

**Computers in Chemistry, 1/e**

P Riyazuddin

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**About the Book**

The book describes the fundamentals of computers to enable students to develop and write simple programs related to chemistry. The attempt here has been to trigger the interest of the students in the direct application potential of computers in the field of chemistry. The languages discussed are BASIC, FORTRAN and C. Beginning first of a language, the book describes control statements and gives a brief introduction to arrays, functions, sub-routines and sequence common examples and calculations in physical, organic and inorganic chemistry have been presented. More than 150 program ranging from simple to complex, interesting exercises, hints and problems are some special features of the book.

**Salient Features**

- Provides an introduction to computer programming, with all important applications of programming in chemistry.
- Programming concepts have been given a detailed treatment before getting on with their applications.
- More than 150 programs with simple to complex treatment, exercises, and problems are provided.
- Appendices provide further elaboration on ASCII codes, student's t values, values of F at 95% confidence level, and rejection quotients, Q, at different confidence limits.

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- ▶ Monte Carlo Methods I
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#### Appendices

Appendices I: ASCII Codes Table-Format of Standard Characters

Appendices II: Student's t Values (one-tailed)

Appendices III: Values of Fat 95% Confidence Level

Appendices IV: Rejection Quotients, Q, at Different Confidence Limits

Bibliography

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#### **About the Author**

**P Riyazuddin** :- P. Riyazuddin is the Head, Dept. of Analytical Chemistry and Chairman, School of Chemical Sciences at the University of Madras. His main research interests include electroanalytical techniques, environmental analytical chemistry (toxic metals speciation), pharmaceutical analysis and chemometrics.

He is author and co-author of several publications in peer reviewed journals. Beside his regular research, he has devoted much of his time to chemical education, taking a particular interest in finding new ways for teachers with limited resources to provide experiments and projects for their students. This interest resulted in publication of several papers on inexpensive equipment and experiments for teaching of analytical chemistry.