

68[L, M, T].—Y. A. KRUGLIĀK & D. R. WHITMAN, *Tablitsy integralov kvantovoï khimii* (*Tables of quantum chemistry integrals*), Computing Center, Acad. Sci. USSR, Moscow, 1965, xlix + 440 pp., 27 cm. Price 4.76 rubles.

Approximations to solutions of the Schrödinger molecular equation are generally constructed with the help of *atomic orbitals*, that is, atomic one-electron functions, centered on the various nuclei in a molecule. In order to carry through this approach, it is necessary to evaluate a great number of difficult integrals between atomic orbitals on various centers. The various known methods for effecting these quadratures all require the evaluation of certain auxiliary functions as intermediate quantities.

The simplest of these auxiliary functions are represented by the integrals

$$A_n(\alpha) = \int_1^{\infty} x^n e^{-\alpha x} dx, B_n(\alpha) = \int_{-1}^1 x^n e^{-\alpha x} dx$$

which are related to the incomplete gamma function. Methods for evaluating these functions are well known, computer programs are available in many institutes, and a number of tables [1] have been published in the past. The numerous and considerable difficulties inherent in a study of molecular integrals are quite unrelated to these simple functions  $A_n(\alpha)$  and  $B_n(\alpha)$ .

The present volume deals exclusively with these two functions. An excellent introduction in Russian, probably the most detailed one on this subject, sets forth the properties of the tabulated functions, the methods used in calculating the tables, and details of interpolation in the tables. Included is a complete, detailed, and accurate review of all tables of  $A_n(\alpha)$  and  $B_n(\alpha)$  hitherto published.

Table I (pp. 1–401) gives values of  $A_n(\alpha)$  and  $B_n(\alpha)$  to 6S (in floating-point form) for  $n = 0(1)15$ ,  $\alpha = 0(0.01)50$ . Table II (pp. 403–439) continues this tabulation to 10, 12, or 14S for  $n = 0(1)17$ ,  $\alpha = 0(0.125)25$ .

This book appears to have been published under the sponsorship of the Computing Center of the Academy of Sciences of the USSR, the Gorky State University in Kharkov, and the Case Institute of Technology in Cleveland. Table I appears to have been calculated essentially at Case Institute and was published in 1961 as a technical report of that institution. Table II is, except for two values, a copy of a previous table by Miller, Gerhauser & Matsen [2].

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1. A. FLETCHER, J. C. P. MILLER, L. ROSENHEAD & L. J. COMRIE, *An Index of Mathematical Tables*, Vol. I, 2nd ed., Addison-Wesley, Reading, Massachusetts, 1962, pp. 305–306.

2. J. MILLER, J. M. GERHAUSER & F. A. MATSEN, *Quantum Chemistry Integrals and Tables*, Univ. of Texas Press, Austin, 1959. (For a review see *Math. Comp.*, v. 14, 1960, pp. 211–212, RMT 36.)

69[M, X].—R. E. BARNHILL & J. A. WIXOM, *Tables Related to Quadratures with Remainders of Minimum Norm*. I, ms. of 22 typewritten pages deposited in the UMT file and reproduced on the Microfiche page attached to this issue.