. A quasirelativistic version of the Bonifacic-Huzinaga model-potential method, using orbitals with nodes, is presented. Bond-length contractions 5.5 and 7.0 pm, respectively.
Krauss and Stevens (1983a)	UH, UH^-, UH^+, UF, UF^-. Potential energy curves found to resemble the analogous alkaline-earth ones.
Krauss and Stevens (1983b)	UO, UO^+. Potential energy curves for the lowest electronic states. The $X(\Omega=9/2)$ state of UO^+ is strongly ionic, $U^{3+}O^{2-}$. Strong, red visible spectral lines predicted. R_e = 184 pm, ω_e = 925 cm^{-1}.
Laskowski et al. (1983a)	CsO. Potential energy curves reported for the $X\ ^2\Sigma^+$ and $A\ ^2\Pi$ states of CsO. Correlating 17 electrons gives satisfactory results. The bond is 20 pm shorter than in a non-relativistic CI calculation by Allison and Goddard.
Laskowski et al. (1983b)	CsH. Potential energy curve for the $X\ ^1\Sigma$ state, including 5s-5p core-to-valence correlation.
Martin and Hay (1983)	$Ag_{26}O$. A model for chemisorbed oxygen on Ag(110). The calculated ω_e for a bridging site 327 cm^{-1} (exp. 310, 325), the SCF D_e much too small.
Martins and Andreoni (1983)	Ag_2. Deformation densities, R_e, ω_e, D_e considered. Pseudopotentials of Bachelet et al. (1982).
Stoll et al. (1983)	M_2^{n+}, MH^{n+} (M = Cu, Ag; n = 0, 1). Combines (a) a "semiempirical" pseudopotential with a direction-dependent core

Table 7.7. (continued).

	polarisation potential, fit to experimental one-electron atomic energies, (b) A LSD correlation potential for valence electrons only and (c) Separate d^{10} - d^{10} core-core interaction corrections. Reports atomic EA and IP, molecular R_e, ω_e, D_e, IP. - Relativistic effects extracted as the DF-HF difference from a fit to Koopmans IP, omitting the polarisation potential.
Stevens and Krauss (1983b)	Xe_2Cl. Equilibrium geometry and excimer transition probabilities calculated.
Teichteil and Spiegelmann (1983)	InH, Ar_2^*. Potential curves. Pseudopotentials of Teichteil et al (1983). In the "quasi-degenerate" perturbation theory used, the molecular spin-orbit effects are not derived from a given atomic configuration, which is important for Ar_2^* g states.
Wang and Pitzer (1983)	PtH, PtH^+. Bonding analysed for ground and excited states. Both the Pt $5d_{zz}$ and 6s AO:s found to be important. Relativistic effects increase the importance of both.
Andzelm et al. (1984)	Xe_2. At the Cowan-Griffin level, relativistic effects diminish the SCF interaction energy by about 20 % and shorten the R_e by 0.3 a.u.
Bagus et al. (1984)	Cu_5CO. Chemisorption discussed, results compared with all-electron calculations.
Balasubramanian (1984)	SnO^+, PbX^+ (X = O - Se). Spectroscopic properties and vertical IP calculated.
Balasubramanian and Pitzer (1984a)	SnH. Potential energy curves for five low-lying states including CI in the s^2p^2 valence space.
Balasubramanian and Pitzer (1984b)	PbH. Potential energy curves for five low-lying states. Calculated ground-state D_e 1.64 eV (exp. 1.59 eV), R_e 195 pm (exp. 184 pm).
Canadell et al. (1984)	C_5H_5M (M = In, Tl, Sn^+). Bonding analysed, found to be largely covalent, with a competition between π bonding and δ antibonding, and with negligible Tl 6d contributions.
Celestino and Ermler (1984)	Hg_2, Hg_2^+, TlHg. Potential energy curves for ground and excited electronic states. No strongly bound states are found with allowed transitions to the ground state.

Table 7.7. (continued).

Christiansen (1984)	Bi_2. The dissociation curve of the 0_g^+ ground state calculated. The D_e and ω_e are in good agreement with experiment. A full-valence CI, including spin-orbit effects, on a Λ - S coupled SCF function. The bond length is too long (279 pm, exp. 266 pm).
Flad et al. (1984)	M_n, M_n^+ (M = Cu, Ag, n<5). Valence correlation from density functionals. Structures, chemical binding energies IP calculated.
Garcia-Prieto et al. (1984)	Cu + H_2. Potential energy surface for the reaction Cu + H_2 $\rightarrow$ CuH + H, including the properties of CuH and CuH_2.
Hay (1984)	$W(PH_3)(CO)_3H_2$. The existence of a stable, symmetric H_2 complex W-H = 215 pm and H-H = 79 pm is confirmed (exp. 194(12) and 75(16) pm, respectively). Cp. 74 pm for H_2.
Huzinaga et al. (1984)	I_2, XeF_2. Relativistic effects on R_e, ω_e, EA and IP reported at the quasirelativistic level, neglecting s-o coupling.
Igel et al. (1984)	CuO, AgO. Potential energy curves, dipole moments for the ground state; X $^2\Pi$ - A $^2\Sigma$ excitation energies.
Illas et al. (1984)	CuOH, $Cu(OH)_2^-$. Geometries determined. CuOH is C_s, $Cu(OH)_2^-$ is C_2 ("H_2O_2-like").
Laskowski and Bagus (1984)	Cu_5Cl. The Cu-Cl distance and vibrational frequency calculated.
Low and Goddard (1984)	H_2 + $Pt(PH_3)_2$, PtH. Potential surface for the reaction. The relative importance of d^{10} and d^9s^1 states explains the differences between Pd and Pt. Ground-state properties of PtH.
Obara et al. (1984)	H_2 + $Pt(PH_3)_2$, CH_4 + $Pt(PH_3)_2$ $\rightarrow$ $Pt(H)(CH_3)(PH_3)_2$. Potential surface for the reactions. H/D isotope effect explained. Both *cis* and *trans* geometries given.
Olson et al. (1984)	CsH. Potential energy curves for H + Cs $\rightarrow$ H^- + Cs^+.
Pelissier and Davidson (1984)	Cs_2. Bonding analysed qualitatively. Core-repulsion of the neighbour found important.
Rubio and Illas (1984)	Sn_3H_6, Sn_4H_8. Geometries optimised, Sn-Sn agrees with experiment. Pseudopotentials of Teichteil et al. (1983a).

Table 7.7. (continued)

Spiegelmann and Malrieu (1984)	Effective Hamiltonians for avoided crossings. The diabatic case.
Stoll et al. (1984)	M_2, MH (M = Cu, Ag). Potential energy curves, IP.
Andzelm et al. (1985)	Mo_2, Ru_2, Ag_2, AgH, AgO, AgF. A Huzinaga-type model-potential approach with nodes, for local-density models. Spin-polarization and quasirelativistic corrections included. For Ag, shells starting from 4p, and for Mo the shells, starting from 3d, have to be included in the valence space. The AgH relativistic bond-length contraction only 4 pm.
Bagus and Mueller (1985)	$Cu_n(CO)$, n = 1 - 29. Bonding and C-O stretching frequency analysed.
Balasubramanian (1985a)	BiH. Potential energy curves for seven low-lying states. Bond lengths about 10 pm above experiment. D_e (theor.) 2.17 eV for X 0^+(I).
Balasubramanian (1985b)	ICl, ICl^+. Potential energy curves for six low-lying states. X 0^+ R_e 21 pm above experiment.
Balasubramanian (1985c)	TlF. Spectroscopic properties for nine low-lying states. X 0^+ R_e 204 pm (exp, 208), ω_e 592 cm^{-1} (exp. 477), D_e 3.86 eV (exp. 4.57).
Balasubramanian (1985d)	PbF The low-lying states are assigned. X $^2\Pi_{1/2}$ R_e 208 pm (exp. 206).
Basch (1985)	Pt(XY), XY = CO, N_2, CN^-, NO^+. Changes of XY R_e and ω_e upon complexation.
Basch et al. (1985)	$Pt(NH_3)_2^{2+}$, $Pt(NH_3)_2Cl_2$, $Pt(NH_3)_3X$, $Pt(NH_3)_2XY$ (X, Y = H_2O, OH^-). Relative energies and geometries at SCF level.
Bauschlicher (1985a)	CO/M, M = Cu, Ni, Pt. Tilting of absorbed CO studied for surface models of Cu(100), Ni(110), and Pt(110) for coverages greater than half a monolayer.
Bauschlicher (1985b)	NH_3/Cu_n. Chemisorption of NH_3 on various sites studied.
Chapman et al. (1985)	HI. Potential curves for six low-lying states. X 0^+ R_e 166 pm (exp. 161).
Christiansen and Ermler (1985)	Xe_2^+, Au_2. The connection between orbital contractions and bond-length contractions studied within the pseudopotential picture.
Fernandez et al. (1985)	SnH_4, SnH_4^+. Jahn-Teller distortions calculated and PES

Table 7.7. (continued).

	interpreted. Relativistic bond-length contractions 1.1 and 1.4 % for SnH_4 and SnH_4^+, respectively.
Hay and Martin (1985)	AgH, Ag_2, AgO. Various 1-, 11- and 19-electron ECP:s compared with all-electron results. The best R_e (AgH) still 5 pm above experiment.
Illas et al. (1985)	CuOH. Molecular structure and dissociation energy calculated with one or 11 elecrons in the valence space. The latter reproduces the experimental D_e.
Jasien and Stevens (1985)	CX, OCX, CX_2, H_2CX, X = Se, Te. Unprotonated and protonated species studied. Good agreement with observed proton affinities.
Koutecky et al. (1985)	RhCO, PdCO. Bonding analysed.
Krauss and Stevens (1985)	MH, MO; M = Fe, Ru. Bonding analysed.
Krauss et al. (1985)	AgH, AuH. Close agreement found with the all-AO DF calculations of Lee and McLean (1982). The 4s4p AO:s of Ag and 5s5p AO:s of Au included in valence space. Relativistic effects give for AuH two bonding σ MO:s: a 5dσ - 1sσ 3σ MO and a 6s - 1s 4σ MO. Relativistic effects almost half the dipole moment.
McMichael Rohlfing and Hay (1985)	MCO, $M(CO)_4$, M = Pd, Pt. Includes correlation at the MP2 level. Correlation enhances back bonding. The relative stability for both series Ni > Pt > Pd, in agreement with experiment.
Miyoshi et al. (1985)	Pd_4, Pt_4. Electronic structures and densities-of-states calculated, neglecting spin-orbit coupling.
Nelin and Bauschlicher (1985)	WO. Four low-lying states considered. All are formed from a d^4s^1 configuration of W^+, in contrast to CrO and MoO.
Ohanessian et al. (1985)	AsN. Potential curves for several low-lying states.
Pacchioni (1985)	Sn_2, Pb_2. Potential energy curves without spin-orbit splitting.
Ross and Ermler (1985)	M_2, M_2^+, MH, M = Ag, Au; AgAu. No f AO:s included. Even the correlated calculations with the shape-consistent EP:s give too large bond lengths, e.g. for Au_2 264 pm (exp. 247 pm).

Table 7.7. (continued).

Ruffolo et al. (1985)	M/Rg; M = Cu, Ag, Au, Rg = Ar, Kr, Xe. Matrix cage distortions and consequent splittings of metal-atom P levels studied by using a crystal-field model.
Wadt and Hay (1985)	TlH, Xe_2^+. Potential curves with 3- and 13-electron pseudopotentials compared for TlH.
Wang (1985)	Cu_n, Cu_n^+ (n = 1 - 3). Local-spin-density calculations with and without self-interaction corrections. Geometry and binding energy reported for Cu_2 and Cu_3.

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

Reference	Comments
Snijders et al. (1979)	I_2, HgI_2. The central article, introducing the method. The calculation of the matrix elements and the group-theoretical aspects are described. Photoelectron spectra interpreted. For the non-relativistic version, see Baerends et al. (1973), Baerends and Ros (1978).
Jonkers et al. (1980)	TeX_2 (X = Cl, Br). Photoelectron spectra interpreted. Second-order spin-orbit effects found to be important in these C_{2v} cases.
Ros et al. (1980)	MCl_2 (M = Zn, Cd, Hg). Relativistic effects on electron densities considered; shown to be of observable magnitude for $HgCl_2$.
Ziegler et al. (1980)	Au_2, AuH, AuCl. The relativistic bond lenght contraction is interpreted as a first-order relativistic effect, involving $\langle \Psi^0 \| h_m + h_d \| \Psi^0 \rangle$; the numerical values of the contraction (46, 23 and 13 pm, respectively) agree with the pseudopotential ones. Relativistic effects on D_e and ω_e also calculated.
Pyykkoe et al. (1981)	CsH, BaH^+, MX_4 (M = Zr, Hf; X = H, Cl). The role of d orbitals in bonding analysed. Important 5d contributions found for CsH, BaH^+. They diminish the relativistic bond length contraction by diminishing the 5s coefficients, not by the relativistic d AO expansion. The chemical similarity of Zr and Hf explained by a cancellation of the shell-structure expansion from Zr to Hf by the larger relativistic contraction of Hf.
Ziegler et al. (1981)	MH, MCl, (M = Cu, Ag, Au, Cs), Cs_2, AuCs, MH^+, MCl_2, M_2^{2+} (M = Zn, Cd, Hg). The transition-state method for calculating potential energy curves is used. R_e, D_e and ω_e calculated in all cases. The rôle of relativity in stabilizing Hg_2^{2+} is directly confirmed. The conclusions agree with earlier pseudopotential ones, when available.
Egdell et al. (1982)	BiX_3 (X = Cl - I). Photoelectron spectrum assigned. A new, relativistic hybridization, caused by Bi 6p spin-orbit splitting, found for the Bi-X σ-bonds.
Jonkers et al. (1982a)	CI_4. Photoelectron spectrum assigned.

Table 7.8. (continued).

Jonkers et al. (1982b)	C_2I_4. Photoelectron spectrum assigned.
Snijders and Baerends (1982)	A review.
Jonkers et al. (1983a)	GeI_2. Photoelectron spectrum assigned. The role of second-order spin-orbit effects discussed.
Ziegler (1983)	CH_3M, (M = Cu, Ag, Au). Potential energy curves. The non-relativistic stability $CuCH_3 > AgCH_3 > AuCH_3$ is changed into $AuCH_3 > CuCH_3 > AgCH_3$ by relativistic effects.
Ziegler (1983b)	$H_3W \equiv WH_3$. Bond lengths and energies calculated, compared with Cr_2H_6 and Mo_2H_6. Relativity contracts R(W - W) by 5 pm to 231 pm (exp. for W_2L_6 226 - 229 pm) and strengthens the $W \equiv W$ bond by 113 kJ mol^{-1} to 535 kJ, making it stronger than the $Mo \equiv Mo$ one. Experimentally $D(W \equiv W)$ and $D(Mo \equiv Mo)$ are 558 and 398 kJ mol^{-1}, respectively.
Baerends et al. (1984)	A review on applications in PES.
DeKock et al. (1984a)	UO_2^{2+}. The HOMO is found to be a δ_u with 71 % 5f character. It is the HOMO, partially due to "pushing from below" by the 6p (8 % of it), and partially due to the 5f relativistic destabilization.
DeKock et al. (1984b)	HgX_2 (X = CH_3, CN, $CCCH_3$), CH_3CN, Me_3PAuMe, HgCN. PES and bonding interpreted. Only a small 6p contribution found, indicating a three-centre-two-electron bond involving the Hg or Au 6s, and thus not 6s-6p hybridization. In the radical HgCN, however, the 6p AO is important. A larger 5d bonding contribution for Au than for Hg. (40 versus 10 %). Competition between 5d s-o splitting and 5d-ligand hybridization analysed for the various molecules. The relativistic contraction of the Hg-C bond in $HgMe_2$ about 10 pm, the relativistic stabilization 9.1 kcal/mol of a total of 56.2 (exp. 57.5).
Dyke et al. (1984)	XY (X, Y = F - I). Photoelectron spectra, especially the MO s-o splitting, interpreted. The explanation of Wittel (1972) for $\Delta\varepsilon(\pi_g) > \Delta\varepsilon(\pi_u)$ of I_2 confirmed.
Louwen et al. (1984a)	*trans*-$[(PH_3)_2M(C \equiv CR)_2]$, M = Pd; R = H, CH_3, *trans*-$[(PH_3)_2M(C \equiv N)_2]$, $[(PH_3)_2MCl(C \equiv N)]$. Orbital energies and orbital characters given. The δ^{u}_{M-C} orbitals are relativistically stabilized in the dicyanides and bisacetylides. Metal $d\pi$ - acetylide π^* back-

Table 7.8. (continued).

	bonding insignificant. The "d_{zz}" a_1 MO actually contains both Pt 5d and 6s character and only suffers minor relativistic effects.
Louwen et al. (1984b)	trans-[$(EH_3)_2MCl_2$] E = N, P; M = Pd, Pt. Orbital energies and orbital characters given. Only minor relativistic effects.
Ziegler (1984)	$M_2Cl_4(PH_3)_4^{n+}$ (M = Re, W). Relativistic contributions to the $M \overset{4}{-} M$ bond strength small, 9 and 7 kJ mol^{-1} for Re and W, respectively.
Ziegler (1985a)	$M_2(CO_2H)_4$, M = Cr - W, $W_2(CO_2CF_3)_4$, $M_2(PH_3)_4Cl_4$. Bonding and PES interpreted.
Ziegler (1985b)	$Pt(PH_3)_2$ or $Ir(PH_3)_2^+$ complexed to O_2, C_2H_2 or C_2H_4. The stability order for a homologous series is 3d > 5d > 4d. The back donation to ligands more important than the donation to metal.

Table 7.9. First-order perturbation theory on molecules.

Reference	Comments
Ladik (1959, 1961a)	H_2 using a Wang wave function. Result ten times too large.
Kolos and Wolniewicz (1964)	H_2. Claims that D_e is diminished by $2.4 \cdot 10^{-6}$ au due to relativistic effcts. (This calculation includes both correlation effects and the Breit-Pauli terms.)
Veseth (1970)	S-o interactions in diatomics.
Bersuker et al. (1972, 1974)	Formulates a "quasirelativistic" HF model.
Matcha (1973, 1976)	Alkali halides. All BP terms. Finds a relativistic decrease of D_e.
Matsuoka (1973)	Relativistic molecular integrals.
Aoyama and Yamakawa (1977)	H_2CO. A "Tamm-Dancoff" approximation including BP terms in the Hamiltonian. Numerical results apparently erroneous.
Langhoff and Kern (1977)	A review on molecular fine structure.
Bishop and Cheung (1978a, 1980, 1981a)	H_2. Relativistic and radiative terms from PT for many (v, J) of the X and a states.
J.S. Cohen et al. (1979)	S-o coupling explains quenching of $O(^1D)$ by Ar-Xe.
Michels et al. (1979b)	Noble-gas dimer ions.
Langhoff (1980)	S-o coupling in rare-gas oxides, up to XeO.
Richards et al. (1980)	Review on s-o effects in molecules.
Hess (1981)	BP-PT for molecules.
Marian (1981)	BP-PT for molecules.
Phillips and Davidson (1981)	H_2CO.
Cooper and Wilson (1982b)	Fine structure of 2nd-row diatomics.
Phillips and Davidson (1982)	CH_2.
Chandra and Buenker (1983ab); Buenker et al. (1984)	Evaluation of BP matrix elements for molecules.
Martin (1983a)	AgH.
Martin (1983b)	Cu_2.
Cooper et al. (1984)	Identifies new contributions to molecular fine structure.
Faegri and Almloef (1984)	$Ni(CO)_4$ Ni-C bond contraction 2.6 pm.
Katriel et al. (1984)	M_2, M_2^+, M = Li, Na.
Luethi et al. (1984)	The Fe-C contraction in $Fe(C_5H_5)_2$ only 0.7 pm.
Cooper (1985)	S-o splitting of OH.
Havriliak and Yarkony (1985)	Spin-forbidden line strengths for NF.
Scharf et al. (1985)	Cu_2. CI, with the Cowan-Griffin operator in 1st order.
Werner and Martin (1985)	Cu_2. CI and CEPA, with the CG operator.

Table 7.10. Density functional calculations.

Reference	Comments
Gordon and Kim (1972)	The "Gordon-Kim Model", relating interatomic interaction potentials between closed-shell atoms to atomic densities.
Gilbert et al. (1975)	Radii and softnesses for np^6 systems (n=2-6) (alkali ions, rare gases and halide ions) from DF calculations.
Baylis (1977)	Hg_2. Compares rel. and n.r. cases, estimates correlation effects.
Grant and Pyper (1977)	Molecular and crystal energies of group 14 (Pb, 114) and 16 (Te, Po, 116) salts.
Pyper et al. (1977)	The Hg-Hg interaction potential is halved by relativistic effects.
Catlow (1978); Catlow and Pyper (1979)	UO_2(s), U/PuO_2(s). Cohesive, electronic and redox properties using an ionic model.
Clugston and Pyper (1978, 1979); Pyper et al. (1977)	Gordon-Kim calculations. Negligible relativistic effects for Xe_2, Rn_2, increasingly important ones for Zn_2-Hg_2. Large deviation from the experiments of Stefanov et al. J. Phys. B 15 (1982) 239, and Hilpert (1982).
Bister et al. (1979)	A "mean DF" interatomic potential for stopping-power calculations.
J.S. Cohen (1979)	U-U Gordon-Kim potentials.
Wood and Pyper (1981a)	Lattice energies for fluorides of Ag, Pb, 113 and 116.
Wood and Pyper (1981b)	Interatomic potentials for inert-gas dimers (up to Rn), Ag-F, Tl-Cl, Na-Cl.
Gollisch (1982)	A QR density-functional scheme based on molecular densities. A basis of QR AO:s. Reports R_e, ω_e, D_e, IP_1 for Cs_2, Au_2, CsAu and their cations.

Table 7.11. Semiempirical methods.

Reference	Comments
Mulliken (1949)	Foundations of semiempirical quantum chemistry. Introduces the $h_{ij}=S_{ij}(h_{ii} + h_{jj})/2$ approximation.
Wolfsberg and Helmholz (1952)	Multiply the previous formula by K=1.6 - 2.0.
Hoffmann (1963)	The "extended Hueckel theory" applied to hydrocarbons. For an inorganic application, see Lohr and Lipscomb (1963).
Newman (1965)	Pi-bonding in the uranyl ion. The importance of relativistic overlap integrals is underlined.
Newton et al. (1966)	An approximation, where kinetic energy terms are calculated exactly and others related to the overlap integrals S_{ij}.
Hafemeister (1967)	Relativistic effects on overlap integrals between alkali metals or halogens.
Dixon et al. (1970)	Halomethanes. S-o coupling.
Brogli and Heilbronner (1971)	Alkyl halides. Competition between s-o splitting and chemical bonding in PES of molecules.
Hayes and Edelstein (1972)	$M(C_8H_8)_2$, M=U, Np, Pu. EHT using DF orbitals.
Jungen (1972)	S-o splitting of I_2 and C_2I_2.
Berkosky et al. (1973)	MWH + s-o. PX_3, PYX_3, (X = Cl - I, Y = O, S) PES.
Wittel et al. (1974); Manne et al. (1975)	Include s-o effects in an EHT calculation by doubling the diagonalized n.r. matrix. Applications on halogen compounds. Uses s-o parameters of Wittel and Manne (1974).
Trautwein et al. (1975); Reschke et al. (1977)	EHT calculations on ^{57}Fe isomer shifts using DF atomic EO integrals.
Bersuker et al. (1977)	A "Mulliken-Wolfsberg-Helmholtz" (MWH) model using jj-coupled basis and experimental energy parameters. $PtCl_6^{2-}$. See also Bersuker et al. (1974).
Freed (1977)	Theoretical basis for semiempirical theories.
Denning et al. (1979)	Experimental determination and parameterized models for the energy levels of uranyl.
Lohr and Pyykkoe (1979)	The Relativistically Parameterized Extended Hueckel ("REX") method. I_2, Bi_4.
Boudreaux and Carsey (1980); Carsey and Boudreaux (1980)	Pt complexes. A charge-iterative s-o-split EHT model.
del Re et al. (1980)	Review on semiempirical methods.
Harris et al. (1980)	The "FAKE" method. See Newton et al. (1966) above.

Table 7.11. (continued).

Lohr et al. (1980a)	The "REX" program.
Lohr et al. (1980b)	REX results for tetrahalides and -methyls of groups 4 and 14.
Richtsmeier et al. (1980)	Geometries of group 11 trimers using the "diatomics-in-molecules (DIM)" approach.
Tatsumi and Hoffmann (1980)	EHT with averaged DF orbitals for MoO_2^{2+} and UO_2^{2+}: why is uranyl linear?
Glebov and Nefedov (1981ab)	Uranyl complexes. Uses a semiempirical method, roughly at the CNDO level, in jj-coupling, and relativistic energy parameters but with n.r. DZ radial functions.
Liska et al. (1981)	S-o splitting in halogen compounds at the CNDO or INDO level, using the method of Manne and Wittel.
Lohr (1981)	REX calculations on cluster compounds of Ge, Sn, Pb and Bi.
Pyykkoe and Wiesenfeld (1981); Pyykkoe (1982)	Applications of the REX method on nuclear spin-spin tensors.
Viste et al. (1982)	Ditto. DZ parameters for Zn-Hg, O-Po.
Pyykkoe and Lohr (1981)	Applications of the REX method on energy levels, bonding and geometries of U, Ln, Po, I, At and Rn compounds. Lists single-zeta parameters for all elements, 1-120.
Woolley (1981)	Theoretical basis for Extended Hueckel methods. Discusses differences between s or p and d AO:s.
Egdell et al. (1982)	REX and P-HFS calculations compared for Bi trihalides. A novel Bi 6p s-o dominated hybridization found for the δ levels. DZ radial functions for N-Bi, F-117.
Pyykkoe (1982b)	The D_e of dihalogens related to Pitzer's relativistic hybridization rules.
Glebov (1983)	Uranyl compounds. A review.
Roesch (1983a)	Simplifies the REX program (by factors of 2 in memory and 5 in running time) using quaternionic algebra.
Roesch (1983b)	Implements these ideas in program "QATREX".
Bigot and Minot (1984)	Pt_n (n=2-13). An EHT model with s-o coupling. Solved using quaternions.
Gleghorn and Hammond (1984)	M_2H_4 (M=Ge, Sn, Pb) geometries optimized using a charge-iterative REX model.
Larsson et al. (1984)	A REX treatment of $PdCl_4^{2-}$ and $PtCl_4^{2-}$. Compared to a DS-DVM one.
Larsson et al. (1984b)	UF_6 using a charge-iterative REX model.
Lohr (1984)	Electronegativity equalization and main-group anionic clusters.
Lyudchik and Borkovskii (1984)	Diagonalize h_{so} in a doubled EHT basis, like Manne et al. (1975), but using the relation between Kramers pairs. CI_4.

Table 7.11. (continued).

Pyykkoe and Laaksonen (1984)	Double-zeta parameters for Th-Am. Application on uranyl.
Trinquier and Hoffmann (1984)	PbO (solid).
Viste and Pyykkoe (1984)	$I+I_2$ using REX: a spin conservation rule explained.
Alves and Larsson (1985)	W to Hg impurities in Si. (Si_{17}). Default REX. Energy levels, relative to the band gap.
Borkovskii and Lyudchik (1985)	EHT + s-o levels for uranyl halides.

Table 7.12. Relativistic crystal field theory.

Reference	Comments
Bethe (1929)	Foundations of crystal-field theory.
Griffith (1960)	Fundamentals of crystal-field theory.
Kneubuehl (1962)	Anisotropic s-o coupling in ESR.
Misetich and Buch (1964)	g-factors and s-o coupling in ligand-field theory.
Rajnak and Wybourne (1964)	Spin-orbit interactions in l^N configurations.
Wybourne (1965, 1966)	Gd^{3+} $^8S_{7/2}$ using relativistic crystal-field theory. Different radial functions for $J = l \pm 1/2$.
van Heuvelen (1967)	Mn^{2+}.
Lulek (1969)	S-o splitting arising from the anisotropic crystal field.
Jorgensen (1970); Nugent (1970)	Interpretation of the "tetrad effect" in stabilities of lanthanoid complexes.
Lewis et al. (1970)	Various $<r^n>$ parameters for actinoids. DS and DF.
Jorgensen (1971)	"Modern aspects of ligand field theory".
Lewis (1971)	Various $<r^n>$ parameters for lanthanoid atoms and ions. DS.
Varga et al. (1971)	Interpretation of $5f^4$ AmO_2^+ spectra.
Buckmaster et al. (1972)	S-o matrix elements in crystal field theory.
Andriessen et al. (1973, 1974)	Crystal-field theory with 4-component radial wave functions.
Chatterjee et al. (1973)	Formulates the relativistic crystal field. Includes overlap and covalency. The isotropic contribution to S-state splitting.
Hagston and Lowther (1973)	Ground-state splitting of Mn^{2+} ions.
Rosen and Waber (1974)	Relativistic $<r^n>$ integrals for lanthanoids.
Lulek (1975)	Spin-orbit coupling in a cubic crystal field. The contribution from the anisotropic crystal field to S-state splitting.
Newman and Urban (1975)	EPR spectra of S-state ions.
Parrot (1975)	Dipole strengths of d^5 ions in cubic fields for forbidden transitions.
de Beer et al. (1976)	Electric-field effects on Mn^{2+} EPR.
Lander et al. (1976)	Neutron diffraction from UO_2.
Zevin et al. (1978)	Relativistic nuclear quadrupole coupling in systems with $L > 0$.
Chatterjee et al. (1981)	Relativistic radial integrals for Sm^{2+} in tetragonal compounds. DF ones of Freemann and Desclaux (1979) good, DS ones of Lewis (1971) too large.
Goovaerts et al. (1981)	A relativistic MBPT treatment of the Tl atom hfs in a tetragonal crystal field.

Table 7.12. (continued).

Basu and Chakravarty (1982)	Intermediate-coupling scheme for complexes of d^n atoms.
Van Puymbroeck et al. (1982)	Hfs and g-tensor of Ga^0 and In^0 in KCl.
Kibler et al. (1984)	Energy levels of Sm^{2+} in BaClF and SrClF.
Pastusiak (1984)	Crystal-field contributions to the zero-field splittings of S-state $4f^7$ ions. References to earlier work.
Spitsyn et al. (1984)	Interpretation of intra-row periodicity effects.
Tuszynski and Chatterjee (1984)	Effective operators in relativistic crystal-field theory.

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

Reference	Comments
Mullikan (1930)	"Hund's case (c)", or ω - ω-coupling.
Ramsey (1953)	The n.r. theory of nuclear spin-spin coupling.
Nikitin (1961)	Wave functions of diatomic molecules with strong spin-orbit coupling.
A.J. Stone (1963)	Gauge invariance of the g-tensor.
Lin (1967)	Theory of nuclear magnetic shielding.
Hegstrom (1969)	Magnetic screening in the hydrogen atom.
Lipas et al. (1973)	Calculation of magnetic-dipole hyperfine matrix elements in molecules.
Eisenberger and Reed (1974)	Relativistic theory of the Compton effect.
Manninen et al. (1974)	Relativistic theory of the Compton effect.
Ribberfors (1975ab)	Relativistic theory of the Compton effect.
Pyykkoe (1977)	Relativistic theory of nuclear spin-spin coupling. Predicts a relativistic increase of the relative anisotropy of the coupling tensor, and a new isotropic term.
Hegstrom (1979)	Magnetic properties of H_2^+.
Pyykkoe and Wiesenfeld (1981)	The increased anisotropy attributed to a "s-$p_{1/2}$ mechanism".
Kolb et al. (1982)	Theory of nuclear magnetic shielding in atoms.
Pyper (1983bc)	Theory of nuclear magnetic shielding in molecules.
Pyykkoe (1983)	Theory of nuclear magnetic shielding in molecules.
Zhang and Webb (1983)	Theory of nuclear magnetic shielding in molecules.
Hunt (1985)	Magnetic screening in H_2.

8. SOLID-STATE THEORY

Solid-state calculations fall, strictly speaking, outside the present review. Because of some methodological points of contact, and because of the interest in chemical properties in Ch. 9, a small sample of the available literature is included in Table 8.1. For the particular case of the Kronig-Penney model (a chain of delta-functions), see Table 2.4.

Table 8.1. Band-structure calculations.

Reference	Comments
Altmann et al. (1957)	Relation between bond hybrids and metallic structures.
Callaway et al. (1957)	Relativistic effects on the cohesive energies of alkali metals.
Herman et al. (1963)	Relativistic corrections for tetrahedrally bonded semiconductors.
L.E. Johnson et al. (1963)	Relativistic effects in the band structure of PbTe.
Animalu (1966)	S-o interaction in metals and semiconductors.
Harrison (1966)	Pseudopotentials in the theory of metals.
Onodera and Okazaki (1966a)	The RKKR method. Theory only.
Loucks (1967)	The relativistic, augmented plane wave method.
M.L. Cohen and Heine (1970); Heine and Weaire (1970)	Review on PP methods.
Ellis and Painter (1970)	The discrete variational method (DVM)
Christensen and Seraphin (1971); Christensen (1982)	Relativistic band-structure of Au explains the optical properties especially the interband edge; a n.r. one does not.
Dimmock (1971)	Review on augmented-plane-wave methods.
Ziman (1971)	Bloch functions.
Phillips (1973)	Bonds and bands in semiconductors.
Davis (1974)	Actinoid compounds with NaCl structure.
Freeman and Koelling (1974)	Actinoids.
Krogh Andersen (1975)	Linear methods in band theory.
Moore (1975ab)	The g-shift in metals.
Neto and Ferreira (1976)	Relativistic Green's function method.
Singh et al. (1976)	Theory of g-factors in Fe and Ni.
Koelling and Harmon (1977); MacDonald et al. (1980)	Simultaneous inclusion of relativistic effects and spin polarization.
Catlow (1978); Catlow and Pyper (1979)	Cohesive electronic and redox properties of UO_2, U/PuO_2 using an ionic model.
Skriver et al. (1978)	The actinoid metals.
Zevin et al. (1978)	Relativistic quadrupole coupling.

Table 8.1. (continued).

Gloetzel and McMahan (1979)	The isostructural ("6s-to-5d-bonding", fcc-to-fcc) phase transition of Cs.
Keller et al. (1979)	Densities-of-states for the coinage metals using a cluster model.
Wertheim et al. (1979)	CsCl-structure intermetallic compounds (including CsAu).
Freeman (1980)	Lanthanoids and actinoids.
Herbst (1980-1984); Herbst and Wilkins (1982)	Core-level excitations in metals.
Takeda (1980)	Au.
Borstel et al. (1981, 1982); J. Braun et al. (1985)	Relativistic theory of photoemission from solids.
Burdett and Lin (1981)	EHT-type calculations on the crystal structures of PbO etc.
Doniach and Sommers (1981); Cortona et al. (1985)	Spin-polarized LDF models.
Jepsen et al. (1981)	Band structure of the coinage metals.
Kambe (1981)	Two-dimensional band theory for adsorbates.
Koelling (1981)	Review on band-structure calculations.
MacDonald et al. (1981)	Pd and Pt.
Tulkki and Keski-Rahkonen (1981)	X-ray satellites in metallic Zr, Rh, Ag.
Zhang (1981)	Scalar relativistic Green's function methods.
Christensen and Wilkins (1982)	Electronic pressures in heavy-element materials.
Godreche (1982)	Relativistic muffin-tin orbital methods.
MacDonald (1982)	g-factors of transition metals.
MacDonald et al. (1982)	Coinage metals Cu - Au. Influence of the transverse-photon term on the exchange potential studied.
Mallett (1982)	Actinoid monocarbides.
Misra et al. (1982)	MBPT of magnetic susceptibility in solids.
Nemoshkalenko et al. (1982ab)	X-ray spectra of 5d transition metals. A review.
Tripathi et al. (1982, 1985)	Theory of the Knight shift.
von Boehm and Isomaeki (1982)	Anisotropic semiconductors.
Weinberger (1982)	Actinoids. A review.
Benbow and Smith (1983)	Relativistic theory of photoemission of d-band metals.
Brooks (1983, 1985)	Atomic volumes of the actinoids.
Bylander and Kleinman (1983, 1984)	Cohesive properties of W.
Christensen and Kollar (1983)	CsAu.
Hedegard and Johansson (1983)	Auger energy shifts for the 5d transition metals.
Koelling and MacDonald (1983)	Relativistic effects in solids. A review.

Table 8.1. (continued).

Ladik et al. (1983)	Formulates a DF-LCAO theory for crystals.
Nemoshkalenko et al. (1983)	The relativistic, linear muffin-tin orbital method, applied on Au.
Weinert and Freeman (1983)	Knight shift of Pt (001).
Christensen (1984)	A review on relativistic band-structure calculations.
Davenport(1984)	"Linear augmented STO method". QR.
Eckhardt et al. (1984)	Noble metals.
C. Koenig et al. (1984)	Alkali metal-gold compounds.
Skriver (1984)	The LMTO method.
Thoerner and Borstel (1984)	Theory of photoemission from solids.
Trinquier and Hoffmann (1984)	PbO.
Davenport et al. (1985)	Cohesive energies of Lu - Au.
Dirl et al. (1985)	Relativistic cubic harmonics.
Fournier and Manes (1985)	Actinoids and their compounds.
Hoshino and Hasegawa (1985)	Relativistic corrections for an atom, imbedded in jellium.
Naegele et al. (1985)	Hybridization of actinoid 5f electrons.
Satpathy and Andersen (1985)	Bonding in $Gd_{10}C_4Cl_8$.
Yasui and Shimizu (1985)	Magnetic susceptibility of V.

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 development of this story is outlined in Table 9.1.

As to particular properties, references on bond lengths are summarized in Table 9.2., dissociation energies are discussed in Table 9.3. and force constants in Table 9.4.

For electronic spin-spin (or "zero-field") splittings, we mainly refer to the reviews, also given in Table 9.5. The other magnetic-resonance parameters are discussed in Table 9.6. and the molecular, electric dipole moments and charge distributions in Table 9.7. Data on molecular energy levels are summarized in Table 9.8 and those on molecular ionization potentials and electron affinities in Table 9.9.

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
Biron (1915)	"Secondary periodicity": $N/^{P}\backslash As/^{Sb}\backslash Bi$, etc. Quotes Abegg's electronic valence theory.
Sommerfeld (1916)	The relativistic stabilization and splitting of one-electron levels.
Grimm and Sommerfeld (1926)	Discuss the various valencies of main-group elements using Sommerfeld's relativistic atomic model.
Sidgwick (1933)	Introduces the term "inert pair" for $6s^2$.
Lakatos (1955)	Experimental thermochemical periodicities. Quotes the "transition metal contraction" for row 3.
Mayers (1957)	The indirect relativistic 5d destabilization in Hg.
Drago (1958)	Gives thermodynamic data on the "inert-pair effect".
Viswanathan (1959)	"Relativistic theory of chemical binding".
Boyd et al. (1963)	The indirect relativistic 5f destabilization in uranium.
Woods Halley and Shore (1965)	Molecular binding at the limit of large s-o interaction.
Larson and Waber (1968)	Where does the 5g series start?
Powell (1968); Szabo (1969)	Pedagogical articles on "relativistic quantum chemistry" (shapes of one-electron orbitals).
Waber (1969)	Quantum chemistry of the superheavy elements.
M.L. Cohen and Heine (1970); Heine and Weaire (1970)	Quotes the $6s^2$ inert pair and the related valence change (Sn (IV) vs. Pb (II) etc.) as "usually considered" due to relativistic effects (see pp. 59, 420).
Fricke and Waber (1971); Fricke et al. (1971)	Relativistic increase of the $5d^n6s^2$ configurations for 5d elements. S-o induced local maxima of IP_1 at the $5d^46s^2$ W and the $6p^2$ Pb. Predictions for the superheavies.
Penneman et al. (1971)	Chemistry of the superheavy elements.
Fricke and Waber (1972a)	Cs the largest atom in nature, due to the ns-shell relativistic contraction.
Desclaux (1973)	Presents a DF/HF comparison for energies and $\langle r^n \rangle$ of Z = 1-100, including evidence for the "gold maximum" of relativistic effects at Z = 29, 47, 79. See also Pyykkoe and Desclaux (1979b).
Smith and Davis (1973)	Review monovalent, Bi^+, chemistry. Attributed to $(p_{1/2})^2$ closed shells.
Desclaux and Pyykkoe (1974)	The relativistic bond-length contraction of CH_4 - PbH_4. See Table 9.2.
Silva et al. (1974)	Find experimentally that the No^{2+} ionic radius resembles the Yb^{2+} one.

Table 9.1. (continued).

Bagus et al. (1975)	The "lanthanoid contraction" studied by n.r. HF on "pseudo" 6th row atoms without a 4f shell.
Fricke (1975)	Properties of the superheavies, up to 172-184. Mentions the aurides CsAu, RbAu.
Liebman (1975)	Discusses s-o effects on Rn chemistry.
Pitzer (1975ab)	Points out that h_{so} perturbs both sigma and pi bonds, suggests that the elements 112, 114 and 118 may be relatively inert gases.
Smith (1975)	The anomalous IP_1 of Bi explained by final-state s-o stabilization.
Desclaux and Pyykkoe (1976)	"The chemical difference between Ag and Au may mainly be a relativistic effect".
Pyykkoe and Desclaux (1976)	Transition from 6p to $6p_{1/2}$ bonding in TlH.
Krasnov et al. (1976)	The lanthanoid contraction of Ln-X bond lengths in trihalides related to DS 5p radii.
Keller and Seaborg (1977)	Chemistry of the elements 104-107.
Pyper et al. (1977)	The Hg-Hg interaction potential is halved by relativistic effects.
Saeger and Rodies (1977)	The colour of gold and its alloys (experimental).
Seppelt (1977)	Synthesizes $AsCl_5$, despite of the transition-metal contraction (exp.).
Mikheev (1978)	Chemistry of Po.
Pyykkoe (1978)	(Ch. XI). Review on relativistic effects in chemistry. Mentions the nobility of Au, stability of Au^- and Hg_2^{2+}, liquidity of Hg. Compares lanthanoids and actinoids. Proposes a valency rule, implying higher valencies for 5d elements than for 4d elements.
Pyykkoe and Desclaux (1978)	Proposes that relativistic effects make sigma bonds of W as short as, and stronger than those of Mo. Relativistic contribution to the lanthanoid contraction about 3 pm (of 19 pm).
Rajnak and Shore (1978)	Regularities in electron binding energies in $l^N s^M$ configurations.
Rose et al. (1978a)	Compares direct and indirect relativistic effects for the valence electrons of Lu, Au, Tl. The direct ones found to dominate for 6s and 6p electrons!
Skriver et al. (1978)	The increased binding in actinoid metals from Ac to Pu ascribed to 5f electrons. A sudden localization occurs at Am.
Harris and Jones (1979)	N.r. bonding trends for the dimers C_2 - Pb_2. Discusses the anomalously small p-shell radii for C (no p core), Ge and Pb (partial screening by 3d- and 4f-shells, respectively).
Jones (1979)	Be_2 - Ra_2. d contributions discussed.
Jorgensen (1979)	A review on the Periodic System.

Table 9.1. (continued).

Pitzer (1979)	Review on relativistic effects in chemistry
Pyykkoe (1979a)	An introduction for first-year students.
Pyykkoe (1979b)	Analyses (n-1)d contributions to the bonds of alkaline earths. A relativistic decrease from Ba to Ra found.
Pyykkoe (1979bc)	Relativistic, covalent radii of late actinoids similar to those of the late lanthanoids.
Pyykkoe (1979d)	Confirms that the 4th-row anomaly in the "secondary periodicity" of Biron (1915) can be assigned to a (non-relativistic) "transition-metal contraction" due to the filled 3d shell, as proposed by Shchukarev (1954) or Nyholm (1961). The corresponding 6th-row anomaly is partly relativistic,partly an analogous "lanthanoid contraction".
Pyykkoe and Desclaux (1979b)	Review on relativistic effects in chemistry. Mentions the yellow colour of gold.
Seppelt (1979)	Reviews the structural chemistry of fluorides and oxide fluorides of non-metals.
Christiansen and Pitzer (1980); Pitzer and Christiansen (1981); Christiansen et al. (1982)	Transition from 6pσ bonding to $6p_{1/2}$ bonding in TlH confirmed.
Desclaux and Fricke (1980)	$_{103}$Lr ground state $7s^2 7p^1$, not $7s^2 6d^1$. See also Nugent et al. (1974).
Hulet et al. (1980); Hulet (1982, 1983)	Chemistry of the elements 99-105.
Pyper (1980bc, 1982a); Wood and Pyper (1981c)	Proposes a "kappa valence method", corresponding, for sigma bonds, to a normal sigma bond and a triplet pi bond. Pitzer and Christiansen (1981) show the latter contribution to be negligible.
Tatsumi and Hoffmann (1980)	Discuss "6p activation" of 5f AO:s in uranyl.
Ziegler et al. (1980,1981)	Interpret the nature of the relativistic bond-length contraction. Explicitly treat Hg_2^{2+}.
Burdett and Lin (1981)	Solid structures derived from the CsCl one; the stereochemically active $6s^2$ pair in red PbO.
Christiansen and Pitzer (1981); Christiansen (1983)	Verify for Tl_2 the idea of Pitzer (1975ab), that spin-orbit effects give a very weak bond for the ground state.
Hafner et al. (1981)	Effect of s-o coupling on bond strengths and -angles.
Hay (1981)	Compares M=Pd, Pt in Zeise's anion $MCl_3(C_2H_4)^-$.
Pyykkoe (1981)	Review on relativistic effects in structural chemistry.

Table 9.1. (continued).

Pyykkoe and Desclaux (1981)	Review on relativistic effects in chemistry.
Pyykkoe et al. (1981)	Effects of d AO:s on the bond-length contraction analysed. The similarity of Zr and Hf interpreted as cancelling relativistic and shell-structure effects, not the cancelling of s-p contractions and d expansions (Pyykkoe and Desclaux ,1977).
Tossell and Vaughan (1981)	Relationships between valence AO energies and crystal structures of compounds of Cu - Au and Zn - Hg.
Wadt (1981)	Why uranyl is linear and ThO_2 bent? Proposes simply a larger 6d participation for Th.
Cole and Perdew (1982)	Relativistic effects increase the Au EA from 1.5 to 2.5 eV.
Egdell et al. (1982)	A novel hybridization of the Bi-X sigma bonds found for BiX_3. Dominated by the 6p s-o splitting.
Ionova et al. (1982, 1983)	A review on relativistic effects in f-element chemistry.
Jorgensen (1982)	Emphasizes the "pushing from below" by 6p states on "ungerade" valence MO:s of uranium compounds.
Migdalek and Baylis (1982a)	Role of relativity, relaxation and core polarization in IP_1 of Cu - Au.
Trautmann (1982)	Status of superheavy element research.
Balasubramanian and Pitzer (1983)	Spin-orbit effects make the Pb_2 bond weak. A PP calculation with and without s-o.
Bylander and Kleinman (1983b)	The shift from d^5s ground state for Mo to a d^4s^2 one for W attributed to relativistic effects. Already mentioned by Fricke and Waber (1971), Fricke (1975).
Flerov and Ter-Akopian (1983)	Superheavy nuclei.
Grant (1983a)	Review on relativistic effects in atoms.
Haaland (1983)	Periodic trends in the bond lengths, of main-group methyl, hydride and chloride compounds. Row 6 found anomalous.
McKelvey (1983)	A pedagogical introduction to "relativistic effects on chemical properties".
Pitzer (1983, 1984)	Reviews on the author's own pseudopotential work.
Roesch and Streitwieser (1983); Roesch (1984)	Explains the success of n.r. $X\alpha$ work on thorocene and uranocene as cancelling occupation-number and relativistic effects.
Yan (1983)	Review on relativistic effects in chemistry.

Table 9.1. (continued).

Chamizo (1984)	The anomalously small EA of Pb attributed to s-o stabilization of neutral Pb.
Christiansen (1984)	Bi_2 has a bond-order (m_j=3/2) of close to 1.
de Kock et al. (1984a)	Role of "6p pushing" and 5f relativistic destabilization in the bonding of uranyl.
de Kock et al. (1984b)	Bonding of linear Hg, Au complexes analysed.
Ionova and Spitsyn (1984)	A review on relativistic effects in heavy-element chemistry (mainly of transition metals).
Low and Goddard (1984)	Relativistic effects and the chemistry of Pd and Pt.
Rabii and Yang (1984)	Compares Ag_2 and Au_2, finds larger s-d hybridisation in the latter.
Spitsyn and Ionova (1984)	Unusual oxidation states of lanthanoids and actinoids.
Trinquier and Hoffmann (1984)	PbO.
Banna (1985)	"Relativistic effects at freshman level", illustrated by x-ray PES.
Christiansen et al. (1985)	A review on relativistic effects in chemistry.
Christiansen and Ermler (1985)	Analyzes the bond-length contraction.
Nelin and Bauschlicher (1985)	Compares diatomic WO with MoO. Some excited states in different order, due to different atomic ground states.
Pacchioni (1985)	Compares Sn_2 and Pb_2 at the "scalar relativistic" level. See Balasubramanian and Pitzer (1983) above.

Table 9.2. Bond lengths.

Reference	Comments
Luke et al. (1969)	H_2^+ bond-length contraction 0.0016 pm.
Desclaux and Pyykkoe (1974)	CH_4 - PbH_4. The contraction of the Pb-H bond 11 pm or 5.6 per cent. (For slightly improved E(R) fits, see Pyykkoe (1979b)).
Desclaux and Pyykkoe (1976)	CuH - AuH.
Pyykkoe and Desclaux (1976)	BH - TlH.
Pyykkoe and Desclaux (1977)	MH_4 (M = Ti - Hf).
Hay et al. (1978)	AuH, AuCl, $HgCl_2$.
Pyykkoe and Desclaux (1978)	MH_4 (M = Ce, Th) and MH_6 (M = Cr, Mo, W).
Basch and Topiol (1979)	AuCl, $HgCl_2$, PtH. ODC.
Lee et al. (1979)	Au_2.
Michels et al. (1979)	Hg_2^+.
Pyykkoe (1979b)	MH^+ and MH_2 (M = Be-Ba, Zn-Hg, Yb). Proposes the estimates for the contraction $C = (R_{nr} - R_{rel})/R_{nr}$: C/per cent = 9.8 (2.7) x $10^{-4}Z^2$ C/pm = 17 (6) x $10^{-4}Z^2$.
Pyykkoe (1979c)	MH (M = La, Lu).
Basch (1980)	PtH (ODC), Ag_2 (CI) ground-state contractions 29, 11 pm, respectively.
Lee et al. (1980)	TlH.
Snijders and Pyykkoe (1980)	Verify the interpretation of Ziegler et al. (1980, 1981) using DF-OCE wave functions. AuH, TlH.
Ziegler et al. (1980, 1981)	Interpret the relativistic contraction of bond lengths as an orthogonality effect, involving the mass-velocity and Darwin terms in semi-core s AO:s mixed to the valence MO:s by the orthogonalization. Applications for M_2, MH, MCl (M = Cu, Ag, Au); MH^+, M_2^{2+}, MCl_2 (M = Zn, Cd, Hg), CsH, Cs_2, CsAu.
Pyykkoe et al. (1981)	Effect of d AO:s on the contraction, using both the DF-OCE and P-HFS approaches. CsH, BaH^+, RaH^+, MH_6 (M = Mo, W); MH_4 (M = Ti - Hf); MCl_4 (M = Zr, Hf). The Ziegler et al. (1980, 1981) explanation still holds but d AO:s diminish the core s character in valence MO:s.
Lee and McLean (1982); McLean and Lee (1982)	AgH, AuH.

Table 9.2. (continued).

Klobukowski (1983)	AgH, Ag_2.
Laskowski et al. (1983)	CsH contraction about 3 pm.
Martin (1983a)	AgH.
Martin (1983b)	Cu_2.
McLean (1983)	AgH, AuH and Ag_2. Deduces relativistic bond-length contractions from a comparison of n.r. CI results and experiment.
Pélissier (1983)	Cu_2.
Schwarz et al. (1983)	Analyses the relativistic bond-length contraction, finds that the Ziegler et al. (1980, 1981) one has an alternative.
Stoll et al. (1983)	Ag_2, AgH.
Ziegler (1983b)	W_2H_6. The relativistic contraction of the W≡W bond from 236 to 231 pm leaves it longer than the Mo≡Mo one of 223 pm.
De Kock et al. (1984b)	$Hg(CH_3)_2$. Contraction 10 pm.
Faegri and Almloef (1984)	$Ni(CO)_4$ Ni-C bond contraction 2.6 pm from PT.
Katriel et al. (1984)	Verify the interpretation of the relativistic bond-length contraction by Ziegler et al. (1980, 1981). M_2, M_2^+ (M = Li, Na)
Luethi et al. (1984)	The Fe-C contraction in $Fe(C_5H_5)_2$ only 0.7 pm.
Pelissier and Davidson (1984)	Cs_2.
Wallmeier (1984)	LiH. C = 0.010 %
Andzelm et al. (1985)	QR PP. Ag_2, AgH, AgO, AgF contractions 7, 4, 5 and 4 pm, respectively.
Christiansen and Ermler (1985)	Analyses the bond-length contraction (of Xe_2^+ and Au_2) using PP.
Fernandez et al. (1985)	SnH_4 and SnH_4^+ contractions 2 pm, from a PP calculation.
Hay and Martin (1985)	Ag_2 and AgO.
Ross and Ermler (1985)	Ag_2, Au_2, AgAu, AgH, AuH.
Scharf et al. (1985)	Cu_2.
Werner and Martin (1985)	Cu_2.

Table 9.3. Dissociation and interaction energies.

Reference	Comments
Ladik (1959, 1961a)	PT using a wave function. Result ten times too large.
Ladik (1961b, 1965)	Radiation corrections for H_2.
Kolos and Wolniewicz (1964)	H_2 D_e diminished 2.4 10^{-6} a.u. by relativistic effects. (Correlation, Breit terms and QED corrections included).
Luke et al. (1969)	H_2^+ D_e increased by 0.72 10^{-6} a.u.
Matcha (1973, 1976)	Diatomic alkali halides by PT. Up to ($_{19}$K)F, Li($_{35}$Br). A decrease by a few per cent found.
Desclaux and Pyykkoe (1976)	CuH - AuH.
Hay et al. (1978)	AuH,AuCl, $HgCl_2$.
Basch and Topiol (1979)	AuCl, $HgCl_2$. ODC.
Ermler et al. (1979); Lee et al. (1979)	Relativistic Au_2 D_e agrees with experiment. Relativistic increase about 1 eV.
Michels et al. (1979)	Hg_2^+.
Basch (1980); Basch and Topiol (1979)	Ag_2 ground-state rel. (n.r.) D_e/eV 1.12 (0.95), PtH 2.8 (1.0), respectively. CI.
Lee et al. (1980)	TlH.
Ziegler et al. (1980,1981)	Several molecules, see Table 9.2.
Lee and McLean (1982); Mclean and Lee (1982)	AgH, AuH.
Laskowski et al. (1983b)	CsH D_e decreased by relativity.
Martin (1983a)	AgH.
Martin (1983b)	Cu_2.
Pelissier (1983)	Cu_2.
Ziegler (1983b)	W_2H_6, as a model of W≡W bonds. Stronger than Mo≡Mo, due to relativity.
Andzelm et al. (1984)	The Xe-Xe interaction. QR PP.
de Kock et al. (1984)	$Hg(CH_3)_2$.
Ziegler (1984)	$M_2Cl_4(PH_3)_4$ Relativistic stabilization of the M≡M bond only 9 and 7 kJ/mol for Re and W, respectively.
Andzelm et al. (1985)	Ag_2, AgH, AgO, AgF.
Hay and Martin (1985)	Ag_2, AgO.
Ross and Ermler (1985)	Ag_2, Au_2, AgAu, AgH, AuH.

Table 9.4. Force constants.

Reference	Comments
Desclaux and Pyykkoe (1974)	CH_4 - PbH_4.
Desclaux and Pyykkoe (1976)	CuH - AgH.
Pyykkoe and Desclaux (1976)	BH - TlH.
Hay et al. (1978)	AuH, AuCl, $HgCl_2$.
Basch and Topiol (1979)	AuCl, $HgCl_2$, PtH. ODC.
Basch (1980)	Ag_2, PtH, CI.
Ziegler et al. (1980, 1981).	Several molecules, see Table 9.2.
Klobukowski (1983)	AgH, Ag_2.
Martin (1983a)	AgH.
Martin (1983b)	Cu_2.
Pelissier (1983)	Cu_2.
Andzelm et al. (1985)	Ag_2, AgH, AgO, AgF.
Hay and Martin (1985)	Ag_2, AgO.
Ross and Ermler (1985)	Ag_2, Au_2, AgAu, AgH, AuH.

Table 9.5. Molecular fine-structure splittings. See also the Tables 7.9., 7.11. and 9.8.

Reference	Comments
Veseth (1970)	Molecular fine structure.
Langhoff and Kern (1977)	A review on molecular fine structure.
Richards et al. (1980)	Review on s-o effects in molecules.
Case (1984)	Relativistic theory of zero-field splittings.
Dyke et al. (1984)	S-o splittings in dihalogens. The P-HFS model verifies the explanation of Wittel (1972) for $\Delta_u > \Delta_g$.

Table 9.6. Magnetic resonance parameters.

Reference	Comments
A.J.Stone (1963)	Gauge-invariance of the g-tensor.
Atkins and Jamieson (1967)	Derive the g tensor through a FW transformation. A new mass-velocity term found.
Hegstrom (1969)	Magnetic shielding in atomic hydrogen.
Nomura et al. (1969)	Relate the "heavy-atom chemical shift" to s-o coupling using 3rd-order PT. Quotes Nakagawa et al. (1967).
Morishima et al. (1973)	Proton chemical shifts in hydrogen halides.
Hegstrom (1975b)	Relates the g tensor to NMR chemical shifts. H_2^+.
Singh et al. (1976)	Theory of g-factors in metals.
Pyykkoe (1977); Pyykkoe and Wiesenfeld (1981)	Relativistic theory of nuclear spin-spin coupling. Contains a new isotropic term. Predicts an increase of the relative anisotropy, related to the "s-p term". See also Table 7.11.
Veseth (1977)	Interpretation of g-factors in diatomic molecules.
Volodicheva and Rebane (1978)	Proton chemical shifts in hydrogen halides.
Zevin et al. (1978)	Relativistic quadrupole coupling.
Hegstrom (1979)	g factors and other magnetic properties of H_2^+. Includes radiative and nuclear mass terms.
Cheremisin and Schastnev (1980)	3rd-order PT treatment of the ^{13}C chemical shift in halomethanes.
Sham et al. (1980)	Interpret nuclear quadrupole coupling in linear Au complexes using "renormalized" 5d and 6p DF AO:s.
Cheung and Merer (1982)	S-o distortion of the isotropic hyperfine Hamiltonian of high-spin states.
Kolb et al. (1982)	Magnetic shielding in atoms.
Tripathi et al. (1982, 1985)	Theory of the chemical shift in solids.
Arratia-Perez and Case (1983)	M1 hyperfine tensors of XeF and CsO.
Asada and Terakura (1983)	Relativistic corrections and the M1 hfs-induced nuclear spin-lattice relaxation in transition metals.
Pyper (1983bc)	Relativistic theory of chemical shifts.
Pyykkoe (1983)	Relativistic theory of chemical shifts.
Zhang and Webb (1983)	Relativistic theory of chemical shifts.
Case and Lopez (1984)	Relativistic theory of molecular M1 hfs.

Table 9.7. Electric dipole moments and molecular charge distributions.

Reference	Comments
Ros et al. (1980)	Relativistic effects on the deformation densities of MCl_2 (M = Zn, Cd, Hg) may be observable for Hg.
Krauss et al. (1985)	Relativistic dipole moments for AgH and AuH. The latter is about 1/2 of the n.r. one.
Sundholm (1985)	Relativistic dipole moment decrease of -0.00026 -0.00010 a.u. (electronic + bond-length) estimated for LiH.

Table 9.8. Molecular energy levels and energy transfer.

Reference	Comments
Rosen and Ellis (1974, 1975)	Relativistic effects on the energy levels of XeF_2, H_2X, InX, MCl.
Ellis and Rosen (1977)	ReF_6. Relativistic effects diminish the e_g - t_{2g} splitting from 5.5 to 3.8 eV. Surprisingly, no 5d relativistic destabilization in the molecule. t_{2g} s-o splittings for WF_6 - PtF_6.
Boring and Wood (1979ab)	Orbital energies of UO_2^{2+}, UF_6.
Rosen and Fricke (1979)	UF_5.
Bursten et al. (1980, 1983b); Cotton (1980)	Orbital energies of $Re_2Cl_8^{2-}$, Re_3Cl_9.
Feller and Davidson (1980)	The singlet-triplet separation in methylene.
Jonkers et al. (1980)	$TeCl_2$, $TeBr_2$.
J.H.Wood et al. (1981)	UO_2^{2+} levels with and without self-consistency of relativistic effects.
Chermette et al. (1982)	WO_6^{6-}. Relativistic effects place 4f above 5p.
Cotton et al. (1982)	Relativistic effects on quadruple Mo-Mo and W-W bonds.
Goursot and Chermette (1982)	One-electron energy levels of $IrCl_6^{3-}$. MS Xα.
Jonkers et al. (1982a)	CI_4.
Jonkers et al. (1982b)	C_2I_4.
Le Beuze et al. (1982)	$Mo_6S_8^{2-}$.
Sontum and Case (1982)	Coinage-metal porphines.
Goursot et al. (1983)	One-electron energy levels of $PtCl_6^{2-}$. MS Xα.
Jonkers et al. (1983)	GeI_2.
Avery (1984)	Relativistic, S-matrix theory of resonance energy transfer in molecules.
de Kock et al. (1984a)	One-electron energy levels of uranyl. The (largely 5f)δ_u HOMO due to both 6p pushing and relativistic destabilization.
de Kock et al. (1984b)	Competition between 5d s-o splitting and bonding in linear Hg and Au compounds.
Louwen et al. (1984)	$(PH_3)_2Pt(CCH)_2$.
Yang et al. (1984)	$W(CO)_6$.
Braydich et al. (1985)	$W_2(O_2CH)_4$.

Table 9.9. Molecular ionization potentials and electron affinities. For assignment of photoelectron spectra, see also Table 9.8.

Reference	Comments
Hay et al. (1979a)	UF_6 IP and EA.
Rosen et al. (1979)	MF_6 (M = Mo, W, 106) IP.
Berkowitz et al. (1980)	AgX (X = Cl - I) IP.
Lee et al. (1980)	PbS, PbSe, Au_2 IP.
Basch (1981)	Ag_n (n = 1 - 3) IP and EA.
Roesch and Streitwieser (1983); Streitwieser et al. (1985)	$M(C_8H_8)_2$ (M = Ce, Th, U) IP.
Stoll et al. (1983, 1984); Flad et al. (1984)	M_2, MH (M = Cu, Ag) IP.
Wang and Pitzer (1983)	PtH.
Balasubramanian (1984)	SnO, PbX (X = O - Se) IP.
Topol' and Zhilinskii (1984)	UF_4 (T_d) IP and EA.
Balasubramanian (1985b)	ICl IP.
Fernandez et al. (1985)	SnH_4 IP.
Ross and Ermler (1985)	Ag_2, Au_2 IP_1.

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 terminology "lanthanoid" and "actinoid", and 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.

$\mathbf{A}$	Magnetic vector potential.
$\underline{A}$	Hyperfine coupling tensor.
$\underline{\boldsymbol{\alpha}}$	Dirac matrix.
α	Fine structure constant (1/137.035 981 (12), 1985).
AE	All-electron.
AL	Average level.
α_L	Electric polarizability of multipolarity L.
An	An actinoid (Ac - Lr).
AO	Atomic orbital.
$\mathbf{B}$	Magnetic field.
β	Dirac matrix.
BP	Breit-Pauli.
c	Speed of light.
CEPA	Coupled electron-pair approximation.
CI	Configuration interaction.
D_e	Dissociation energy.
DF	Dirac-Fock. (Not "density-functional").
DS	Dirac-Slater.
DVM	Discrete Variational Method.
DZ	Double-zeta (radial function).
$\mathbf{E}$	Electric field.
EA	Electron affinity.
EAL	Extended average level.
ECP	Effective core potential.
EM	Electromagnetic.
ESR	Electron spin resonance.
FAKE	Fast, Accurate Kinetic Energy method.
FS	Fine structure.
FW	Foldy-Wouthuysen.
g	The electron g-factor.
$\mathbf{g}$	The electron g-tensor (in ESR).
γ_L	Electric screening constant of multipolarity L.
GTO	Gaussian type orbital.
GVB	Generalized valence bond.
h_D	The Dirac Hamiltonian (see eq.(2.4)).
h_d	The Darwin term at the n.r. limit.
h_m	The mass-velocity term.
HF	Hartree-Fock
Hfs	hyperfine structure.
HFS	Hartree-Fock-Slater.
IP	Ionization potential.
χ_L	Magnetic susceptibility of multipolarity L.
KG	Klein-Gordon.
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.
Ln	A lanthanoid (La - Lu).
LMTO	Linear Muffin-Tin Orbital method.

List of acronyms and symbols (continued).

MBPT	Many-body perturbation theory.
MCDF	Multiconfiguration Dirac-Fock.
MCHF	Multiconfiguration Hartree-Fock.
Me	Methyl (CH_3-).
MO	Molecular orbital.
MRCI	Multi-reference CI.
MS	Multiple Scattering.
MWH	Mulliken-Wolfsberg-Helmholtz (= EHT).
N	Number of electrons.
N.r.	Non-relativistic.
OCE	One-centre expansion.
ODC	Optimised Double-Configuration method.
ω_e	Vibrational frequency.
PES	Photoelectron spectrum, -spectroscopy.
P-K	Phillips-Kleinman.
PP	Pseudopotential.
PT	Perturbation theory.
QED	Quantum electrodynamics.
QM	Quantum mechanics.
QR	Quasirelativistic ("one-component").
ρ	Electron density.
R_e	Bond length.
REX	Relativistically parameterized Extended Hueckel.
RPA	Random phase approximation.
S	Overlap matrix.
σ_L	Magnetic screening constant of multipolarity L.
S-O	Spin-orbit.
STO	Slater-type orbital.
TD	Time-dependent.
T_e	Electronic excitation energy.
TF	Thomas-Fermi.
TP	Transition probability.
TS	Transition state.
V	A potential.
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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