68[L, M, T].—Y. A. KRUGLIAK & D. R. WHITMAN, *Tablitsy integralov kvantovoĭ 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].

KLAUS RUEDENBERG

Iowa State University
Ames, Iowa

Eidgenössische Technische Hochschule
Zürich, Switzerland

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.

These tables contain the weights w_k for a family of quadrature formulas of the following type:

$$\int_{-1}^{+1} f(x)dx = \sum_{k=1}^{n} w_k f(x_k) + R_n ,$$

where R_n denotes the error associated with using the sum in place of the integral. Different groups of weights are tabulated, one for each of ten sets of abscissas $x_1, x_2, \cdots, x_n$. These sets of abscissas are identical to those used in the following rules: trapezoidal, Simpson, Weddle, and Gauss 2, 3, 4, 5, 7, 10, 16 point rules. A bound for the quadrature error of the form

$$|R_n| \leq ||R_n||\, ||f||$$

exists. The norm $||R_n||$ (cf. [1]) is also tabulated. The norm $||f||$ is defined by

$$||f|| = \iint_{\epsilon(a)} |f(z)|^2 dxdy$$

or by the same relation with $f(z)$ replaced by $f'(z)$, the first derivative of $f(z)$, depending on the choice of tabulated weights; the double integral is taken over an ellipse in the complex plane with semimajor axis a and semiminor axis $b = (a^2 - 1)^{1/2}$. Weights are tabulated for different a ranging from 1.0001 to 5.0. These weights have been determined for each a and each set of abscissas by the condition that the norm $||R_n||$ be minimized. It is therefore possible for these weights to yield a smaller quadrature error than that associated with the corresponding "ordinary" weights and same abscissas; comparison of the quadrature errors for some special cases is given in reference 1.

Eleven-digit numbers are tabulated; the calculations were carried out in double precision (16 digits). The results of $||R_n||$, using the standard weights, agreed with the results obtained by Lo, Lee and Sun [2], which gives an external check on the computations. An explanation of the headings—No Precision—and—Precision for Constants—can be found in [1].

LLOYD D. FOSDICK

University of Illinois
Department of Computer Science
Urbana, Illinois

1. R. E. BARNHILL & J. A. WIXOM, "Quadratures with remainders of minimum norm. I," *Math. Comp.*, v. 21, 1967, pp. 66–75.
2. Y. T. LO, S. W. LEE & B. SUN, *Math. Comp.*, v. 19, 1965, p. 133.

70[P, S, X, Z].—BERNI ALDER, SIDNEY FERNBACH & MANUEL ROTENBERG, Editors, *Methods in Computational Physics: Advances in Research and Applications, Vol. 5: Nuclear Particle Kinematics*, Academic Press, New York, 1966, xi + 264 pp., 23 cm. Price $11.50.

The fifth volume of this admirable series describes some applications of computers and computing technology to high-energy physics experiments and to the reduction of data from such experiments.

The last three of the five chapters are devoted to methods (hardware and software) for reclaiming experimental information from photographic records. The first