

1. Record Nr.	UNINA9910974903703321
Autore	Fitts Donald D. <1932->
Titolo	Principles of quantum mechanics as applied to chemistry and chemical physics // Donald D. Fitts
Pubbl/distr/stampa	New York, : Cambridge University Press, 1999
ISBN	0-511-00763-9 0-511-81354-6 0-511-14905-0 0-511-05224-3
Edizione	[1st ed.]
Descrizione fisica	1 online resource (ix, 351 pages) : digital, PDF file(s)
Disciplina	541.2/8
Soggetti	Quantum chemistry
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Title from publisher's bibliographic system (viewed on 05 Oct 2015).
Nota di bibliografia	Includes bibliographical references (p. 344-346) and index.
Nota di contenuto	Cover; Half-title; Title; Copyright; Contents; Preface; 1 The wave function; 2 Schrodinger wave mechanics; 3 General principles of quantum theory; 4 Harmonic oscillator; 5 Angular momentum; 6 The hydrogen atom; 7 Spin; 8 Systems of identical particles; 9 Approximation methods; 10 Molecular structure; Appendix A Mathematical formulas; Appendix B Fourier series and Fourier integral; Appendix C Dirac delta function; Appendix D Hermite polynomials; Appendix E Legendre and associated Legendre polynomials; Appendix F Laguerre and associated Laguerre polynomials Appendix G Series solutions of differential equations Appendix H Recurrence relation for hydrogen-atom expectation values; Appendix I Matrices; Appendix J Evaluation of the two-electron interaction integral; Selected bibliography; Index
Sommario/riassunto	This text presents a rigorous mathematical account of the principles of quantum mechanics, in particular as applied to chemistry and chemical physics. Applications are used as illustrations of the basic theory. The first two chapters serve as an introduction to quantum theory, although it is assumed that the reader has been exposed to elementary quantum mechanics as part of an undergraduate physical chemistry or atomic physics course. Following a discussion of wave motion leading to

Schrodinger's wave mechanics, the postulates of quantum mechanics are presented along with essential mathematical concepts and techniques. The postulates are rigorously applied to the harmonic oscillator, angular momentum, the hydrogen atom, the variation method, perturbation theory, and nuclear motion. Modern theoretical concepts such as hermitian operators, Hilbert space, Dirac notation, and ladder operators are introduced and used throughout. This text is appropriate for beginning graduate students in chemistry, chemical physics, molecular physics and materials science.
