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Additions and Revisions to the Algorithms and Fortran Programs to Calculate Quantum Collision Integrals for Realistic Intermolecular Potentials

J. J. Hurly,* G. T. McConville, and W. L. Taylor

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*Chemistry Department, University of Cincinnati

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1. Introduction

This report is an addendum to MLM-3321, Algorithms and Fortran Programs to Calculate Quantum Collision Integrals for Realistic Intermolecular Potentials, by William L. Taylor [1].

The programs presented in MLM-3321 were written for the Mod-Comp computer that is now essentially obsolete; in this report, those programs have been revised for the IBM 3090, a much faster and larger machine. Several procedures were used by Taylor to minimize program run times, and most of the calculation was limited to single precision. When using the IBM 3090, the importance of time saving and conservation of storage locations is far less and this has allowed improvements to be made in the accuracy of the calculations.

Historically, the original version of the quantum mechanical collision integral program, QCOLL.FOR, was written in the 1960s by W. L. Taylor and J. M. Keller and was used to study interaction potentials for helium [2,3]. QCOLL.FOR utilized the Runga-Kutta scheme for numerical integration of the wave equation to obtain the phase shifts. The perturbed wave function containing the potential was integrated out to a large value of R, where the influence of the potential was essentially zero; then, the phase at a node was compared to the phase of the unperturbed wave function (spherical Bessel function). This we call the R_0-R method. Finally phase shifts according to the formulae of Wood [4], and Gauss-Laguerre quadrature [5] over the energy distribution completed the evaluation of the quantum collision integrals. In 1979, Aziz and Carley at the University of Waterloo, and Taylor and McConville at Mound Laboratory, collaborated on the quantum calculations of transport properties and virial coefficients for a new helium potential, HFDHE2 [6]. Carley independently wrote a computer code for calculation of the transport collision integrals using an algorithm for numerical integration of the wave equation due to Hepburn and LeRoy [7]. The cross section and energy integrations were adapted from the work of O'Hara and Smith [8,9]. Comparison of the numerical calculations from the two codes revealed very nearly identical results for the transport collision integrals.

More recently McConville [10] has investigated in some detail the calculation of the quantal phase shifts used to obtain the second virial coefficient at low temperatures. New low temperature virial coefficient data [11] prompted new and more precise calculations of quantum phase shifts using new helium potentials with deeper well depths. McConville used two codes [12] to calculate quantum phase shifts: (1) the phase shift portion of QCOLL.FOR and (2) a code written by LeRoy [13] which was supplied by R. A. Aziz and is designated herein by AZIZPH.FOR. This code utilizes Numerov's method of numerical integration, stopping the integration of the wave function after a relatively small number of cycles, typically eight nodes. A small Jeffreys-Wentzel-Kramers-Brillouin (JWKB) correction by Gaussian quadrature is applied to account for the balance of the phase shift from that point out to infinity. The phase shift is calculated by the arc tangent method. McConville has found that the arc tangent algorithm (ATAN) converges more quickly than the currently used comparison of asymptotic zeros. More importantly, however, McConville found that with the same potential function the two codes produced somewhat different sums of phase shifts which are used directly in calculating the second virial coefficients below 4 K. The calculations were further studied in this report, and reasons for the differences in the two computer codes are postulated. McConville's finding on the superiority of the ATAN method is upheld. These changes have been incorporated in the program, and a discussion of relative accuracies is presented.

Since the QCOLL program package was originally written for the study of helium-helium interactions, a disscusion of the modifications required to study other systems is presented, with the neon-argon system presented as an example.

2. Analysis of the Accuracy of Calculated Phase Shifts

The definition of the phase shift requires that the zero of the perturbed wave function be determined. The zero of the wave function is the distance R at which the wave function is equal to zero, and the zero is approached from a negative value. Each wave function has an infinite number of zeros, each called a node. The phase shift formula must be applied to a node or zero at the asymptotic limit.

In QCOLL.FOR, the perturbed wave function is calculated using a Runga-Kutta integration out to the asymptotic limit, which is approximated by the value of R at the cut off parameter VTEST. VTEST is a small fraction of the potential well depth, originally set at 10^{-6}. Each wavelength is divided into evenly spaced NK sections. The zero of the wave function is then found by interpolation. The interpolation to zero uses four points from the integration, two positive and two negative. The closer these four points are to the zero, the more accurate the interpolation.

In the R_0-R method, the zero of the unperturbed wave function, or spherical Bessel function, must also be determined. In the original version of QCOLL.FOR, this was done by integrating the wave function with the potential set equal to zero to produce a table of Bessel function zeros. For helium, it was found that a table of 100 L values with 49 zeros per Bessel function was adequate. Subsequently, the table was extended to L = 175 to accommodate heavier systems.

In AZIZPH.FOR, the program integrates the perturbed wave function until the difference in wavelength, from one cycle to another, meets a predetermined criterion; then, the position of the node is determined. The phase shift is determined by the arc tangent method, and a small JWKB correction is added; finally, the correct multiple of π is applied. A small error in the value of R at the node generates a significant error in the first and second order Bessel functions, which are calculated at that R. Any error in the Bessel functions will lead to a significant inaccuracy in the value of the calculated phase shift. Therefore, for both programs, the determination of the zeros must be very accurate.

A. Phase Shift Calculations Performed with QCOLL.FOR for 4He–4He Using the HFDHE–B [14] Interatomic Potential

As previously stated, the phase shift must be calculated at the asymptotic limit, and it must be determined at which node, or distance R, the approach to this limit is sufficiently achieved. The phase shift for energy 10.0633 K and L = 2 was calculated at several nodes with the results are presented in Table 1 and Figure 1. For Table 1 and succeeding tables, the percent deviation was obtained by taking the difference of the calculated value less the "correct value" (given at the bottom of the tables), then dividing this difference by the correct value and multiplying by 100. In Figure 1 the approach to the limit can be observed, as well as the node at which satisfactory results are achieved.

It was discovered that at larger nodes, greater than 20, the program failed to determine an accurate value of the zero with the usual integration step size. To correct this, the step size was made smaller. In program QCOLL, the integration step size is determined by the parameter NK, which defines the number of integration points per wavelength. In Table 1 the phase shifts are presented for the different values of NK. When NK=400, the phase shift approaches a truly asymptotic limit with increasing node number, as theory predicts.

Table 1

COMPARISON OF PHASE SHIFTS CALCULATED WITH QCOLL.FOR
USING R_0-R AND ARC TANGENT METHODS
AT E = 10.0633 K AND L = 2

VTEST	Radius (A)	Node No.	Phase Shift (R_0-R)	% Dev. (R_0-R)	Phase Shift (arc tan)	% Dev. (arc tan)
NK=40						
10^{-4}	23.48	6	+0.456791	+0.64	+0.453860	-0.01
10^{-5}	30.41	8	+0.455617	+0.38	+0.453866	-0.01
10^{-6}	37.33	10	+0.455029	+0.25	+0.453865	-0.01
10^{-7}	51.15	14	+0.454482	+0.13	+0.453861	-0.01
10^{-8}	78.75	22	+0.454111	+0.05	+0.453848	-0.01
10^{-9}	106.34	30	+0.453980	+0.02	+0.453836	-0.01
10^{-10}	154.62	44	+0.453882	-0.00	+0.453814	-0.02
10^{-11}	223.58	64	+0.453817	-0.02	+0.453817	-0.02
10^{-12}	327.01	94	+0.453753	-0.03	+0.453737	-0.04
NK=125						
10^{-4}	23.48	6	+0.456817	+0.64	+0.453887	-0.00
10^{-5}	30.41	8	+0.455647	+0.39	+0.453896	-0.00
10^{-6}	37.33	10	+0.455062	+0.26	+0.453898	+0.00
10^{-7}	51.15	14	+0.454521	+0.14	+0.453899	+0.00
10^{-8}	78.75	22	+0.454162	+0.06	+0.453899	+0.00
10^{-9}	106.34	30	+0.454043	+0.03	+0.453899	+0.00
10^{-10}	154.62	44	+0.453967	+0.01	+0.453899	+0.00
10^{-11}	223.58	64	+0.453931	+0.01	+0.453899	+0.00
10^{-12}	327.01	94	+0.453913	+0.00	+0.453898	+0.00
NK=400						
10^{-4}	23.48	6	+0.456818	+0.64	+0.453887	-0.00
10^{-5}	30.41	8	+0.455647	+0.39	+0.453896	-0.00
10^{-6}	37.33	10	+0.455063	+0.26	+0.453899	-0.00
10^{-7}	51.15	14	+0.454521	+0.14	+0.453900	-0.00
10^{-8}	78.75	22	+0.454163	+0.06	+0.453900	-0.00
10^{-9}	106.34	30	+0.454044	+0.03	+0.453900	-0.00
10^{-10}	154.62	44	+0.453968	+0.02	+0.453900	-0.00
10^{-11}	223.58	64	+0.453933	+0.01	+0.453900	-0.00
10^{-12}	327.01	94	+0.453915	+0.00	+0.453900	-0.00

NOTE: The correct value of the phase shift is taken to be
L = +0.4538976

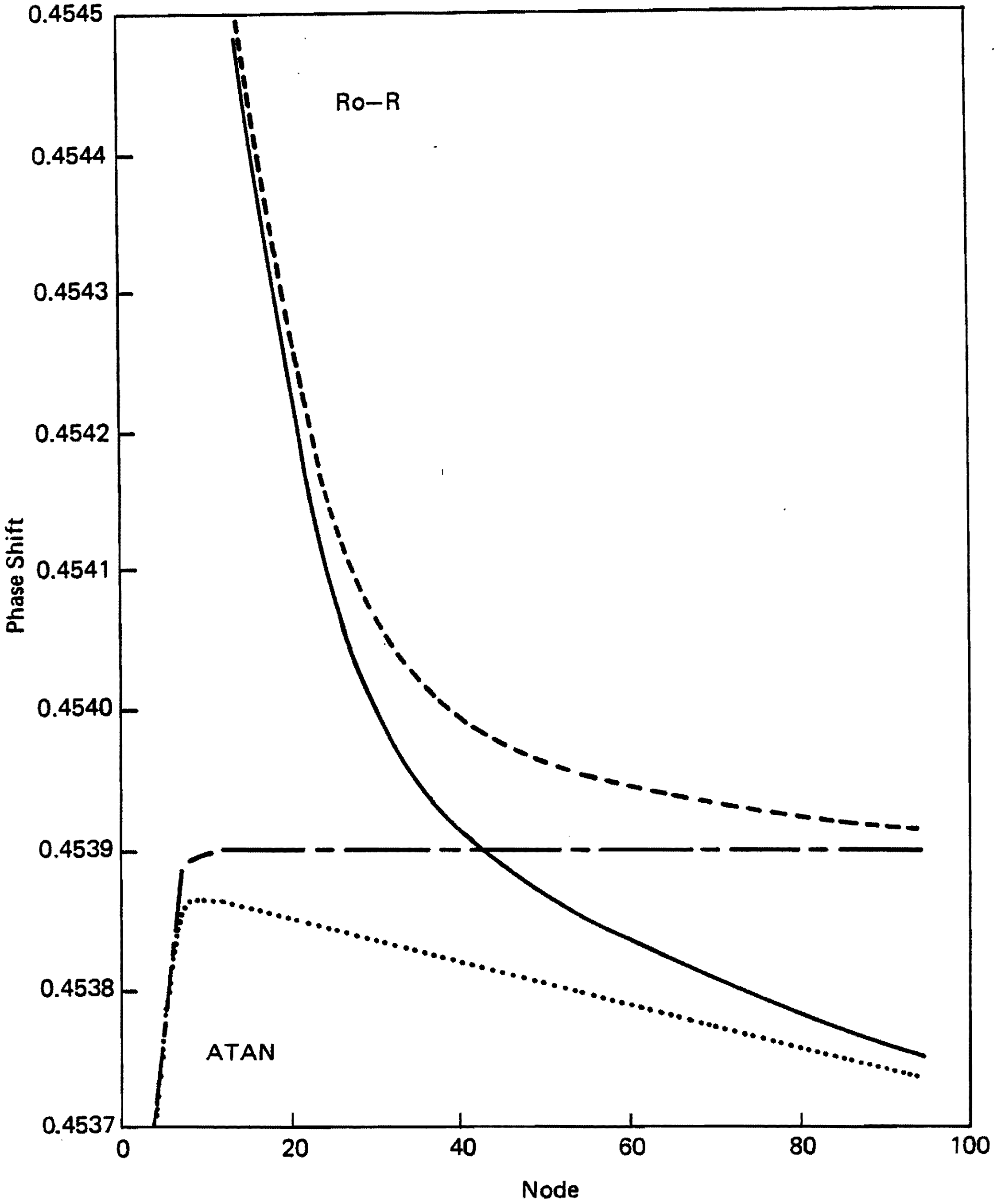

Figure 1 - Absolute phase shift calculated with QCOLL.FOR using both R_o-R and ATAN methods for E=10.0633 K and L=2 vs. increasing node number. The curves are: ——— and ...... , N=40; and ------ and —— —, NK=400.

Sums of the phase shifts are important because they are necessary in the calculation of the total cross section and the virial coefficient. Weighted sums, known as moments, are needed in the calculation of the various transport collision integrals. Table 2 presents the sums of the even phase shifts as used in the virial coefficient calculation for several values of NK. The original value of NK used was 40, which proved to be insufficient. Figure 2 shows the values of the sums of the even phase shifts at 10.0633 K for different values of NK.

B. Phase Shift Calculations Performed with AZIZPH.FOR

A program recently obtained to calculate the phase shifts was compared to QCOLL.FOR. This program was written by LeRoy [13] at the University of Waterloo and was supplied by R. A. Aziz. Although written completely independently, this program (AZIZPH.FOR) should produce the same results as QCOLL.FOR. Program AZIZPH.FOR evaluates the phase shift at a lower number node than that of QCOLL, typically less than 10. The program then adds a JWKB correction, to compensate for failure to reach the asymptotic limit. The JWKB correction was temporarily removed from the program, and the phase shifts were calculated at different nodes as done for QCOLL. At lower node numbers, both programs generate essentially the same value as QCOLL, but at higher node numbers the inaccuracy of the original Numerov step size, RH=0.35, becomes evident. Program AZIZPH.FOR uses a variable called RH to set the integration step size. Table 3 and Figure 3 present the L=2 phase shift calculated at E=10.0633 K with the AZIZPH.FOR program. Figure 3 compares the phase shift calculated with and without the JWKB correction for two different values of RH. Table 4 shows the sums of the even phase shifts for ^{4}He for different step sizes and cutoff parameters. The two

Table 2

COMPARISON OF SUMS OF PHASE SHIFTS CALCULATED WITH QCOLL.FOR USING R_0-R AND ARC TANGENT METHODS AT E = 10.0633 K AND L = 2

VTEST	Radius (A)	Node No.	Sum (R_0-R)	% Dev. R_0-R	Sum (arc tan)	% Dev. (arc tan)
NK=40						
10^{-4}	23.48	6	+2.743882	+3.05	+2.660464	-0.09
10^{-5}	30.41	8	+2.707251	+1.67	+2.661607	-0.04
10^{-6}	37.33	10	+2.685837	+0.87	+2.661544	-0.05
10^{-7}	51.15	14	+2.674078	+0.42	+2.660967	-0.07
10^{-8}	78.75	22	+2.666177	+0.13	+2.659892	-0.11
10^{-9}	106.34	30	+2.652289	-0.39	+2.649044	-0.52
10^{-10}	154.62	44	+2.646687	-0.60	+2.645087	-0.66
10^{-11}	223.58	64	+2.640157	-0.85	+2.639406	-0.88
10^{-12}	327.01	94	+2.632573	-1.13	+2.632228	-1.15
NK=125						
10^{-4}	23.48	6	+2.744249	+3.06	+2.660813	-0.07
10^{-5}	30.41	8	+2.707895	+1.69	+2.662223	-0.02
10^{-6}	37.33	10	+2.636850	+0.91	+2.662525	-0.01
10^{-7}	51.15	14	+2.675747	+0.49	+2.662603	-0.00
10^{-8}	78.75	22	+2.668925	+0.23	+2.662611	-0.00
10^{-9}	106.34	30	+2.665773	+0.11	+2.662597	-0.00
10^{-10}	154.62	44	+2.664158	+0.05	+2.662572	-0.01
10^{-11}	223.58	64	+2.663291	+0.02	+2.662534	-0.01
10^{-12}	327.01	94	+2.662829	+0.00	+2.662476	-0.01
NK=400						
10^{-4}	23.48	6	+2.744253	+3.06	+2.660817	-0.07
10^{-5}	30.41	8	+2.707902	+1.70	+2.662230	-0.02
10^{-6}	37.33	10	+2.686861	+0.91	+2.662536	-0.01
10^{-7}	51.15	14	+2.675764	+0.49	+2.662620	-0.00
10^{-8}	78.75	22	+2.669188	+0.24	+2.662725	-0.00
10^{-9}	106.34	30	+2.665971	+0.12	+2.662729	+0.00
10^{-10}	154.62	44	+2.664348	+0.06	+2.662730	+0.00
10^{-11}	223.58	64	+2.663502	+0.03	+2.662729	+0.00
10^{-12}	327.01	94	+2.663090	+0.01	+2.662729	+0.00

NOTE: The correct value of the sum is taken to be $\Sigma = +2.6627282$

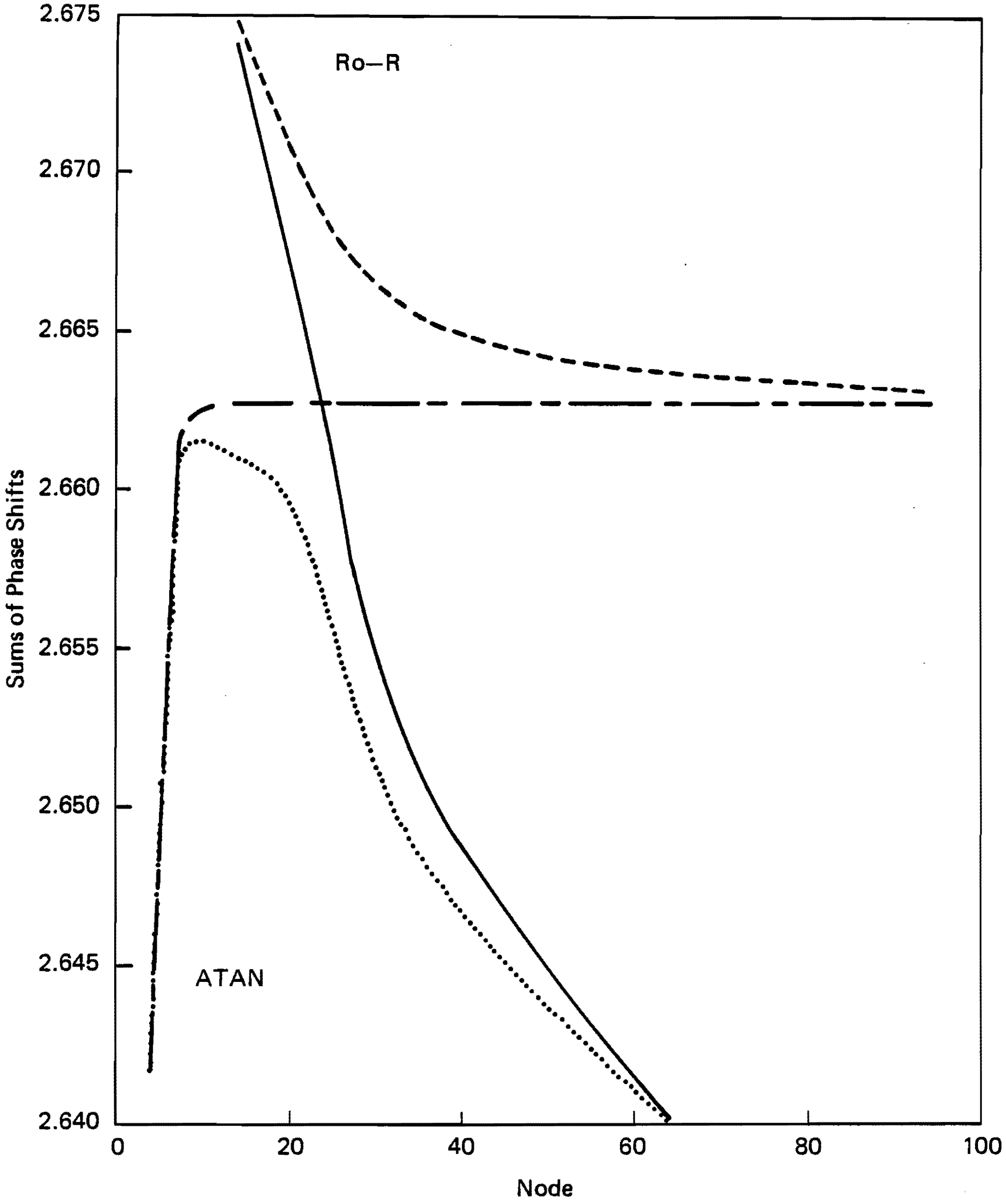

Figure 2 - Sums of phase shifts calculated with QCOLL.FOR using both the R_0-R and ATAN methods for E=10.0633 K and L=2 vs. increasing node number. The curves are the same as for Figure 1.

Table 3

COMPARISON OF PHASE SHIFTS CALCULATED WITH AZIZPH.FOR
USING ARC TANGENT METHOD WITH AND WITHOUT JWKB CORRECTION
AT E = 10.0633 K AND L = 2

Delta	Radius (A)	Node No.	Phase Shift (w/corr)	% Dev.	Phase Shift (w/o corr)	% Dev.
RH=0.35						
	23.48	6	+0.453899	+0.000	+0.453886	-0.003
	30.41	8	+0.453899	+0.000	+0.453895	-0.001
	37.33	10	+0.453899	+0.000	+0.453898	-0.000
	51.15	14	+0.453899	+0.000	+0.453899	-0.000
	78.75	22	+0.453900	+0.000	+0.453900	-0.000
	106.34	30	+0.453900	+0.001	+0.453900	-0.000
	154.62	44	+0.453901	+0.001	+0.453901	+0.001
	223.58	64	+0.453902	+0.001	+0.453902	+0.001
	327.01	94	+0.453904	+0.001	+0.453904	+0.001
RH=0.20						
	23.48	6	+0.453898	+0.000	+0.453885	-0.003
	30.41	8	+0.453898	+0.000	+0.453894	-0.001
	37.33	10	+0.453898	+0.000	+0.453897	-0.000
	51.15	14	+0.453898	+0.000	+0.453898	-0.000
	78.75	22	+0.453898	+0.000	+0.453898	+0.000
	106.34	30	+0.453898	+0.000	+0.453898	+0.000
	154.62	44	+0.453898	+0.000	+0.453898	+0.000
	223.58	64	+0.453898	+0.000	+0.453898	+0.000
	327.01	94	+0.453898	+0.000	+0.453898	+0.000
RH=0.05						
	23.48	6	+0.453898	+0.000	+0.453885	-0.003
	30.41	8	+0.453898	+0.000	+0.453894	-0.001
	37.33	10	+0.453898	+0.000	+0.453896	-0.000
	51.15	14	+0.453898	+0.000	+0.453897	-0.000
	78.75	22	+0.453898	+0.000	+0.453898	-0.000
	106.34	30	+0.453898	+0.000	+0.453898	-0.000
	154.62	44	+0.453898	+0.000	+0.453898	-0.000
	223.58	64	+0.453898	+0.000	+0.453898	-0.000
	327.01	94	+0.453898	+0.000	+0.453898	-0.000

NOTE: The correct value of the phase shift is taken to be L = +0.4538976

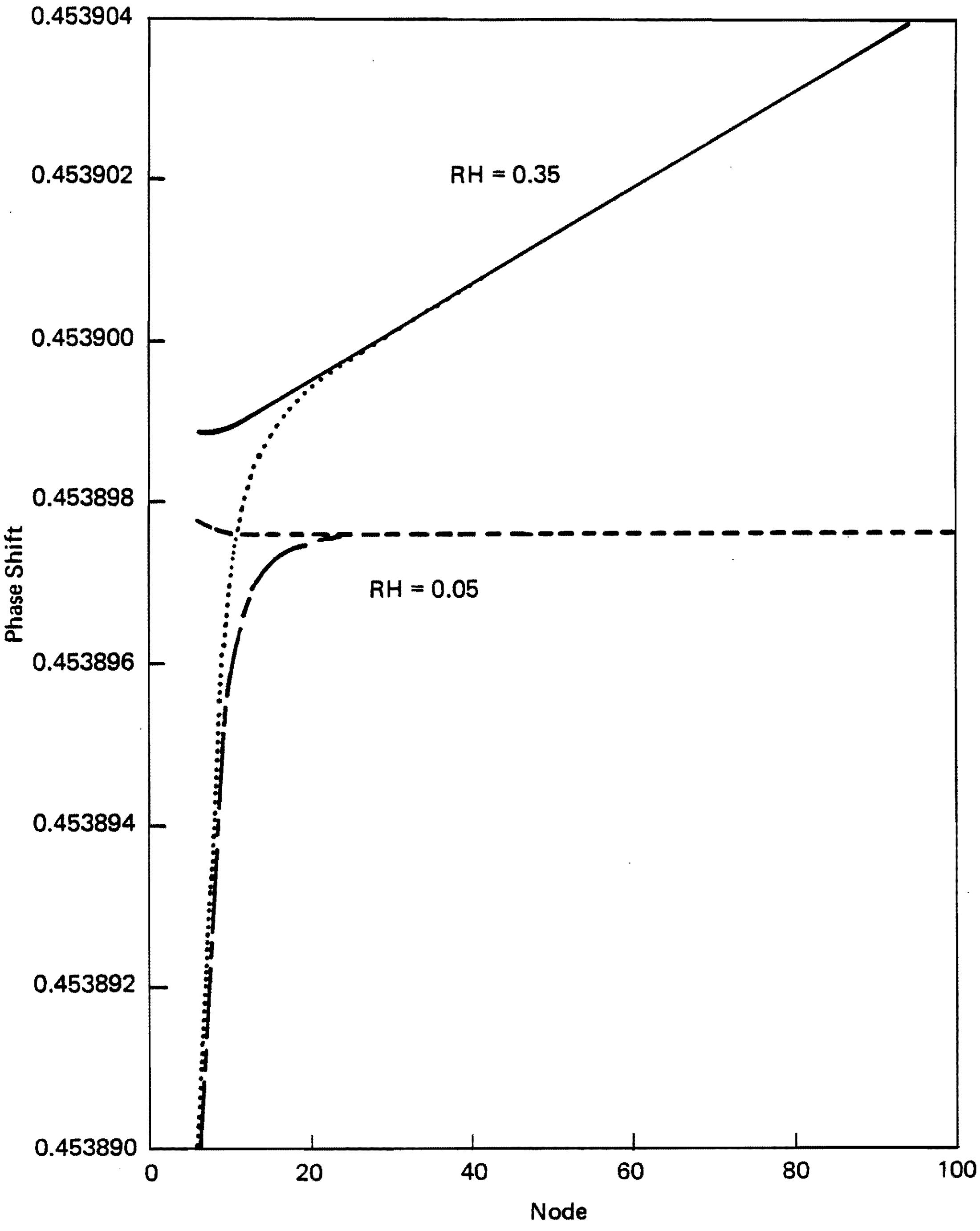

Figure 3 - Absolute phase shift calculated with AZIZPH.FOR using the ATAN method for E=10.0633 K and L=2 and with (w.) and without (w/o) the JWKB correction vs. increasing node number. The curves are: —— (w.) and . . . . (w/o), RH=0.35; ------- (w.) and —— –(w/o), RH=0.05.

cutoff parameters are PHTEST and ERR. PHTEST is the convergence criterion for the individual phase shifts, and ERR is the convergence criterion for the sum of the phase shifts. Figure 4 shows the calculated sums versus PHTST for different values of RH. It should be kept in mind that the program originally never evaluated the phase shift past a node number of 10, hence this discrepancy from the correct value was not observed. Obviously a smaller step size, RH=0.20 to 0.05, is required, especially at larger nodes, as well as a more stringent value of PHTST.

C. Analysis of Sections A and B

A major consideration in the present work was to determine whether the arc tangent or R_0-R method was superior. Figure 1 shows the absolute phase shift calculated from QCOLL at different nodes. It is apparent that both methods, ATAN and R_0-R, approach the same limit, but the ATAN method does so sooner. At any given node, the results from the ATAN method will be more accurate than those from the R_0-R method. For this reason, the ATAN method is the method of choice in these calculations. Figure 1 also shows the effect of the step size in the integration when NK=40; when NK=400, the approach to the limit is obvious. Figure 2 demonstrates the same behavior for the sums of the phase shifts, indicating that the deviations are not a function of L. Figure 3 shows the phase shift calculation for the LeRoy program. A small step size for the integration in the LeRoy program creates a positive error in the phase shift. Figure 4 is a plot of the sum of the phase shifts versus the cutoff criteria, PHTST, for the individual phase shifts. The figure not only illustrates the small error in the calculation due to the step size but a much larger error due to an insufficiently stringent value of PHTST. The original value used by Aziz was 10^{-4}, and this is shown by the solid square.

Table 4

COMPARISON OF SUMS OF PHASE SHIFTS CALCULATED WITH AZIZPH.FOR WITH DIFFERENT INTEGRATION STEP SIZES AND CUTOFF PARAMETERS AT E = 10.0633 K AND L =2

PHTEST	ERR	Sum (arc tan)	% Dev. (arc tan)
RH=0.35			
10^{-4}	10^{-3}	+2.657321	-0.203
10^{-4}	10^{-4}	+2.661626*	-0.041
10^{-5}	10^{-5}	+2.662599	-0.005
10^{-6}	10^{-6}	+2.662804	+0.003
10^{-7}	10^{-6}	+2.662828	+0.004
RH=0.20			
10^{-4}	10^{-3}	+2.657310	-0.203
10^{-4}	10^{-4}	+2.661607	-0.042
10^{-5}	10^{-5}	+2.662567	-0.006
10^{-6}	10^{-6}	+2.662744	+0.001
10^{-7}	10^{-6}	+2.662738	+0.000
RH=0.05			
10^{-4}	10^{-3}	+2.657308	-0.204
10^{-4}	10^{-4}	+2.661604	-0.042
10^{-5}	10^{-5}	+2.662563	-0.006
10^{-6}	10^{-6}	+2.662738	+0.000
10^{-7}	10^{-6}	+2.662728	+0.000

NOTE: The correct value of the sum is taken to be $\Sigma = +2.6627282$. The asterisk denotes the value calculated with the original parameters of AZIZPH.FOR.

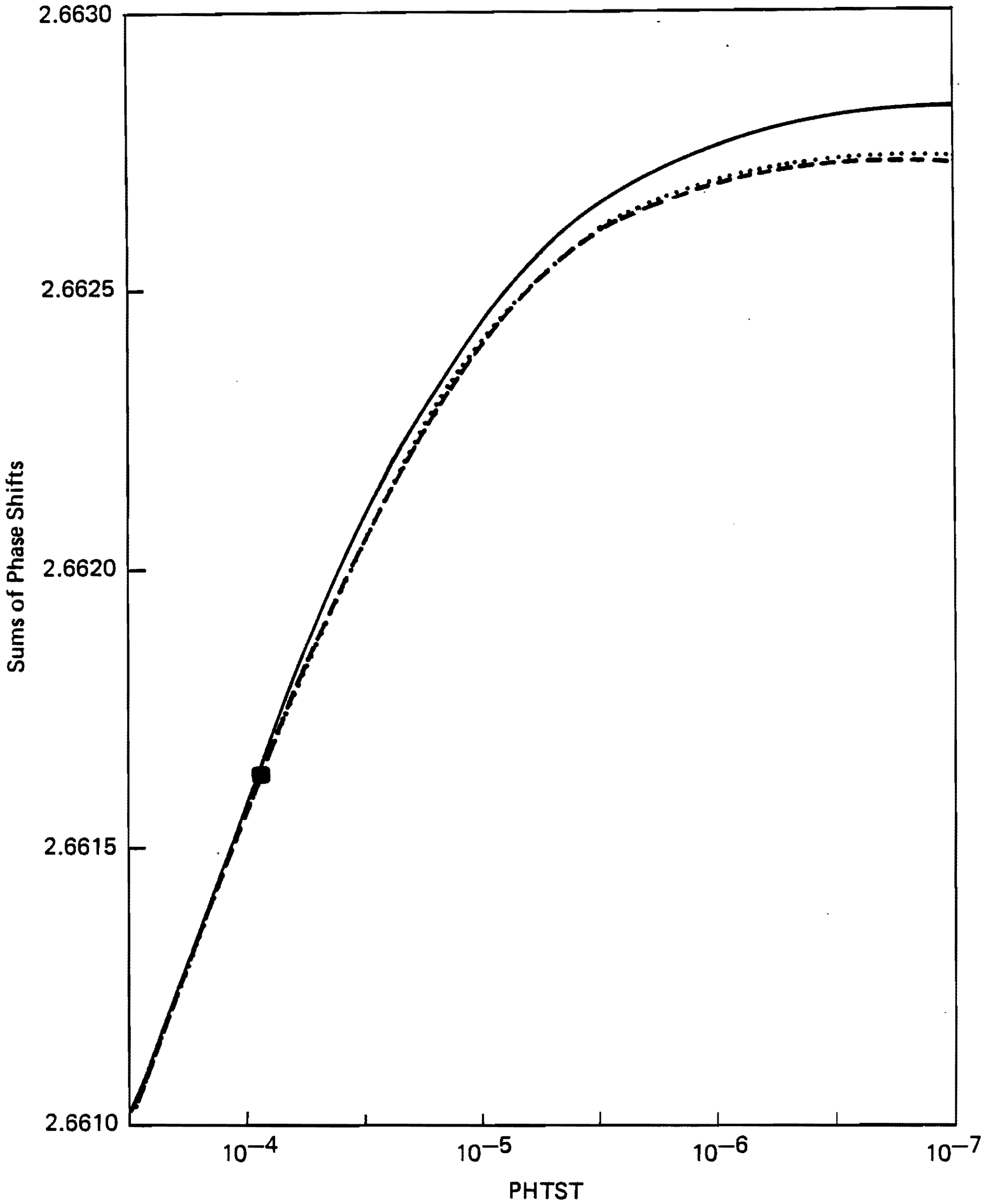

Figure 4 - Sums of phase shifts calculated with AZIZPH.FOR using the ATAN method for E=10.0633 K and L=2 vs different phase shift convergence criteria, PHTST. The curves are: —— , RH=0.35; . . . . , RH=0.20; and - - - -, RH=0.05. The solid square is the value calculated with the original parameters used by Aziz in the program.

Figure 5 shows the sums of the phase shifts calculated with the two programs as a function of VTEST or PHTST. QCOLL.FOR uses VTEST as a cutoff and AZIZPH.FOR uses PHTST as a cutoff. All curves approach the same asymptotic limit, indicating consistency.

Figures 6a and 6b show the $\Omega^{(2,2)*}$ collision integral calculated at different values of VTEST. Once again, the superiority of the ATAN technique is obvious. The collision integrals are not so sensitive to the approach to the asymptotic limit as the sums used in calculating the virial coefficient.

Since both programs produce essentially the same results with stringent parameters, it is concluded that this value is the asymptotic limit. The integration parameters needed to achieve these results are, however, unacceptable in a practical sense. Calculations with NK=400 and RH=0.05 required all quad precision (REAL*16) and excessive computer time. The minimal stringent parameters, which will still yield the desired accuracy, must be determined.

D. Determination of the Optimal Method for Calculating the Second Virial Coefficient

The calculation of the quantal second virial coefficient requires an integration over the sums of the phase shifts versus energy as given by Equation 6.4-11 in Reference [15]. Thus, differences that appear in different calculations of the second virial coefficient can appear from two sources: differences in various codes to calculate phase shifts (and hence their sums) or in the numerical integration over energy. Because the energy integrand has the form $e^{-E/kT}$ f(E), where f(E) is the sum over phase shifts, the Gauss-Laguerre quadrature was considered to be the logical method for its evaluation. This method was found, however, to be less accurate than the Newton-Coats methods for temperatures below approximately 10 K for a subtle reason.

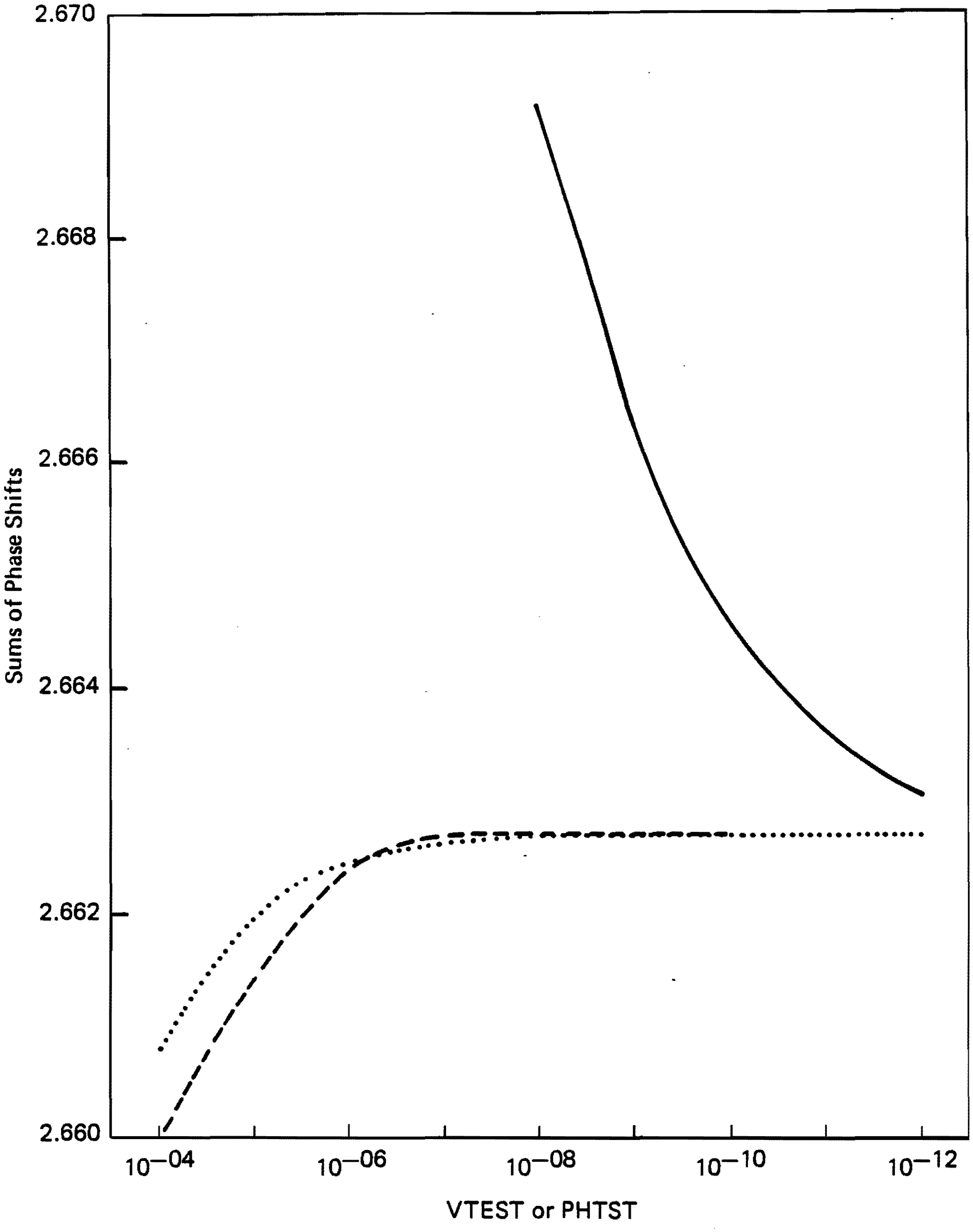

Figure 5 - Comparison of the sums of phase shifts for the two programs vs. equivalent convergence criteria (VTEST or PHTST). The curves are: ——— , QCOLL.FOR, R_0-R method with NK=400; . . . . , QCOLL.FOR, ATA method with NK=400; and - - - -, AZIZPH.FOR, ATAN method with RH=0.05.

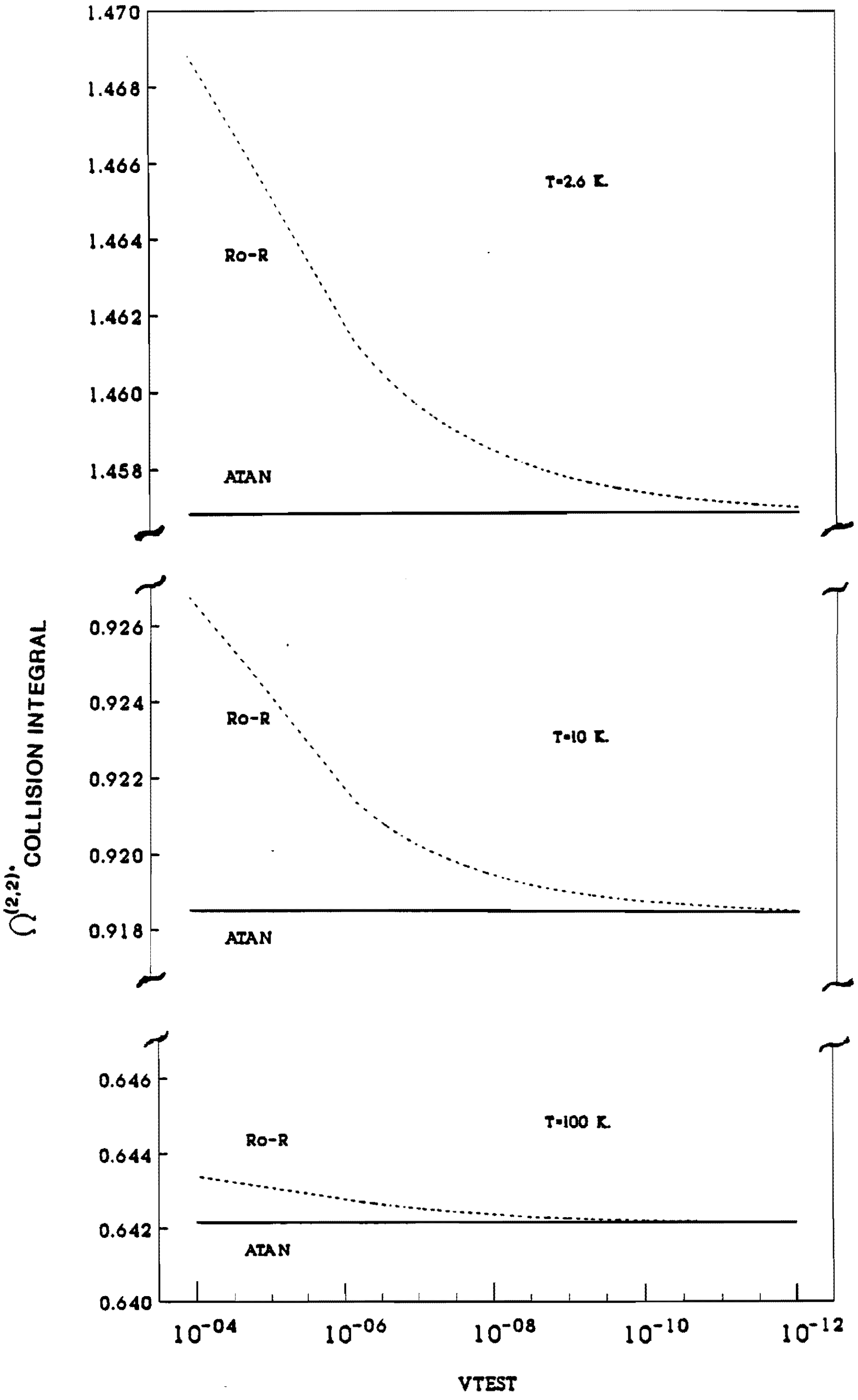

Figure 6 - Comparison of the $\Omega^{(2,2)*}$ collision integral at E = 2.6, 10 and 100 K calculated from QCOLL.FOR using both the ATAN and R_o-R methods vs increasing value of VTEST.

The difference in the second virial coefficient due to the differences in the phase shift calculations is illustrated by comparing a calculation using QCOLL.FOR in the real asymptotic limit with the results obtained from the AZIZPH.FOR program with the original input parameters. The JWKB correction for the excluded potential tail, for R larger than node 6, is included. The values of the virials were calculated at the temperatures of the Berry [11] virial coefficient data, and the differences are shown in Table 5. The differences in the calculations for the same potential and energy integration are less than 10% of the experimental uncertainty.

Table 5

COMPARISON OF SECOND VIRIAL COEFFICIENTS FOR ^{4}He CALCULATED WITH THE QCOLL.FOR AND AZIZPH.FOR PHASE SHIFT CODES VS. EXPERIMENT

Temp. (K)	Exp. Ref[11]	Exp. Unc. (+ or -)	QCOLL.FOR	Difference (QCOLL-AZIZ)
2.60	-142.5	1.0	-142.29	-0.09
2.75	-133.2	0.7	-133.27	-0.09
3.33	-105.8	0.7	-106.14	-0.07
4.22	- 79.5	0.5	- 79.62	-0.05
7.20	- 39.0	0.7	- 39.13	-0.02
13.80	- 11.7	0.4	- 11.90	0.00
20.27	- 2.4	0.2	- 2.54	0.00
27.10	+ 2.5	0.3	+ 2.40	0.00

NOTE: The units of the virial coefficients and the difference are given in cm^3 mole^{-1}.

To elucidate the difference between different quadrature methods for the energy integral, a code was written to fit the phase shift sums from Q = 0 to 40 to a cubic spline function. The integration was then performed using the Gauss-Laguerre (G-L) and several other quadrature methods of different levels of sophistication, e.g., square intervals (SQ), half-square (HA) intervals, Simpson's Rule (SM), and Weddle's Rule (WED). A Simpson's Rule code (AZIZ.SM) was also obtained from Aziz that is somewhat different from the Mound Simpson's Rule code. The results are shown in Table 6. It is clear from Table 6 that the Gauss-Laguerre integration differs significantly from the Newton-Coats methods for T < 10 K. This difference occurs because, in order to get all of the low energy contribution to the integral, one has to include the interval between Q=0 and the smallest x value in the Gauss-Laguerre quadrature table because the sum is equal to π at Q=0.

The problem with the Newton-Coats and simpler rules is that the answer depends on the grid size down to very fine grids. The first part of Table 6 shows the different methods using the original grid employed by Aziz. The methods differ as much as 0.1 cm^3 $mole^{-1}$. With the finer grid in the second part of Table 6, the differences converge to 0.02 cm^3 $mole^{-1}$. Thus, the calculated second virial coefficients for helium, using different codes but the same potential function, HFD-B [15], has a calculational uncertainty of less than 0.1 cm^3 $mole^{-1}$ for 2.6 < T < 27 K.

E. Discussion of the Optimal Integration Methods and Parameters for QCOLL.FOR

This section addresses choosing integration methods and parameters for QCOLL.FOR that will balance the requirements of numerical accuracy of the results with the practical problem of computer running time. The more rapid convergence of the arc tangent method over the R_0-R method has been shown in the foregoing and the program has been converted to this calculational method with

Table 6

THERMAL AVERAGING FOR SECOND VIRIAL COEFFICIENT USING QUADRATURES DESCRIBED IN TEST WITH BEST QCOLL.FOR SUMS

Temp (K)	G-L	AZIZ.SM	WED	SM	HA	SQ
	cm^3 mole^{-1}					
A[a]						
2.60	-125.2429	-125.4877	-125.5099	-125.5090	-125.4877	-125.5027
2.75	-117.5883	-117.7332	-117.7548	-117.7543	-117.7332	-117.7501
3.33	- 94.3959	- 94.5531	- 94.5740	- 94.5744	- 94.5531	- 94.5761
4.22	- 71.4083	- 71.5106	- 71.5311	- 71.5323	- 71.5106	- 71.5384
7.20	- 35.4544	- 35.4931	- 35.5051	- 35.5061	- 35.4931	- 35.5112
13.80	- 10.5219	- 10.5313	- 10.5171	- 10.5120	- 10.5313	- 10.5011
20.27	- 1.7566	- 1.7591	- 1.7357	- 1.7051	- 1.7591	- 1.6719
27.10	+ 2.9015	+ 2.9025	+ 2.9345	+ 3.0078	+ 2.9025	+ 3.0712
B[b]						
2.60	-125.2427	-125.4945	-125.4967	-125.4969	-125.4945	-125.4945
2.75	-117.5082	-117.7390	-117.7410	-117.7411	-117.7390	-117.7390
3.33	- 94.3956	- 94.5566	- 94.5578	- 94.5578	- 94.5566	- 94.5566
4.22	- 71.4081	- 71.5124	- 71.5130	- 71.5131	- 71.5124	- 71.5124
7.20	- 35.4544	- 35.4936	- 35.4938	- 35.4938	- 35.4936	- 35.4936

the added advantage of eliminating the large table of Bessel function zeros.

It is unrealistic to calculate the phase shifts in every instance with the most stringent parameters considered, e.g., the 200th node with NK=400, as this will result in a great consumption of computer time. If only the collision integrals are required, the program may be run with NK=40 and a VTEST as low as 10^{-4} if the arc tangent method is used. If the R_0-R method is used, a VTEST of 10^{-6} or better will yield collision integrals with an accuracy better than 0.3% at very low temperatures (≈2 to 15 K) and better than 0.1% at higher temperatures. The rapid Gauss-Laguerre integration method is sufficiently accurate.

If, however, the sums of the phase shifts are to be used in the calculation of the second virial coefficient at low temperatures, more stringent parameters and integration methods are required. Figure 1 shows that NK=40 is not sufficiently accurate, particularly at higher nodes, and from Tables 1 and 2 it is seen that NK≈100 with VTEST=10^{-8} will yield quite accurate results. Table 6 shows the virial coefficients calculated with various integration methods and two energy grids at different temperatures. When performing the energy integration for the virial coefficient at low temperatures, it is advisable to use an integration method such as Simpson's rule rather than the Gauss-Laguerre, as the G-L weight functions apparently do not sufficiently sample the low energy region of the integrand. It is also advisable to use a fine energy grid.

QCOLL.FOR has been set up for rapid calculation of the collision integrals and it is left to the reader to make the programmatic changes suggested in the previous paragraph.

3. Modifications to QCOLL.FOR

A. Changes Made for Convenience of Operation

1. The entire program, including all subroutines, has been rewritten in double precision, i.e., REAL*8. This increases the program's accuracy and helps to eliminate overflow and underflow errors by allowing the machine to handle larger numbers.

2. The program contains several parameters that determine the limits to which a certain calculation is performed. Where feasible, these variables have been changed to more stringent values thereby forcing a more rigorous calculation. An example of this is the variable ELIMIT. ELIMIT determines at which energy the calculation switches from quantal to classical calculations. Here ELIMIT is increased from 650 to 1000 K. The variable VTEST has been left unchanged at 1.0E-06 and NK=40, as disscused earlier. The first parameter determines the limits of the integration over the perturbed wave function as a function of the intermolecular potential and the second determines the integration step size. Wherever these changes have been made, a comment card is included to clarify the purpose.

3. Originally, the parameters calculated by Program SCAN.FOR were supplied to the calculation via the input file QCOLL.INP. In the present arrangement, Program SCAN.FOR has been incorporated into the main program as Subroutine SCAN. This eliminated the need to alter the input file continually to accommodate frequent changes in the intermolecular potential which in turn affect the region of integration due to the centrifugal potential. This does not apply to the force constants of the potential, SIGMA and EPSILN.

4. Because the program is written in double precision in its entirety, Subroutine POT.FOR is no longer needed and has been removed.

5. Subroutine OVERFL and Function ZERO have been incorporated into the main body of the program.

B. Modifications to Utilize Arc Tangent Calculation

McConville [10] has discussed the two different methods for the calculation of phase shifts. The first is the R_0-R definition, where the phase shift is assumed to be the difference between the zero of the spherical Bessel function, R_0, and the zero of the perturbed wave function, R, at an asymptotic limit where the effect of the perturbing potential is negligible, e.g., VTEST is very small. This is the formula used in the original code for Program QCOLL. The second method is known as the arc tangent formula, where the phase shift is the arc tangent of the ratio of the spherical Bessel function to the Neumann function evaluated at some node of the perturbed wave function. AZIZPH.FOR typically uses the sixth node which is not at the asymptotic limit and requires a small correction.

It was determined that both methods essentially will yield accurate results, although the arc tangent formula does so with less rigorous limits placed on the precision of the calculations. That is, both methods will give the correct answer, but because of numerical convergence problems, it is easier to achieve a desired accuracy with the second method. For a detailed discussion of these calculations see Reference [2].

An additioal advantage gained from using the arc tangent formula lies in its use of the first and second order spherical Bessel functions which are evaluated at a given distance, r_0. These values may be easily and rapidly calculated from recursion formulae, thereby eliminating the need for the large table of

Bessel function zeros used in the original version of QCOLL. Thus, the values of the Bessel functions are calculated as needed, eliminating the restrictions placed on the calculations imposed by having a fixed set of Bessel zeros. The spherical Bessel functions are determined in Subroutine BESLFX.

The determination of the phase shifts via the arc tangent formula is performed in Subroutine ATANPHAS. In this subroutine, Subroutine BESLFX is called to determine the first and second order spherical Bessel functions, and the arc tangent of their ratio is determined. Since the arc tangent can only yield a value between $+\pi/2$ and $-\pi/2$, and a phase shift can have any value, a specific number of multiples of π must be added to the results of the arc tangent calculation. This value is a function of the L value, the argument, and the energy. It is also calculated in Subroutine ATANPHS.

4. Modifications Required for Other Systems

Program QCOLL was written by Taylor [1] specifically for the helium-helium system which was under investigation at the time. The quantal nature of a "particle" is directly dependent on its de Broglie wavelength. When the wavelength of the particle is of the same order of magnitude as the size of the particle, or the region in which the particle is bound, quantal effects make themselves evident as diffraction and dispersion of the wave function. When this occurs, quantal calculation of the phase shifts is required. Otherwise the classical calculation is sufficient, being much easier and faster. The size, or diameter, of a particle is assumed not to change. Helium, the smallest free atom, has the greatest probability of its de Broglie wavelength being the same order of magnitude as its size. On the other hand, however, the de Broglie wavelength is dependent on temperature. The lower the temperature of the free particle, the longer the wavelength. Therefore, quantal effects are more apparent at lower temperatures and the quantal calculation is required.

A. Modifications to Input Data and Mainline

In order to execute the calculation for an atomic or molecular system other than helium, a number of modifications must be made. For the present discussion, Subroutines POTEN and POT are considered to be "input data," as they are normally changed from system to system. The values of SIGMA and EPSILON, which apply to the potential programmed in POTEN and POT, must be set in the input file QCOLL.INP. In this version, the scan parameters are calculated internally and do not need to be entered.

In the mainline, Program QCOLL, the atomic weights in the binary mixture are specified. For any system other than helium-helium, the new atomic weights must be provided. The value of the spin of the system must also be supplied. The spin for any system composed of an unlike pair is zero, as the particles are distinguishable and the system follows Boltzmann statistics. The spin for a like-like system is determined by the number of elementary particles in the atom. If the number is even, then the system obeys Bose-Einstein statistics. If the number of particles is odd, then the system obeys Fermi-Dirac statistics. The program automatically calculates, with the proper statistics provided, the correct value of the program branching parameter, KASE, which is supplied in QCOLL.INP: 0 = Boltzmann, +1 = Bose-Einstein, and -1 = Fermi-Dirac.

B. Modifications to Subroutines

Other parameters that require modification are found in the initialization of Subroutine PHASE. The constants WF0 and WFP0 define the initial approximation of r_0 to the wave function and its first derivative. The value 1.0D+50 for both parameters should be adequate for most systems. The other two parameters that demand attention are RINT and RMAXX, which set the initial conditions for the Runga-Kutta integration of the wave function. RINT and RMAXX tell the program at what distances, r, to search for the first zero of the wave function. First, set RINT and RMAXX at excessively large values; for example, for the neon-argon case, RINT = 0.8*R1 and RMAXX = 50.0*R1. Although the program should run with these values, it will not give correct results. Because RINT was set too large, the program will not find the first zero, but rather a larger one, and will give the wrong answer for the phase shift. However, once the program is executing, the value of RINT must be reduced. The values of the phase shifts will continue to change. This should be continued until the values of the phase shifts remain constant. If RINT is made too small, a message will appear that the interval is too small. Once the proper range has been determined, correct results will be obtained. In order to optimize the calculation, RMAXX should also be reduced until the program no longer runs.

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Appendix A

Revised Computer Program
QCOLL.FOR

```
      PROGRAM QCOLL
CJJH  REVISED SUMMER 89 TO UTILIZE ARC-TANGENT METHOD OF CALCULATING
CJJH  PHASE SHIFTS
CJJH
CJJH  THIS VERSION IS WRITTEN TO RUN ON THE MOUND 'IBM 3090'
CJJH  ON THE 3090 RUN TIME IS APPROX. 15 MIN
CJJH
C     CALCULATION OF COLLISION INTEGRALS BY QUANTUM FORMULAS AT LOW
C     TEMPERATURES AND CLASSICAL FORMULAS AT HIGH TEMPERATURES
C     REVISED FOR PCW/MODCOMP BY W. L. TAYLOR, MOUND LABORATORY, 9-9-85
C
C     THIS PROG. IS SPECIALIZED FOR HELIUM. IT CAN BE CHANGED TO
C     ANOTHER SYSTEM BY CHANGING DEFINITIONS OF WT1, WT2, AND SPIN
C     IN STMNTS, 145 THRU 160 BELOW (NOTE THAT KASE DEFINES BOTH THE
C     SYSTEM AND STATISTICS). IT MAY ALSO BE NECESSARY TO CHANGE
C     DEFINITION OF ELIMIT BELOW AND THE DEF. OF PARAMETERS USED IN
C     PHASE SHIFT CALC., WHICH ARE GIVEN AT BEGINNING OF SUBROUTINE
C     PHASE, ESPECIALLY THE INTIAL CONDITIONS.
C     THE INTERMOLECULAR POTENTIAL IS INPUT TO THIS PROGRAM IN THE
C     FORM OF THREE FORTRAN SUBPROGRAMS
C     FUNCTION PHI(R)  CALC. POTENTIAL AT DISTANCE R
C     SUBROUTINE POTEN(R,V,DV,DDV)  CALC. POTENTIAL-V, ITS FIRST DERIV-
C                                                 ATIV
C                                                 DDV
C     SUBROUTINE POT(R,V)  CALC. POTENTIAL-V AT DISTANCE R. R AND V
C                        MUST BE DOUBLE PRECISION, BUT CALC. OF V
C                        SHOULD BE DONE IN SINGLE PRECISION.
C     ANY SET OF UNITS MAY BE USED, OF COURSE SAME SET MUST BE USED IN
C     ALL THREE SUBPROGRAMS. THIS PROGRAM IS INFORMED OF UNITS USED
C     BY THE INPUT PARAMETERS EPSILN AND SIGMA, SEE DEF. OF INPUT DATA
C     BELOW. DISTANCE UNITS SHOULD BE SUCH THAT SIGMA IS OF ORDER ONE
C     E.G. DO NOT USE CENTIMETERS
CJJH  THE ENTIRE PROGRAM HAS BEEN SWITCHED TO DOUBLE PRECISION(REAL*8)
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION Q(4),QS(200,4),QL(200,4),E(200),EL(200),PE(8),PQ(8,4),
     1        A(8),B(8),ETA(300),ETAO(15),OMEGA(16),T(200),
     2        OMEGAS(200,16),TITLE(20)
      DIMENSION QSCAT(200)
      COMMON U(50),W(50),UL(50),WL(50)
      CALL ERRTRA
CJJH  ERRTRA IS AN ERROR HANDLING SUBROUTINE FROM THE BUILT IN LIB.
C     UNIT ASSIGNMENTS:
C     LUQUAD.INP - CONTAINS GAUSS QUAD. TABLES,
C     LUBES.INP - CONTAINS BESSEL ZEROES (READ IN FROM PHASE),
C     LUPH.OUT - PHASE SHIFTS WRITTEN HERE,
C     LUCS.OUT - CROSS SECTIONS WRITTEN HERE,
C     LUCI.OUT - COLL.INTEGRALS WRITTEN HERE
C     ELIMIT IS ENERGY (IN DEG.) AT WHICH CROSS SEC. CALC. SWITCH TO
C     CLASSICAL CALCULATION.
C
CJJH  UNIT 6 IS WHERE THE 'PRINT OUT' WILL GO, ALL PHASE SHIFTS,
CJJH  CROSS SECTIONS, COLLISION INTEGRALS, AND OTHER MESSAGES ARE SENT
CJJH  HERE.
      NW=6
      ELIMIT=1000.
CJJH  ELIMIT HAS BEEN CHANGED FROM 600 TO 1000, IT IS THE MAX ENERGY FOR
CJJH  WHICH PHASE SHIFTS ARE CALCULATED.
      HBAR=1.05443D-27
      AVO=6.0247D+23
      BOLTZ=1.38049D-16
C     OPEN DISK FILES
C     10 IS ASSIGNED TO FILE 'LUQUAD.INP' ON PC DISK
      NR = 10
C     READ QUADRATURE TABLES, FIRST TABLE IS GAUSS TABLE(RECOMMEND 40
C     POINTS), SECOND TABLE IS GAUSS-LAGUERRE TABLE(REC. 28 POINTS)
      READ(NR,910) NGS
      N=NGS/2
  910 FORMAT(10X,I2)
      READ(NR,911) (U(I),W(I),I=1,N)
  911 FORMAT(2E20.6)
      READ(NR,910) NGSL
      READ(NR,911) (UL(I),WL(I),I=1,NGSL)
C
C     READ INPUT DATA, THE DEFINITIONS OF INPUT DATA ARE:
C     R1-ZERO OF POTENTIAL,
C     R3-INFLECTION POINT IN ATTRACTIVE REGION,
C     RC-DISTANCE OF CLOSEST APPROACH CORRESPONDING TO EC,
C     EC-MAXIMUM ORBITING ENERGY,
C     EINF-ENERGY ABOVE WHICH POTENTIAL IS UNDEFINED
C     (E.G. FOR L-J EINF IS INFINITE, FOR EXP.-6 IT IS FINITE)
C     THESE QUANTITIES ARE CALC. BY PROG. SCAN. THEY MUST BE EXPRESSED
C     IN UNITS OF EPSILN AND SIGMA, WHERE
C     EPSILN-ENERGY UNITS USED IN POTENTIAL SUBPROGRAMS, IN DEGREES K.
C     I.E., IF ENERGIES ARE EXPRESSED IN UNITS OF THE DEPTH OF THE WELL,
C     SAY 1.411E-16 ERGS, THEN EPSILN=10.22
C     IF ENERGIES ARE EXPRESSED IN ERGS, EPSILN=1/1.38E-16
C     SIGMA-UNIT OF LENGTH USED IN POTENTIAL SUBPROGRAMS, IN ANGSTROMS.
C     ALSO USED TO REDUCE CROSS SECTIONS AND COLLISION INTEGRALS.
C     KASE-SPECIFIES SYSTEM. -1 FOR HE3-HE3, 0 FOR HE3-HE4, +1 FOR
C
C     T(I,I=1,NT)-TEMPERATURES(IN DEG.K) AT WHICH COLL. INTEGRALS ARE
C     CALCULATED. NT IS NO. OF TEMPERATURES.
C     NOTE THAT FIRST ITEM READ IS A TITLE CARD.
C
C     11 IS ASSIGNED TO 'QCOLL.INP' ON PC DISK
      NR = 11
      READ(NR,901) TITLE
C     READ(NR,*) R1,R3,RC,EC,EINF
CJJH  THE SCAN PARAMETERS ARE CALCULATED RATHER THAN READ IN.
CJJH  THIS JUST MAKES IT EASIER TO RUN DIFFERENT POTENTIALS
CJJH  WHEN POSSIBLE THE FORMAT FOR READ STATMENTS IS UNSPECIFIED
CJJH  FOR CONVENIENCE
      CALL SCAN(R1,R3,RC,EC,EINF)
      READ(NR,*) EPSILN,SIGMA,KASE,NT
      READ(NR,*) (T(I),I=1,NT)
  901 FORMAT(20A4)
  902 FORMAT(5E10.4)
  903 FORMAT(2E10.4,2I5)
      CALL POTEN(R3,V,DV,DDV)
      V=EPSILN*V
      DV=EPSILN*PHI(R3)
      DM1=R3
CJJH  SINCE THE ENTIRE PROGRAM IS IN REAL*8 THERE IS NO NEED FOR THE
CJJH  SUBROUTINE POT.  IT'S ELIMINATION MAKES RUNNING DIFFERENT POTEN-
TIALS
CJJH  EASIER.
      DM2=PHI(DM1)
      DDV=EPSILN*DM2
      ER=SIGMA*R3
      WRITE(NW,913) TITLE,ELIMIT,SIGMA
      WRITE(NW,908) EPSILN
      WRITE(NW,914) ER,V,DV,DDV
      WRITE(NW,909)
      WRITE(NW,915)
      READ(NR,*)WT1,WT2,SPIN
C     INITIALIZE FOR SYSTEM SPECIFIED BY KASE
C     IF(KASE) 145,150,155
C     INDISTINGUISHABLE PARTICLES, FERMI-DIRAC STATISTICS
C 145 WT1=3.01603D0
C     WT2=3.01603D0
C     SPIN=0.5D0
C     WRITE(NW,916)
C     GO TO 160
C     DISTINGUISHABLE PARTICLES, BOLTZMANN STATISTICS
C 150 WT1=3.01603D0
C     WT2=4.00260D0
C     SPIN=0.0D0
C     WRITE(NW,917)
C     GO TO 160
C     INDISTINGUISHABLE PARTICLES, BOSE-EINSTEIN STATISTICS
C 155 WT1=4.00260D0
C     WT2=4.00260D0
C     SPIN=0.0D0
C     WRITE(NW,918)
C 160 CONTINUE
C     WRITE(NW,919) WT1,WT2,SPIN
C     INITIALIZE SUBROUTINE PHASE
      RWT=(WT1*WT2)/(AVO*(WT1+WT2))
      B11=(2.0D0*RWT*EPSILN*SIGMA*SIGMA)/HBAR
      B12=BOLTZ/HBAR
      B1=B11*B12*1.D-16
      ETA(1)=B1
      ETA(2)=R1
      ETA(3)=EC
      ETA(4)=RC
      ETA(5)=SIGMA
      CALL PHASE(ER,ETA,NR,-1,ERR)
C     SET UP ENERGY GRID
```

```
C     THIS ENERGY GRID IS BASED ON THE BEHAVIOR OF THE CROSS SECTIONS
C     FOR HELIUM
CJJH  THIS GRID IS ACCEPTABLE FOR CALCULATING VIRIALS WITH THE GAUSS-
CJJH  LAGUERRE INTEGRATION METHOD; FOR SIMPSON'S RULE THE STEP SIZE IS
CJJH  TOO LARGE
      EMAX=1.10D0*T(NT)*UL(NGSL)
      EMIN=T(1)*UL(1)/1.10D0
      KE=1
      E(1)=.010D0
      DE=.070D0
      NO=17
      NSTOP=1
  220 NSTART=NSTOP+1
      NSTOP=NSTOP+NO
      DO 225 I=NSTART,NSTOP
      E(I)=E(I-1)+DE
  225 CONTINUE
      GO TO (235,240,245,250,260),KE
  235 KE=2
      DE=.140D0
      NO=77
      GO TO 220
  240 KE=3
      E(NSTOP)=12.0D0
      DE=2.0D0
      NO=19
      GO TO 220
  245 KE=4
      DE=10.0D0
      NO=15
      GO TO 220
  250 KE=5
      DE=50.0D0
      NO=16
      GO TO 220
  260 NSTART=NSTOP+1
      DO 270 I=NSTART,200
      E(I)=1.40D0*E(I-1.0D0)
      IF(E(I)-EMAX) 270,270,275
  270 CONTINUE
      WRITE(NW,920)
      STOP
  275 NE=I
C     END SET UP OF ENERGY GRID
C     START CALC. OF CROSS SECTIONS
C     CALC. PHASE SHIFTS AND QUANTUM CROSS SECTIONS FIRST
C     QCONST IS USED FOR SUBROUTINE QCROSS
      QCONST=4.0D0*EPSILN/B1
      DO 302 I=1,300
  302 ETA(I)=0.0D0
      DO 303 I=1,200
  303 QSCAT(I)=0.0D0
      WRITE(NW,929) TITLE
```

```
C     20 IS ASSIGNED TO 'LUPH.OUT ON PC DISK
      NP = 20
      WRITE(NP,901) TITLE
      LAST=1
      DO 400 I=1,NE
      IF(E(I+1)-ELIMIT) 310,305,305
  305 LAST=-1
  310 ER=E(I)/EPSILN
      LSW=0
      CALL PHASE(ER,ETA,N,LSW,ERR)
C     OUTPUT PHASE SHIFTS
      WRITE(NW,930) E(I)
      WRITE(NP,931) E(I),N,LAST
      DO 330 J=1,N,5
      L=J-1
      WRITE(NW,932) L,ETA(J),ETA(J+1),ETA(J+2),ETA(J+3),ETA(J+4)
  330 CONTINUE
      IF(LSW) 340,342,338
  338 CONTINUE
      WRITE(NW,939) LSW
      GO TO 342
  340 CONTINUE
      LSW=-LSW
      WRITE(NW,939) LSW
      WRITE(NW,940) ERR
  342 CONTINUE
      WRITE(NP,933) (ETA(J),J=1,N)
C     END OUTPUT OF PHASE SHIFTS
      WL2=QCONST/E(I)
      CALL QCROSS(WL2,SPIN,KASE,ETA,N,Q,QSCAT(I))
      DO 350 L=1,4
      QS(I,L)=Q(L)
  350 CONTINUE
      IF(I-15) 385,385,390
C     STORE ZERO ORDER PHASE SHIFTS FOR 15 LOWEST ENERGIES
  385 ETAO(I)=ETA(1)
  390 CONTINUE
      IF(LAST) 410,400,400
  400 CONTINUE
  410 NQ=I
C     OUTPUT ZERO ORDER PHASE SHIFTS
      WRITE(NW,936) TITLE
      DO 415 I=1,15
      WRITE(NW,937) E(I),ETAO(I)
  415 CONTINUE
C     CALC. REMAINING CROSS SECTIONS BY CLASSICAL FORMULAS
C     CONST IS USED IN SUBROUTINE CROSS
      CONST=-PHI(4.0D0*R3)*((4.0D0*R3)**6)*1.D+04
      EOLD=-1.0D0
      KE=NQ-5
      DO 525 I=KE,NE
      ER=E(I)/EPSILN
      IF(ER-EINF) 430,430,475
  430 CONTINUE
      CALL CROSS(ER,Q,EC,RC,R1,EOLD,CONST,NGS,NGSL)
      IF(I-NQ) 450,450,475
  450 J=I+1-KE
      PE(J)=E(I)
      DO 455 L=1,4
      PQ(J,L)=100.*(QS(I,L)-Q(L))/QS(I,L)
  455 CONTINUE
      GO TO 500
  475 CONTINUE
      DO 485 L=1,4
      QS(I,L)=Q(L)
  485 CONTINUE
  500 EOLD=ER
  525 CONTINUE
C     OUTPUT CROSS SECTIONS
      WRITE(NW,950) TITLE,SIGMA,EPSILN,WT1,WT2
C     OUTPUT COMPARISON BETWEEN QUANTUM AND CLASSICAL SECTIONS
      WRITE(NW,951) E(NQ+1)
      J=NQ+1-KE
      DO 550 I=1,J
      WRITE(NW,952) PE(I),(PQ(I,L),L=1,4)
  550 CONTINUE
C     21 IS ASSIGNED TO 'LUCS.OUT' ON PC DISK
      NP = 21
      WRITE(NP,957) NE,(TITLE(I),I=2,20)
      WRITE(NW,953)
      DO 560 I=1,NE
      WRITE(NW,954) E(I),(QS(I,L),L=1,4),QSCAT(I)
      WRITE(NP,955) E(I),(QS(I,L),L=1,4)
  560 CONTINUE
C     END OUTPUT OF CROSS SECTIONS
C     END CALCULATION OF CROSS SECTIONS
C     BEGIN CALCULATION OF COLLISION INTEGRALS
      DO 585 I=1,NE
      EL(I)=DLOG(E(I))
      DO 585 L=1,4
      QL(I,L)=DLOG(QS(I,L))
  585 CONTINUE
  600 DO 750 I=1,NT
      TS=T(I)
      DO 610 L=1,16
  610 OMEGA(L)=0.0D0
      DO 700 K=1,NGSL
      EK=TS*UL(K)
      EX=EK
C     BEGIN INTERPOLATION
C     FOR E LESS THAN 100 INTERPOLATION OF CROSS SECTIONS IS Q VS. E
      K100=0
      IF(EX-100.0D0) 617,617,615
  615 K100=1
      EX=DLOG(EX)
  617 CONTINUE
```

```
C     NUM IS NUMBER OF AITKEN INTERPOLATION POINTS
      NUM=5
      ISN=NUM/2
      ITN=(NUM-1)/2
      DO 625 JNT=1,NE
      IF(EK-E(JNT))630,625,625
  625 CONTINUE
  630 IS=JNT-ISN
      IT=JNT+ITN
      JNT=NUM
  631 IF(IS)632,632,635
  632 IS=IS+1
      JNT=JNT-1
      GO TO 631
  635 IF(IT-NE) 640,640,637
  637 IT=IT-1
      JNT=JNT-1
      GO TO 635
  640 LNT=JNT
      JNT=JNT-1
      DO 660 L=1,4
      DO 645 J=1,LNT
      KKK=IS+J-1
      IF(K100) 642,642,644
  642 A(J)=QS(KKK,L)
      B(J)=E(KKK)
      GO TO 645
  644 A(J)=QL(KKK,L)
      B(J)=EL(KKK)
  645 CONTINUE
      DO 650 N=1,JNT
      DO 650 J=N,JNT
      A(J+1)=(A(N)*(B(J+1)-EX)-A(J+1)*(B(N)-EX))/(B(J+1)-B(N))
  650 CONTINUE
      Q(L)=A(JNT+1)
      IF(K100) 660,660,655
  655 Q(L)=DEXP(A(JNT+1))
  660 CONTINUE
C     END INTERPOLATION
C     CALCULATION OF THE (1,S) INTEGRALS
  675 JS=2
      DO 680 L=1,7
      OMEGA(L)=OMEGA(L)+WL(K)*(UL(K)**JS)*Q(1)
  680 JS=JS+1
C     CALCULATION OF THE (2,S) INTEGRALS
      JS=3
      DO 685 L=8,12
      OMEGA(L)=OMEGA(L)+WL(K)*(UL(K)**JS)*Q(2)
  685 JS=JS+1
C     CALCULATION OF THE (3,S) INTEGRALS
      JS=4
      DO 690 L=13,15
      OMEGA(L)=OMEGA(L)+WL(K)*(UL(K)**JS)*Q(3)
  690 JS=JS+1
C     CALCULATION OF THE (4,4) INTEGRAL
      OMEGA(16)=OMEGA(16)+WL(K)*(UL(K)**5)*Q(4)
  700 CONTINUE
C     DIVISION OF INTEGRALS BY (S+1) FACTORIAL
      JS=2
      DO 725 J=1,15
      N=1
      DO 715 L=2,JS
  715 N=L*N
      EOLD=N
      OMEGAS(I,J)=OMEGA(J)/EOLD
      IF(J-7)725,718,720
  718 JS=2
      GO TO 725
  720 IF(J-12)725,722,725
  722 JS=3
  725 JS=JS+1
      OMEGAS(I,16)=OMEGA(16)/120.0D0
  750 CONTINUE
C     OUTPUT OF COLLISION INTEQRALS
      WRITE(NW,960) TITLE,SIGMA,EPSILN,WT1,WT2
      WRITE(NW,961) (J,J=1,7)
C     22 IS ASSIGNED TO 'LUCI.OUT' ON PC DISK
      NP = 22
      WRITE(NP,957) NT,(TITLE(I),I=2,20)
      DO 810 I=1,NT
      WRITE(NW,963) T(I),(OMEGAS(I,L),L=1,8)
      WRITE(NP,964) T(I),(OMEGAS(I,L),L=1,8)
  810 CONTINUE
      WRITE(NW,965) (J,J=3,6),(I,I=3,5)
      DO 815 I=1,NT
      WRITE(NW,963) T(I),(OMEGAS(I,L),L=9,16)
      WRITE(NP,964) T(I),(OMEGAS(I,L),L=9,16)
  815 CONTINUE
C     END OUTPUT OF COLLISION INTEGRALS
  908 FORMAT (05X,'ENERGIES IN ANY MESSAGE PRINTED BY SUBPROGRAMS WILL
     2 BE IN UNITS OF',E12.4,' DEGS.',/)
  909 FORMAT (/05X,'PHASE SHIFTS WRITTEN ON B:LUPH.OUT'/
     1         05X,'CROSS SECTIONS WRITTEN ON B:LUCS.OUT'/
     2         05X,'COLLISION INTEGRALS WRITTEN ON B:LUCI.OUT'/)
  913 FORMAT(1H1,25X,'CALCULATION OF REDUCED COLLISION INTEGRALS',
     1/10X,20A4,///05X,'CROSS SECTIONS CALC. BY QUANTUM EQS. FOR
     2 ENERGIES LESS THAN',F8.2,' DEGS.',/05X,'THE CROSS SECTIONS AND CO
     3LLISION INTEGRALS ARE REDUCED AS DEFINED IN',/05X,'HIRSCHFELDER, C
     4URTISS, AND BIRD, CHAPTER 8.',/05X,'THE VALUE OF THE RIGID SPHERE
     5DIAMETER USED IN THESE CALCULATIONS IS',F10.5,' ANGSTROMS',/5X,
     6'ENERGIES OUTPUTTED BY MAIN PROG. ARE IN DEGREES (I.E. ENERGY
     7 DIVIDED BY BOLTZMAN CONST.)')
  914 FORMAT(/05X,'FOLLOWING FOUR NUMBERS SHOULD BE OF ORDER ONE AND LAS
     1T THREE SHOULD BE EQUAL',/5X,'OTHERWISE SOMETHING IS WRONG WITH
     2POTENTIAL SUBPROGRAMS AND/OR INPUT DATA',/4E17.5/)
  915 FORMAT(///25X,'THESE CALCULATIONS ARE FOR')
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916 FORMAT(12X,'INDISTINGUISHABLE PARTICLES, FERMI-DIRAC STATISTICS')
917 FORMAT(14X,'DISTINGUISHABLE PARTICLES, BOLTZMANN STATISTICS')
918 FORMAT(12X,'INDISTINGUISHABLE PARTICLES, BOSE-EINSTEIN STATS')
919 FORMAT(/11X,'MASS(1)=',F9.5,5X,'MASS(2)=',F9.5,5X,'SPIN=',F5.2,/)
920 FORMAT(//1X,44H ENERGY GRID CONTAINS MORE THAN 200 POINTS  ,/,
   130H AND HENCE EXCEEDS DIMENSIONS                     )
929 FORMAT (30X,'PHASE SHIFTS',/15X,20A4,////)
930 FORMAT(1H0,40X,12HPHASE SHIFTS,/34X,7HENERGY=,F8.3,8H DEGREES,//
   110X,1HL)
931 FORMAT(F10.4,2I5)
932 FORMAT(1X,I10,5F10.4)
933 FORMAT(8F10.4)
936 FORMAT(1H1,//10X,35HLOW ENERGY ZERO ORDER PHASE SHIFTS ,/5X,20A4,/
   1/15X,07HE(DEG.),10X,5HETA-0,/)
937 FORMAT(1X,F22.4,F15.4)
939 FORMAT(/1X,54H   PHASE SHIFTS CALC. BY WKB APPROX. BEGINNING WITH
   1L=,I3)
940 FORMAT(1X,30H   SWITCHED TO WKB BY DEFAULT  ,/,
   143H   AVERAGE DIFF. BETWEEN WKB AND RADIAL FOR  ,/,
   232H   4 PRECEEDING PHASE SHIFTS WAS ,F7.4,8H RADIANS)
950 FORMAT(31X,22HREDUCED CROSS SECTIONS,20X,/,10X,20A4,/,/,
   1' SIGMA=',
   1F7.4,13H     EPSILON=,E11.4,'   WT1=',F9.5,'   WT2=',F9.5,/,/)
951 FORMAT(5X,47HTOTAL SCATTERING CROSS SECTION CALC. Q.M. ONLY  ,
   1/,63H   CROSS SECTIONS CALC. WITH CLASSICAL EQS. BEGINNING WITH
   1E=,F8.3,6H DEGS.,/,82H     PER CENT DIFF. BETWEEN QUANTUM AND CLAS
   2SICAL FOR THE  PRECEEDING ENERGIES ARE,//,
   313H     E(DEGS.),9X,4HQ1-%,9X,4HQ2-%,9X,4HQ3-%,9X,4HQ4-%)
952 FORMAT(1X,F13.3,4F13.2)
953 FORMAT(///30X,23HREDUCED CROSS SECTIONS ,//,
   113H     E(DEGS.),12X,2HQ1,12X,2HQ2,12X,2HQ3,12X,2HQ4,9X,5HTOTAL)
954 FORMAT(1X,F13.4,2X,5F14.4)
955 FORMAT(5F15.6)
957 FORMAT(I3,1X,19A4)
960 FORMAT(23X,28HREDUCED COLLISION INTEGRALS ,20X,2A4,/,9X,20A4,/,/
   1,'    SIGMA=',F7.4,13H     EPSILON=,E11.4,8H    WT1=,F9.5,
   28H    WT2=,F9.5,//)
961 FORMAT(1X,9H     T(K),7(4X,2H1,,I1,3X),4X,3H2,2)
963 FORMAT(1X,F9.2,8F10.5)
964 FORMAT(F8.2,8F9.5)
965 FORMAT(/,1X,'    T(K)',4(4X,2H2,,I1,3X),3(4X,2H3,,I1,3X),4X,3H4,4)
    STOP
    END
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      SUBROUTINE CHIGM (CHI,E,B,RM,N)
C     EVALUATION OF ANGLE OF DEFLECTION BY GAUSS-MEHLER QUADRATURE
C     REVISED FOR IBM PC BY W.L. TAYLOR, MOUND LABORATORY, 9-20-84
C     SUBROUTINE USES FUNCTION PHI(R)
      IMPLICIT REAL*8 (A-H,O-Z)
      K=N+1
      PI=DACOS(-1.0D0)
      M=K/2
      XL=4.0D0*N
      SUM=0.0D0
      DO 200 J=1,M
      AJ=(2*J-1)
      AJ=DCOS(AJ*PI/XL)
      AJN=(2*(K-J)-1)
      AJN=DCOS(AJN*PI/XL)
  158 U=1.0-(PHI(RM/AJ)/E)-(B*B*AJ*AJ/(RM*RM))
      IF(U) 1,1,2
    1 CONTINUE
      U=0.0D0
      GO TO 3
    2 U=AJN/DSQRT(U)
    3 SUM=SUM+U
      IF(JC)173,200,173
  173 JC=0
      IF(J-M)176,174,176
  174 IF(K-2*M)176,200,176
  176 U=AJN
      AJN=AJ
      AJ=U
      GO TO 158
  200 JC=1
      U=N
      CHI=PI*(1.0D0-B*SUM/(U*RM))
      RETURN
      END


      SUBROUTINE OVERFL(JJ)
C     REVISED FOR PCW/MOD COMP BY W. L. TAYLOR, MOUND LABORATORY, 9-9-85
      JJ=2
      RETURN
      END
      SUBROUTINE PHASE (E,ETA,N,LSW,ERR)
C     CALCULATE PHASE SHIFTS BY PARTIAL WAVE USING RUNGA-KUTTA METHOD --
C     REVISED FOR PCW/MODCOMP BY W. L. TAYLOR, MOUND LABORATORY, 9-9-85
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION DB(49,100),TETA(300),ETA(300)
      IF(LSW) 110,180,180
  110 NW = 6
      B1=ETA(1)
      R1=ETA(2)
      EC=ETA(3)
      RC=ETA(4)
C     THE INITIAL CONDITIONS ARE SET HERE, THEY HAVE CAUSED SOME
C     TROUBLE. SUBROUTINES PARWAV AND RUNKA TRY TO CHANGE THEM AND
C     RUNKA PRINTS A MESSAGE TO THIS EFFECT.
C     THE INITIAL CONDITIONS USED SUCCESSFULLY THUS FAR ARE:
C     HELIUM:  WFO=WFPO=1.E-30 AND RINT=.4*R1
C     ARGON: WFO=WFPO=1.E-40 AND RINT=2.0(APPROX. .6*R1 FOR L-J )
C     HE/NE AND NEON: SAME AS FOR HELIUM
CJJH
CJJH  IT WAS FOUND THAT FOR NE/AR WF0 AND WFP0 SHOULD BE 1.0DE-50
CJJH  RINT=.8*R1, AND RMAXX=50*R1.
CJJH
      READ(11,*)VTEST,RINT,RMAXX,WF0,WFP0,NK
CJJH  WF0=1.D-30
CJJH  WFP0=1.D-30
      RINT=RINT*R1
      RMAXX=RMAXX*R1
CJJH  NK=40
      L0=1
      L1=299
      SWTCH=.00010D0
CJJH  SWTCH WAS CHANGED FROM .0001 TO .00001 FOR INCREASED ACCURACY
      LSWMAX=30
CJJH  LSWMAX WAS CHANGED FROM 30 TO INCREASE ACCURACY
      ETASWT=.01D0
      LWKB=10
      WRITE(NW,910) RINT,WF0,WFP0,NK
      WRITE(NW,*)'    VTEST= ',VTEST
      WRITE(NW,911) SWTCH,LSWMAX,ETASWT
C     CALCULATE VO, WHICH IS AN ESTIMATE OF THE WELL DEPTH
C     BO IS USED IN CALCULATING INCREMENT FOR RUNKA
      R=1.2D0*R1
      V=PHI(R)
      VO=V
      BO=B1*VO
C     INITIALIZE PARWAV
      CALL PARWAV(-NK,WF0,WFP0,BO,RINT,DB)
      RETURN
  180 CONTINUE
      Q2=B1*E
      Q=DSQRT(Q2)
      DRMAX=0.1D0*RMAXX
CJJH  VTEST=1.D-07*E
CJJH  VTEST WAS CHANGED FROM 1.0D-06 TO INCREASE ACCURACY
      R=RMAXX
  250 V=PHI(R)
      IF(VTEST-DABS(V))255,260,260
  255 R=R+DRMAX
      GO TO 250
  260 RMAX=R
      R=RINT
C     END OF INITIALIZATION. START DO LOOP TO CALCULATE PHASE SHIFTS.
      DO 301 I=1,300
  301 TETA(I)=0.0D0
      LSW=0
      LKC=5
      DO 400 L=L0,L1
      IF(L-4) 370,310,310
  310 IF(DABS(ETA(L-1))-.1D0) 312,312,365
  312 IF(DABS(ETA(L-2))-.1D0) 314,314,365
  314 IF(DABS(ETA(L-3))-.1D0) 320,320,365
C     DETERMINE WHETHER CALC. IS FINISHED
  320 IF(DABS(ETA(L-1))-.001D0) 322,322,330
  322 IF(DABS(ETA(L-2))-.001D0) 324,324,330
  324 IF(DABS(ETA(L-3))-.001D0)   58,58,330
  330 IF(L-LWKB) 370,336,336
  336 IF(E-EC) 370,370,335
C     DETERMINE WHETHER CALC. CAN SWITCH TO WKB
  335 LS=L-LKC
      LE=L-2
      CALL WKB(E,R1,EC,RC,Q2,LS,LE,TETA)
C     IF(LS) 370,370,340
C 340 CONTINUE
      LKC=2
      LE=LE+1
      LS=LE-3
      SUM=0.0D0
      DO 345 I=LS,LE
      SUM=SUM+DABS(ETA(I)-TETA(I))
  345 CONTINUE
      SUM=SUM/4.D0
      IF(SUM-SWTCH) 350,350,346
C     SWITCH TO WKB BY DEFAULT, INDICATED BY NEGATIVE LSW
  346 CONTINUE
      IF(L-LSWMAX) 370,370,347
  347 CONTINUE
      IF(DABS(ETA(L-1))-ETASWT) 348,348,370
  348 LS=L-1
      LSW=-LS
      ERR=SUM
      GO TO 355
C     SWITCH TO WKB APPROXIMATION
  350 LSW=L-1
      LS=LSW
  355 CONTINUE
      CALL WKB(E,R1,EC,RC,Q2,LS,L1,ETA)
      LTOTAL=LS+1
      GO TO 68
  365 LKC=5
  370 CONTINUE
      CALL PARWAV(L-1,ETAL,Q2,B1,RMAX,DB)
      ETA(L)=ETAL
  400 CONTINUE
      L=L1+1
   58 LTOTAL=L-1
   68 N=LTOTAL
      GO TO 377
  902 FORMAT(3X,7F9.4)
  910 FORMAT(1H1,30X,'CALCULATION OF PHASE SHIFTS',///05X,'SCHROEDINGER
     1EQ. INTEGRATED NUMERICALLY BY RUNGA-KUTTA METHOD',/05X,'INITIAL
     2VALUES USED ARE',/05X,'AT R=',E11.3,05X,'U=',E11.3,05X,'AND DU/DR=
     3',E11.3,/05X,'IF POTENTIAL HAS A SPURIOUS MAX. BE SURE R IS NOT TO
     4O SMALL',/05X,'INTERVAL USED IN RUNGA-KUTTA IS FUNCTION OF ENERGY
     5AND IS',/05X,'DESIGNED TO GIVE',I4,' OR MORE INTEGRATION PTS. PER
     6WAVELENGTH',/)
  911 FORMAT(//05X,'CALC. OF PHASE SHIFTS SWITCHES TO WKB APPROXIMATION
     1WHEN L IS GREATER THAN 8',/05X,'AND AVERAGE DIFFERENCE BETWEEN
     2WKB AND SCHRODINGER EQ. FOR FOUR PHASE SHIFTS',/05X,'IS LESS THAN'
     3,F7.4,' RADIANS',/05X,'IF L IS GREATER THAN',I4,' AND PHASE SHIFT
     4IS LESS THAN',F7.4,' RADIANS',/05X,'PROG. SWITCHES TO WKB BY DEFAU
     5LT',/)
  377 RETURN
      END
      SUBROUTINE QCROSS(WL2,SPIN,KASE,ETA,J,Q,SCAT)
C     CALCULATE QUANTUM MECHANICAL CROSS SECTIONS FROM PHASE SHIFTS --
C     REVISED FOR PCW/MODCOMP BY W. L. TAYLOR, MOUND LABORATORY, 9-9-85
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION ETA(300),Q(4)
      DIMENSION STE(1),STO(1),ST(1),STF(1),STB(1),S1E(1),S1O(1),
     1        S1(1),S1F(1),S1B(1),S2E(1),S2O(1),S2(1),S2F(1),
     2        S2B(1),S3E(1),S3O(1),S3(1),S3F(1),S3B(1),S4E(1),
     3        S4O(1),S4(1),S4F(1),S4B(1)
      SPIN1=(SPIN+1.0D0)/(2.0D0*SPIN+1.0D0)
      SPIN2=SPIN/(2.0D0*SPIN+1.0D0)
      I=1
C     KASE DETERMINES STATISTICS; 0 = BOLTZMANN, -1 = F.D., +1 = B.E.
      ETA(J+1)=0.0D0
      ETA(J+2)=0.0D0
      ETA(J+3)=0.0D0
      ETA(J+4)=0.0D0
C     BEGIN CALCULATION OF CROSS SECTIONS
      STE(I)=0.0D0
      DO 2 N=1,J,2
      EL=N-1
    2 STE(I)=STE(I)+(2.0D0*EL+1.0D0)*DSIN(ETA(N))**2
      STO(I)=0.0D0
      DO 3 N=2,J,2
      EL=N-1
    3 STO(I)=STO(I)+(2.0D0*EL+1.0D0)*DSIN(ETA(N))**2
      ST(I)=WL2*(STE(I)+STO(I))
      STF(I)=2.0D0*WL2*(SPIN1*STO(I)+SPIN2*STE(I))
      STB(I)=2.0D0*WL2*(SPIN1*STE(I)+SPIN2*STO(I))
      S1E(I)=0.0D0
      DO 4 N=1,J,2
      EL=N-1
    4 S1E(I)=S1E(I)+(EL+1.0D0)*DSIN(ETA(N+1)-ETA(N))**2
      S1O(I)=0.0D0
      DO 5 N=2,J,2
      EL=N-1
    5 S1O(I)=S1O(I)+(EL+1.0D0)*DSIN(ETA(N+1)-ETA(N))**2
      S1(I)=WL2*(S1E(I)+S1O(I))
      S1F(I)=2.0D0*WL2*(SPIN1*S1O(I)+SPIN2*S1E(I))
      S1B(I)=2.0D0*WL2*(SPIN1*S1E(I)+SPIN2*S1O(I))
      S2E(I)=0.0D0
      DO 6 N=1,J,2
      EL=N-1
    6 S2E(I)=S2E(I)+(((EL+1.0D0)*(EL+2.0D0))/(2.*EL+3.0D0))
     1*DSIN(ETA(N+2)-ETA(N))**2
      S2O(I)=0.0D0
      DO 7 N=2,J,2
      EL=N-1
    7 S2O(I)=S2O(I)+(((EL+1.0D0)*(EL+2.0D0))/(2.0D0*EL+3.0D0))
     1*DSIN(ETA(N+2)-ETA(N))**2
      S2(I)=WL2*(S2E(I)+S2O(I))
      S2F(I)=2.*WL2*(SPIN1*S2O(I)+SPIN2*S2E(I))
      S2B(I)=2.*WL2*(SPIN1*S2E(I)+SPIN2*S2O(I))
      S3E(I)=0.0D0
      DO 8 N=1,J,2
      EL=N-1
      A=((EL+1.0D0)*(EL+2.0D0)*(EL+3.0D0))/
     1((2.0D0*EL+3.0D0)*(2.0D0*EL+5.0D0))
      B=(3.0D0*(EL+1.0D0)*(EL**2+2.0D0*EL-1.0D0))/
     1((2.0D0*EL-1.0D0)*(2.0D0*EL+5.0D0))
    8 S3E(I)=S3E(I)+A*DSIN(ETA(N+3)-ETA(N))**2+B*DSIN(ETA(N+1)-ETA(N))
     1**2
      S3O(I)=0.0D0
      DO 9 N=2,J,2
      EL=N-1
      A=((EL+1.0D0)*(EL+2.0D0)*(EL+3.0D0))/
     1((2.0D0*EL+3.0D0)*(2.0D0*EL+5.0D0))
      B=(3.0D0*(EL+1.0D0)*(EL**2+2.0D0*EL-1.0D0))
     1/((2.0D0*EL-1.0D0)*(2.0D0*EL+5.0D0))
    9 S3O(I)=S3O(I)+A*DSIN(ETA(N+3)-ETA(N))**2+B*DSIN(ETA(N+1)-ETA(N))
     1**2
      S3(I)=WL2*(S3E(I)+S3O(I))
      S3F(I)=2.0D0*WL2*(SPIN1*S3O(I)+SPIN2*S3E(I))
      S3B(I)=2.0D0*WL2*(SPIN1*S3E(I)+SPIN2*S3O(I))
      S4E(I)=0.0D0
      DO 10 N=1,J,2
      EL=N-1
      C=(EL+1.0D0)*(EL+2.0D0)/((2.0D0*EL+3.0D0)*(2.0D0*EL+7.0D0))
      D=(EL+3.0D0)*(EL+4.0D0)/(2.0D0*EL+5.0D0)
      E=(4.0D0*EL*EL+12.0D0*EL-6.0D0)/(2.0D0*EL-1.0D0)
   10 S4E(I)=S4E(I)+C*(D*DSIN(ETA(N+4)-ETA(N))**2+E*DSIN(ETA(N+2)-ETA(N)
     1)**2)
      S4O(I)=0.0D0
      DO 11 N=2,J,2
      EL=N-1
      C=(EL+1.0D0)*(EL+2.0D0)/((2.0D0*EL+3.0D0)*(2.0D0*EL+7.0D0))
      D=(EL+3.0D0)*(EL+4.0D0)/(2.0D0*EL+5.0D0)
      E=(4.0D0*EL*EL+12.0D0*EL-6.0D0)/(2.0D0*EL-1.0D0)
   11 S4O(I)=S4O(I)+C*(D*DSIN(ETA(N+4)-ETA(N))**2+E*DSIN(ETA(N+2)-ETA(N)
     1)**2)
      S4(I)=WL2*(S4E(I)+S4O(I))
      S4F(I)=2.0D0*WL2*(SPIN1*S4O(I)+SPIN2*S4E(I))
      S4B(I)=2.0D0*WL2*(SPIN1*S4E(I)+SPIN2*S4O(I))
   33 IF(KASE)51,50,52
   50 CONTINUE
C     KASE=0, HE3-HE4
C     BOLTZMANN STATISTICS
      Q(1)=S1(1)
      Q(2)=1.50D0*S2(1)
      Q(3)=S3(1)
      Q(4)=1.250D0*S4(1)
      SCAT=ST(1)
      RETURN
   51 CONTINUE
C     KASE=-1, HE3-HE3
C     FERMI-DIRAC STATISTICS
```

```
      Q(1)=S1F(1)
      Q(2)=1.50D0*S2F(1)
      Q(3)=S3F(1)
      Q(4)=1.250D0*S4F(1)
      SCAT=STF(1)
      RETURN
   52 CONTINUE
C     KASE=1, HE4-HE4
C     BOSE-EINSTEIN STATISTICS
      Q(1)=S1B(1)
      Q(2)=1.50D0*S2B(1)
      Q(3)=S3B(1)
      Q(4)=1.250D0*S4B(1)
      SCAT=STB(1)
      RETURN
      END
      SUBROUTINE WKB(ER,R1,EC,RC,AK2,LS,LE,ETA)
C     REVISED FOR PCW/MODCOMP BY W. L. TAYLOR, MOUND LABORATORY, 9-9-85
C     CALCULATION OF PHASE SHIFTS BY WKB APPROXIMATION
C     SEE F.J. SMITH, PHYSICA, VOL.30, PG.497, EQ.3.7
C     METHOD USED IN THIS ROUTINE ASSUMES EFFECTIVE POTENTIAL IS
C     IF EFFECTIVE POTENTIAL IS NEGATIVE, ROUTINE RETURNS WITH LS=-1
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION ETA(1)
      EFFV(X)=V+B2*E/(X*X)
      NW=6
      N=16
      PI=DACOS(-1.0D0)
      E=ER
      AK=DSQRT(AK2)
      CALL ORBIT(E,RE,ROP,RO,EC,RC,R1,-1.0D0)
      IF(E-EC) 180,180,190
  180 RE=RO
  190 CONTINUE
      B=LS
      B=(B+.50D0)/AK
      B2=B*B
      DR=RE/10.0D0
      R=RE
      DO 200 I=1,40
      R=RE+DR
      CALL POTEN(R,V,DV,DDV)
      X=R
      IF(E-EFFV(X)) 210,210,200
  200 CONTINUE
  210 RM=R-DR
      LAST=0
      DO 500 L=LS,LE
      B=L
      B=(B+.5D0)/AK
      B2=B*B
C     CALCULATE RM
      J1=0
      R=RM
  250 CALL POTEN(R,V,DV,DDV)
      DF=-DV+2.0D0*B2*E/(R*R*R)
      X=R
      DR=-(E-EFFV(X))/DF
      IF(DABS(DR/R)-1.D-06) 275,275,260
  260 R=R+DR
      J1=J1+1
      IF(J1-30) 250,265,265
  265 CONTINUE
      WRITE(NW,905) E,R,DR,L
  905 FORMAT(/1X,11H POOR CONV.,3E16.5,I5)
  275 RM=R+DR
      K=N+1
      M=K/2
      XL=4*N
      JC=1
      SUM=0.0D0
      DO 400 J=1,M
      AJ=(2*J-1)
      AJ=DCOS(AJ*PI/XL)
      AJN=2*(K-J)-1
      AJN=DCOS(AJN*PI/XL)
  358 R=RM/AJ
      CALL POTEN(R,V,DV,DDV)
      X=R
      Q=EFFV(X)
      IF(Q) 362,362,364
  362 CONTINUE
      LS=-1
      WRITE(NW,915) L,E,R
      RETURN
  364 Q=B/DSQRT(Q/E)
      F=DSQRT((E-EFFV(X))/E)
      X=R*R
      U=X*(Q-R)/F
      U=(2.0D0*B2/(X*R)-DV/E)*U
      SUM=SUM+U*AJN
      IF(JC) 373,400,373
  373 JC=0
      IF(J-M) 376,374,376
  374 IF(K-2*M) 376,400,376
  376 U=AJN
      AJN=AJ
      AJ=U
      GO TO 358
  400 JC=1
      ETA(L+1)=AK*PI*SUM/(XL*RM)
      IF(DABS(ETA(L+1))-1.0D-06) 420,420,430
CJJH  VALUE CHANGED FROM 0.0001 TO 1.0D-06
  420 LAST=LAST+1
      IF(LAST-3) 500,520,520
  430 LAST=0
  500 CONTINUE
      L=LE
  520 CONTINUE
      LS=L
  915 FORMAT(/1X,39H EFFECTIVE POTENTIAL IS NEGATIVE FOR L=,I3,
     14H  E=,E12.4,4H  R=,E12.4,/,24H THIS ROUTINE IS INVALID,
     242H IN THIS CASE AND IS RETURNING WITH LS=-1 )
      RETURN
      END
      SUBROUTINE CROSS(E,Q,EC,RC,R1,EOLD,AL,N1,N2)
C     EVALUATION OF CLASSICAL CROSS SECTIONS FOR COLLISION INTEGRALS
C     REVISED FOR PCW/MODCOMP BY W. L. TAYLOR, MOUND LABORATORY, 9-9-85
C     USES SUBPROGRAMS ORBIT, CHIGM, POTEN, PHI
C     ALSO USES GAUSSIAN ABSCISSAS AND WEIGHTS WHICH MUST BE IN COMMON
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION Q(4),M(3,4)
      COMMON U(50),W(50),UL(50),WL(50)
      BF(R)=R*DSQRT((E-V)/E)
      BDBF(R)=R*(2.0D0*(E-V)-R*DV)
      NW=6
      DO 66 I=1,4
   66 M(1,I)=10
      M(3,4)=100
      M(2,1)=20
      M(3,1)=25
      M(2,2)=25
      M(3,2)=35
      M(2,3)=40
      M(3,3)=45
      M(2,4)=70
      DO 150 L=1,4
  150 Q(L)=0.0D0
      K=1
      IF(E-1.25D0*EC)160,200,200
  160 K=2
      IF(E-.1D0*EC)165,200,200
  165 K=3
  200 CALL ORBIT(E,RE,ROP,RO,EC,RC,R1,EOLD)
      IF(E-2.0D0*EC)210,210,375
C     EVALUATE INTEGRAL FROM RE TO ROP (OR RC IF E G.T. EC) BY
C     GAUSSIAN QUADRATURE
  210 A=ROP-RE
      RL=RO
      N=N1/2
      DO 303 J=1,2
      DO 300 I=1,N
      U(I)=-U(I)
      X=0.5D0*(U(I)+1.0D0)
      L=1
      GO TO (225,215),J
  215 L=2
      IF(X-.9D0)225,225,218
  218 L=3
      IF(X-.95D0)225,225,220
  220 L=4
  225 M1=M(K,L)
  227 R=A*X+RE
      CALL POTEN(R,V,DV,DDV)
      B=BF(R)
      CALL CHIGM(CHI,E,B,R,M1)
      Y=DCOS(CHI)
      Z=Y
      BDB=BDBF(R)
      DO 275 L=1,4
      Q(L)=Q(L)+0.5D0*W(I)*BDB*(1.0D0-Y)
  275 Y=Y*Z
  300 CONTINUE
  303 CONTINUE
      DO 305 L=1,4
  305 Q(L)=A*Q(L)
      GO TO 400
  375 RL=RE
C     EVALUATE INTEGRAL FROM RO (RC IF E G.T. EC, RE IF E G.T. 2*EC)
C     TO INFINITY BY GAUSS-LAGUERRE QUADRATURE
  400 SCALE=(((AL/E)**.16667D0)-RL)/UL(N2)
      IF(SCALE) 403,403,404
  403 WRITE(NW,900) E
      STOP
  404 K=1
      M2=10
      IF(E-1.25D0*EC)405,405,410
  405 K=2
      M2=40
  410 DO 500 I=1,N2
      X=UL(I)
      R=X*SCALE+RL
      CALL POTEN(R,V,DV,DDV)
      B=BF(R)
      CALL CHIGM(CHI,E,B,R,M2)
      Y=DCOS(CHI)
      Z=Y
      BDB=SCALE*BDBF(R)*DEXP(X)
      DO 475 L=1,4
      Q(L)=Q(L)+WL(I)*BDB*(1.0D0-Y)
  475 Y=Y*Z
      GO TO (500,480),K
  480 IF(CHI+3.142D0)500,500,482
  482 M2=15
      IF(CHI+1.571D0)500,500,484
  484 M2=10
  500 CONTINUE
      DO 560 L=1,4
      X=L
      X=1.0D0-0.5D0*((1.0D0+(-1.0D0)**L)/(1.0D0+X))
  560 Q(L)=Q(L)/(X*E)
  900 FORMAT(//52H THE APPROXIMATION USED TO EVALUATE THE SCALE FACTOR
     1      ,/,49H IN THE GAUSS-LAGUERRE QUADRATURE FORMULA FOR THE,/,
     2        42H CROSS SECTIONS IS INVALID FOR THE ENERGY=,E13.4)
  580 RETURN
      END
      SUBROUTINE ORBIT(E,RE,ROP,RO,EC,RC,R1,EOLD)
C     CALCULATION OF BOUNDARY CURVE PARAMETERS
C     REVISED FOR PCW/MODCOMP BY W.L. TAYLOR, MOUND LABORATORY, 9-9-85
C     USES SUBROUTINE POTEN
      IMPLICIT REAL*8 (A-H,O-Z)
      NW=6
      ER1=1.0D-06
      ER2=1.0D-06
      ER3=1.0D-06
      J1=0
      J2=0
      J3=0
C     BEGIN CALCULATION OF RE
      BIAS=1.0D0*ER1
  102 R=R1
      DR=R1/100.D0
      IF(EOLD)108,108,104
  104 R=RE
      DR=RE/100.0D0
      IF(E-EOLD)115,115,108
  108 DO 111 J4=1,100
      R=R-DR
      CALL POTEN(R,V,DV,DDV)
      IF(E-V)112,112,109
  109 IF(DDV)115,115,111
  111 CONTINUE
  112 IF(DDV)113,113,115
  113 R=R+.5D0*DR
  115 RE=R
  117 CALL POTEN(RE,V,DV,DDV)
  118 CORR=(E-V)/DV
      J1=J1+1
  120 X=RE+CORR
      CALL POTEN(X,V,DV,DDV)
      IF(DV)123,121,121
  121 CORR=.5D0*CORR
      IF(EOLD)120,120,122
  122 EOLD=-1.0D0
      GO TO 102
  123 IF(DABS (CORR/RE)-ER1)128,128,124
  124 RE=X
      IF(J1-30)118,125,125
  125 IF(DABS (CORR/RE)-100.0D0*ER1)126,126,500
  126 WRITE(NW,901) E
      RE=X-CORR
      BIAS=10.0D0*ER1
  128 RE=RE+CORR
      IF(E-.5D0*EC) 129,135,135
C     BIAS RE TO INSURE THAT E IS GREATER THAN PHI(RE)
  129 RE=RE+BIAS*RE
      CALL POTEN(RE,V,DV,DDV)
      IF(E-V) 129,135,135
  135 CONTINUE
```

```
      IF(RE)500,500,136
  136 IF(RE-(R1+.0001D0*R1))137,500,500
C     END CALCULATION OF RE
  137 IF(E-EC)138,450,450
C     CALCULATE ORBITING PARAMETERS
C     BEGIN CALCULATION OF RO
  138 IF(EOLD)140,140,200
C     INITIAL APPROXIMATION FOR RO
  140 K=0
      U=1.0D0
      X=RC
      DX=RC
  148 X=X+DX
      CALL POTEN(X,V,DV,DDV)
      Y=2.0D0*(E-V)-X*DV
      IF(U*Y) 148,180,153
  153 K=K+1
      U=-U
      DX=-.50D0*DX
      IF(K-10) 148,180,180
  180 RO=X
      U=DX
  200 R=RO
C     END INITIAL APPROXIMATION FOR RO
  205 CALL POTEN(R,V,DV,DDV)
      Y=2.0D0*(E-V)-R*DV
      DY=-3.0D0*DV-R*DDV
      CORR=-Y/DY
      R=R+CORR
      J2=J2+1
      IF(R-RC)230,230,215
  215 IF(DABS(CORR/R)-ER2) 250,250,220
  220 IF(J2-30)205,222,222
  222 IF(DABS(CORR/R)-100.0D0*ER2) 224,224,501
  224 WRITE(NW,902) E
      GO TO 250
C     MODIFY INITIAL APPROXIMATION
  230 IF(EOLD)240,240,235
  235 EOLD=-1.0D0
      GO TO 140
  240 RO=RO+U
      J2=J2-1
      GO TO 200
  250 RO=R
C     END CALCULATION OF RO, CALCULATE BO
      CALL POTEN(RO,V,DV,DDV)
      BO=RO*DSQRT((E-V)/E)
C     BEGIN CALCULATION OF ROP
C     INITIAL APPROXIMATION
      IF(EOLD)275,275,320
  275 ROP=R1
      IK=0
  320 R=ROP
  325 CALL POTEN(R,V,DV,DDV)
      Y=R*R*(E-V)-BO*BO*E
      DY=2.0D0*R*(E-V)-R*R*DV
      CORR=-Y/DY
      J3=J3+1
      X=R+CORR
      IF(X-RC)335,340,340
  335 IF(X-R1)340,340,375
C     MODIFY INITIAL APPROXIMATION
  340 IF(EOLD)345,345,370
  345 IF(IK)365,350,365
  350 IK=1
      U=.05D0*(RC-R1)
      ROP=RC
  355 ROP=ROP-U
      CALL POTEN(ROP,V,DV,DDV)
      Y=ROP*ROP*(E-V)-BO*BO*E
      IF(Y)320,320,355
  365 ROP=ROP+.05D0*U
      GO TO 320
  370 EOLD=-1.0D0
      GO TO 275
  375 IF(DABS (CORR/R)-ER3)400,400,380
  380 R=X
      IF(J3-30)325,385,385
  385 IF(DABS (CORR/R)-100.0D0*ER3)387,387,502
  387 WRITE(NW,903) E
  400 ROP=X
      RETURN
  450 RO=RC
      ROP=RC
      RETURN
  500 WRITE(NW,904) E
      GO TO 510
  501 WRITE(NW,905) E
      GO TO 510
  502 WRITE(NW,906) E
  510 IF(5.EQ.5) STOP
  901 FORMAT(/1X,38H   POOR CONVERGENCE FOR RE,  ENERGY=  ,E14.5)
  902 FORMAT(/1X,38H   POOR CONVERGENCE FOR RO,  ENERGY=  ,E14.5)
  903 FORMAT(/1X,38H   POOR CONVERGENCE FOR ROP, ENERGY=  ,E14.5)
  904 FORMAT(/1X,33H   NO SOLUTION FOR RE,  ENERGY=  ,E14.5)
  905 FORMAT(/1X,33H   NO SOLUTION FOR RO,  ENERGY=  ,E14.5)
  906 FORMAT(/1X,33H   NO SOLUTION FOR ROP, ENERGY=  ,E14.5)
      RETURN
      END
      SUBROUTINE PARWAV(L,ETAL,Q2,B1,RMAX,DB)
C     REVISED FOR PCW/MODCOMP BY W. L. TAYLOR, MOUND LABORATORY, 9-9-85
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION RAD(4),POINT(4)
      IF(L) 120,150,150
C     INITIALIZATION OF PARWAV
  120 CONTINUE
      NW=6
      JM=5000
      NK=-L
      WF0=ETAL
      WFP0=Q2
      B0=B1
      RINTS=RMAX
      PI=DACOS(-1.0D0)
      RETURN
  150 CONTINUE
      EL=L
      Q=DSQRT(Q2)
C     CALCULATE INCREMENT FOR RUNKA, BASED ON NK POINTS PER WAVELENGTH
      PMAX=DSQRT(Q2-B0)
      WAVLGT=2.0D0*PI/PMAX
      H=WAVLGT/NK
C     INITIALIZE RUNKA, FOLLOWING IS NECESSARY BECAUSE
C     RUNKA REQUIRES DOUBLE PRECISION ARQUMENTS
      R=Q2
      WF=B1
      WFP=RMAX
      KZERO=-1
      CALL RUNKA(R,WF,WFP,H,KZERO,L)
      RINT=RINTS
   22 JOF=1
      IF(L) 70,70,71
   71 WF=0.0D0
      WFP=WFP0
      R=RINT
      GO TO 72
   70 WF=WF0
      WFP=WFP0
      R=RINT
C     START RUNGE-KUTTA NUMERICAL INTEGRATION.
   72 CALL RUNKA(R,WF,WFP,H,KZERO,JOF)
      IF(JOF-1)20,20,21
   21 RINT=RINT+H
      GO TO 22
   20 J=1
      J1=1
    3 IF(WF)1,1,2
    1 CALL RUNKA(R,WF,WFP,H,KZERO,JOF)
      J1=J1+1
C     J1 COUNTS NUMERICAL INTEGRATIONS PER HALF WAVE LENGTH. IF JM ARE
C     CALCULATED WITHOUT AN OSCILLATION OCURRING, PROGRAM STOPS.
      IF(J1-JM)3,49,49
   49 WRITE(NW,202) J1,JM
  202 FORMAT(//6X,5HJ1 = ,I5,6X,5HJM = ,I5,6X,18HINTERVAL TOO SMALL,//)
      STOP
    2 POINT(1)=WF
      RAD(1)=R
      CALL RUNKA(R,WF,WFP,H,KZERO,JOF)
      J1=1
    6 POINT(2)=WF
      RAD(2)=R
      CALL RUNKA(R,WF,WFP,H,KZERO,JOF)
      IF(WF)4,4,5
    5 POINT(1)=POINT(2)
      RAD(1)=RAD(2)
      J1=J1+1
      IF(J1-JM)6,49,49
    4 RAD(3)=R
      POINT(3)=WF
      CALL RUNKA(R,WF,WFP,H,KZERO,JOF)
      POINT(4)=WF
      RAD(4)=R
C     PROGRAM DETERMINES ZERO OF WAVE FUNCTION BY INTERPOLATION.
      VAL=0.0D0
      VA=(VAL-POINT(1))
      VB=(VAL-POINT(2))
      VC=(VAL-POINT(3))
      VD=(VAL-POINT(4))
      UA=(POINT(1)-POINT(2))
      UB=(POINT(1)-POINT(3))
      UC=(POINT(1)-POINT(4))
      UD=(POINT(2)-POINT(3))
      UE=(POINT(2)-POINT(4))
      UF=(POINT(3)-POINT(4))
      XO=VB/UA*VC/UB*VD/UC*RAD(1)-VA/UA*VC/UD*VD/UE*RAD(2)
     1+VA/UB*VB/UD*VD/UF*RAD(3)-VA/UC*VB/UE*VC/UF*RAD(4)
      D=XO*Q
      POINT(1)=POINT(3)
      POINT(2)=POINT(4)
      RAD(1)=RAD(3)
      RAD(2)=RAD(4)
    9 CALL RUNKA(R,WF,WFP,H,KZERO,JOF)
      IF(WF)7,8,8
    7 POINT(1)=POINT(2)
      RAD(1)=RAD(2)
      POINT(2)=WF
      RAD(2)=R
      GO TO 9
    8 POINT(3)=WF
      RAD(3)=R
      CALL RUNKA(R,WF,WFP,H,KZERO,JOF)
      POINT(4)=WF
      RAD(4)=R
C     THE NEXT FOLLOWING ZERO OF THE WAVE FUNCTION IS DETERMINED.
      VAL=0.0D0
      VA=(VAL-POINT(1))
      VB=(VAL-POINT(2))
      VC=(VAL-POINT(3))
      VD=(VAL-POINT(4))
      UA=(POINT(1)-POINT(2))
      UB=(POINT(1)-POINT(3))
      UC=(POINT(1)-POINT(4))
      UD=(POINT(2)-POINT(3))
      UE=(POINT(2)-POINT(4))
      UF=(POINT(3)-POINT(4))
      YO=VB/UA*VC/UB*VD/UC*RAD(1)-VA/UA*VC/UD*VD/UE*RAD(2)
     1+VA/UB*VB/UD*VD/UF*RAD(3)-VA/UC*VB/UE*VC/UF*RAD(4)
      D=YO*Q
      KZERO=KZERO/2
CJJH  HERE THE SUBROUTINE ATANPHS IS CALLED TO DETERMINE THE PHASE SHIFT
CJJH  INSTEAD OF ITS DETERMINATION BEING FROM THE DIFFERENCE OF THE
CJJH  WAVE FUNCTION'S ZERO FROM THE BESSEL ZERO.
   31 CALL ATANPHS(L,D,KZERO,ETAL)
      GO TO 18
   32 WRITE(NW,205) KZERO
  205 FORMAT(//6X,10HKZERO/2 = ,I5,6X,23HEXCEEDED RANGE OF TABLE,//)
      STOP
   18 CONTINUE
      RETURN
      END
      SUBROUTINE RUNKA(R,WF,WFP,H,KZERO,JOF)
C     REVISED FOR PCW/MODCOMP BY W. L. TAYLOR, MOUND LABORATORY, 9-9-85
      IMPLICIT REAL*8 (A-H,O-Z)
      IF(KZERO) 120,150,150
C     INITIALIZATION OF RUNKA
  120 Q2=R
      NW=6
      NK=-KZERO
      PI=DACOS(-1.0D0)
      B1=WF
      RMAX=WFP
      EL=JOF
      KZERO=0
      M=1
      RETURN
  150 CONTINUE
      V=PHI(R)
   95 T1=H*(Q2-B1*V-(EL*(EL+1.0D0)/(R*R)))*(-WF)
      RS=R
      R=RS+H/2.0D0
      WF2=WF+H*WFP/2.0D0+H*T1/8.0D0
      V=PHI(R)
      T2=H*(Q2-B1*V-(EL*(EL+1.0D0)/(R*R)))*(-WF2)
      R=RS+H
      WF2=WF+H*WFP+H*T2/2.0D0
      V=PHI(R)
      T3=H*(Q2-B1*V-(EL*(EL+1.0D0)/(R*R)))*(-WF2)
      DWF=H*(WFP+(T1+2.0D0*T2)/6.0D0)
      DWFP=(T1+4.0D0*T2+T3)/6.0D0
      WF=WF+DWF
      WFP=WFP+DWFP
      IF(WF)5,6,6
    5 IF(M)7,8,8
    7 CONTINUE
      GO TO 11
    8 KZERO=KZERO+1
      M=-1
      GO TO 11
    6 IF(M)9,7,7
    9 KZERO=KZERO+1
      M=+1
   11 CONTINUE
      TEST1=100.0D0*WF
      CALL OVERFL(JJ)
      GO TO (2,1,2),JJ
    2 JOF=2
C     WRITE(NW,910) WF
      GO TO 96
    1 TEST2=100.0D0*WFP
      CALL OVERFL(JJ)
      GO TO (4,3,4),JJ
    4 JOF=2
      GO TO 96
    3 IF(R-RMAX)95,96,96
   96 CONTINUE
  910 FORMAT(/1X,23H THE WAVE FUNCTION IS  ,E14.4,/,
     127H IT IS TOO LARGE OR SMALL  ,/,
     253H THE PROGRAM IS CHANGING THE INTIAL VALUE OF WAVE F. ,/)
      RETURN
      END
```

```
      FUNCTION ZERO(RAD,POINT)
C     REVISED FOR PCW/MOD COMP BY W.L. TAYLOR, MOUND LABORATORY, 9-9-85
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION RAD(4),POINT(4)
      VAL=0.0D0
      VA=(VAL-POINT(1))
      VB=(VAL-POINT(2))
      VC=(VAL-POINT(3))
      VD=(VAL-POINT(4))
      UA=(POINT(1)-POINT(2))
      UB=(POINT(1)-POINT(3))
      UC=(POINT(1)-POINT(4))
      UD=(POINT(2)-POINT(3))
      UE=(POINT(2)-POINT(4))
      UF=(POINT(3)-POINT(4))
      ZERO=VB/UA*VC/UB*VD/UC*RAD(1)-VA/UA*VC/UD*VD/UE*RAD(2)
     1+VA/UB*VB/UD*VD/UF*RAD(3)-VA/UC*VB/UE*VC/UF*RAD(4)
      RETURN
      END
      SUBROUTINE ATANPHS(L,D,KZERO,AZAZ)
CJJH  DEVELOPED FROM LEROY'S PHASE SHIFT PROGRAM.
      IMPLICIT REAL*8(A-H,O-Z)
      DATA Z0/0.D0/,ZH/0.5D0/,Z1/1.D0/,Z2/2.D0/,Z3/3.D0/,Z4/4.D0/,
     1  Z5/5.D0/,Z6/6.D0/,PI/3.141592653589793D0/,IFIRST/0/
CJJH  THE SUBROUTINE BSELFX IS CALLED TO CALCULATE THE BESSEL AND
CJJH  NEUMANN FUNCTIONS AT THE GIVEN VALUE OF L AND D.
      CALL BSELFX(L,D,SBJ,SBN)
CJJH  THE PHASE SHIFT IS THE ARC-TANGENT OF THE BESSEL FUNCTION OVER
CJJH  THE NEUMANN FUNCTION
      AZAZ=DATAN(SBJ/SBN)
C** GET ABSOLUTE PHASE SHIFT USING EQ.(9.2.29) OF ABRAMOWITZ AND STEGUN
CJJH  THE NUMBER OF PI'S TO BE ADDED TO THE VALUE IS DETERMINED HERE.
      EJ=L*(L+1)
      ZU=Z4*EJ+Z1
      R4=Z4*D
      SIR4=Z1/R4**2
      TH=D-ZH*L*PI+(ZH+SIR4*((ZU-25.D0)/Z6+SIR4*((1073.D0-ZU*(
     1 114.D0-ZU))/Z5-SIR4*(375733D0-ZU*(54703.D0-ZU*(1535.D0-Z5*
     2 ZU)))/14.D0)))*(ZU-Z1)/R4
      XNDT=(TH+AZAZ)/PI
      NDT=(XNDT+ZH)
      AZAZ=AZAZ+(KZERO*2-NDT)*PI
      RETURN
      END
```

```
      SUBROUTINE BSELFX(L,ARG,SBJ,SBN)
C** SUBROUTINE TO CALCULATE SPHERICAL BESSEL FUNCTIONS OF THE FIRST AND
C   SECOND KINDS,  SBJ  AND  SBN  , RESPECTIVELY, OF ORDER  L  , WITH
C   ARGUMENT  ARG.
      IMPLICIT REAL*8 (A-H,O-Z)
      LH=L/2
      PM=1.0D0
      LE=L
      AR1=1.D0/ARG
      XQ=DSQRT(1.570796326794896*ARG)
      AQ=DCOS(ARG)/XQ
      BQ=DSIN(ARG)/XQ
      XQ=XQ*AR1
   12 CQ=PM
```

```
      IF(LE) 14,28,16
   14 QQ=AQ
      RQ=BQ
      GOTO 18
   16 IF(ARG.LT.(1.D0*L)) GOTO 30
      QQ=BQ
      RQ=AQ
   18 DO 20 IQ=1,L
      PQ=QQ*(CQ+CQ-PM)*AR1-RQ
      CQ=CQ+PM
      RQ=QQ
   20 QQ=PQ
      PQ=PQ*XQ
      IF(PM.LT.0.0D0) GOTO 26
      SBJ=PQ
   22 PM=-1.0D0
      LE=-L
      GOTO 12
   26 SBN=PQ
      K=L-2*LH
      IF(K.EQ.0) SBN=-PQ
      RETURN
   28 SBJ=BQ*XQ
      SBN=-AQ*XQ
      RETURN
C** CALCULATE FX OF 1-ST KIND FOR SMALL ARGUMENT BY ASCENDING POWER
C   EXPANSION.
   30 QQ=1.0D0
      DO 32 I=1,L
   32 QQ=QQ*ARG/(2*I+1)
      SBJ=QQ
      L4=50
      IF(L.GT.12) L4=4*L
      CQ=(2*L+1)
      QQ=-0.5D0*ARG*ARG
      RQ=1.0D0
      PQ=RQ
      DO 34 I=1,L4
      K=I
      RQ=RQ*QQ/(I*(CQ+2*I))
      PQ=PQ+RQ
      IF(DABS(RQ/PQ).LT.1.D-10) GOTO 36
   34 CONTINUE
      RQ=RQ/PQ
   36 SBJ=SBJ*PQ
      GOTO 22
  601 FORMAT('0  ERR   IN   SBJ(',I3,',',E10.5,') . AFTER',I4,' ASCENDIN
     1G TERMS   RATIO =',E10.5 )
      END


      FUNCTION PHI(R)
C     HFD(HE)-B POTENTIAL FOR HELIUM:  E/K = 10.948, RM = 2.963
```

```
C     POTENTIAL IS CALCULATED IN REDUCED FORM
      IMPLICIT REAL*8 (A-H,O-Z)
      A=1.8443101D+05
      MINUS=-1
      ALPHA=10.43329537
      BETA=-2.27965105
      C6=1.36745214D0
      C8=0.42123807D0
      C10=0.17473318D0
      D=1.4826D0
      X=R
      ABX=-1.0D0*ALPHA*X+BETA*X*X
      IF(DABS(ABS).GT.70.0)GOTO 11
      DABX=-1.0D0*ALPHA+2.0D0*BETA*X
      DDABX=2.0D0*BETA
   10 VR=A*DEXP(ABX)
      GO TO 12
   11 VR=0.0D0
   12 X2=X*X
      X4=X2*X2
      X6=X4*X2
      VA=(C6/X6+C8/(X6*X2)+C10/(X6*X4))*MINUS
      IF(X-D) 1,2,2
    1 FX=DEXP(((D/X-1)**2)*MINUS)
      V=VR+VA*FX
      PHI=V
      GO TO 99
    2 V=VR+VA
      PHI=V
   99 RETURN
      END
      SUBROUTINE POTEN(R,V,DV,DDV)
C     HFD(HE)-B POTENTIAL FOR HELIUM:  E/K = 10.948, RM = 2.963
C     POTENTIAL IS CALCULATED IN REDUCED FORM
      IMPLICIT REAL*8 (A-H,O-Z)
      A=1.8443101D+05
      MINUS=-1
      ALPHA=10.43329537
      BETA=-2.27965105
      C6=1.36745214D0
      C8=0.42123807D0
      C10=0.17473318D0
      D=1.4826D0
      X=R
      ABX=-1.0D0*ALPHA*X+BETA*X*X
      IF(DABS(ABS).GT.70.0)GOTO 11
      DABX=-1.0D0*ALPHA+2.0D0*BETA*X
      DDABX=2.0D0*BETA
   10 VR=A*DEXP(ABX)
      GO TO 12
   11 VR=0.0D0
   12 DVR=DABX*VR
      DDVR=DABX*DABX*VR+DDABX*VR
      X2=X*X
      X4=X2*X2
      X6=X4*X2
      VA=(C6/X6+C8/(X6*X2)+C10/(X6*X4))*MINUS
      DVA=(6.0D0*C6/(X6*X)+8.0D0*C8/(X6*X2*X)+10.0D0*C10/(X6*X4*X))
      DDVA=(42.0D0*C6/(X6*X2)+72.0D0*C8/(X6*X4)+110.0D0*C10/(X6*X6))
     1*MINUS
      IF(X-D) 1,2,2
    1 FX=DEXP(((D/X-1)**2)*MINUS)
      DFX=2.0D0*FX*(D*D/(X2*X)-D/X2)
      DDFX=4.0D0*FX*(D**4/X6-2.0D0*D**3/(X4*X)-D*D/(2.0D0*X4)+D/(X2*X))
      V=VR+VA*FX
      DV=DVR+DVA*FX+VA*DFX
      DDV=DDVR+FX*DDVA+2.0D0*DFX*DVA+VA*DDFX
      GO TO 99
    2 V=VR+VA
      DV=DVR+DVA
      DDV=DDVR+DDVA
   99 RETURN
      END
      SUBROUTINE SCAN(R1,R3,RC,EC,EMAX)
C     CALCULATES FOLLOWING  CHARACTERISTIC PARAMETERS OF POTENTIAL
C     ZERO (R1), MINIMUM (R2 AND EMIN), INFLECTION POINT (R3),
C     MAXIMUM ORBITING ENERGY AND ASSOCIATED DISTANCE OF CLOSEST
C     APPROACH (EC AND RC)
C     IF POTENTIAL HAS A SPURIOUS MAXIMUM, CALCULATES MAXIMUM (EMAX
C     AND RMAX) AND INFLECTION POINT (EINF AND RINF)
C     USES SUBROUTINE POTEN
C     INPUT IS AN APPROXIMATION TO R1
C     OUTPUT CONSISTS OF ABOVE QUANTITIES
C     DIMENSION TITLE(20)
      IMPLICIT REAL*8 (A-H,O-Z)
      NR=5
      NW=6
C     OPEN DISK FILE
C     OPEN (UNIT=5,FILE='SCAN.INP',STATUS='OLD',ERR=704)
  105 CONTINUE
      R=0.80D0
      KWIT=-1
C     CLOSE (UNIT=5,ERR=704,STATUS='KEEP')
      R1=R
      IF(R)108,108,109
  108 STOP
  109 CONTINUE
      WRITE(NW,912)
      R=0.40D0
  703 CALL POTEN(R,V,DV,DDV)
  913 FORMAT(' ',7X,4(E10.3,9X))
      IF(7.9-R) 701,701,702
  702 IF(R-.8) 139,140,140
  139 R=R+0.05
      GO TO 703
  140 IF (R-1.195) 137,141,141
  137 R=R+0.01
      GO TO 703
  141 R=R+0.10D0
      GO TO 703
  701 CONTINUE
      R=R1
      WRITE(NW,901)
  120 CALL POTEN(R,PSI,DPSI,DDPSI)
      IF(PSI)130,135,135
  130 IF(DPSI)155,180,180
  135 IF(DDPSI)138,138,145
  138 R=R+0.1*R
C     CALCULATE R1
  145 CORR=-PSI/DPSI
      IF(DABS(CORR/R)-.00001)200,200,150
  150 X=R+CORR
      IF(X)155,155,160
  155 X=R-0.06*R
  160 CALL POTEN(X,PSI,DPSI,DDPSI)
      IF(DPSI)170,170,165
  165 CORR=0.5*CORR
      GO TO 150
  170 R=X
      GO TO 145
  180 IF(DDPSI)185,190,190
  185 R=0.5*R
      GO TO 120
  190 R=0.75*R
      GO TO 120
  200 R1=R+CORR
C     CALCULATE R2
      R=R1
      X=R
      CORR=0.5*R
      GO TO 230
  210 CORR=-DPSI/DDPSI
      IF(DABS(CORR/R)-.00001)275,275,215
  215 X=R+CORR
      IF(X-R1)220,220,230
  220 X=R-0.06*(DABS(DPSI)/DPSI)*R
  230 CALL POTEN(X,PSI,DPSI,DDPSI)
      IF(DDPSI)235,235,240
  235 CORR=0.5*CORR
      GO TO 215
  240 R=X
      GO TO 210
  275 R2=R
      EMIN=PSI
C     CALCULATE R3
      U=1.
      X=R2
      DX=R2-R1
  312 X=X+DX
      CALL POTEN(X,V,DV,DDV)
      IF(U*DDV) 322,370,312
  322 U=-U
      DX=-.5*DX
      IF(DABS(DX/X)-1.D-4) 370,370,312
  370 R3=X
C     CALCULATE RC AND EC
      U=1.
      X=R3
      DX=R3-R2
  422 X=X+DX
      CALL POTEN(X,V,DV,DDV)
      Y=X*DDV+3.*DV
      IF(U*Y) 432,470,422
  432 U=-U
      DX=-.5*DX
      IF(DABS(DX/X)-1.0D-05)470,470,422
  470 RC=X
      EC=V+.5*RC*DV
      BC=RC*DSQRT((EC-V)/EC)
      WRITE(NW,906)
      WRITE(NW,902) R1,R2,R3,EMIN,RC,EC
C     CHECK FOR A SPURIOUS MAXIMUM
      X=-1.E+05*EMIN
      DR=.01*R1
      R=R1
      DO 525 I=1,98
      CALL POTEN(R,V,DV,DDV)
      IF(DDV)540,520,520
  520 IF(V-X)525,530,530
  525 R=R-DR
  530 EINF=0.0
      RINF=0.0
      EMAX=V
      RMAX=R+DR
      WRITE(NW,910) EMAX,RMAX
      RETURN
C     POTENTIAL HAS A SPURIOUS MAXIMUM
C     CALCULATE RINF,EINF,RMAX,AND EMAX
  540 Y=DDV
      X=R
      R=R+DR
  545 CALL POTEN(R,V,DV,DDV)
      IF(DABS(CORR/R)-.0001)560,550,550
  550 Y=DDV
      X=R
      R=R-CORR
      GO TO 545
  560 RINF=R
      EINF=V
      DR=.1*DR
  570 R=R-DR
      IF(DV)570,580,580
  580 CORR=DV/DDV
      IF(DABS(CORR/R)-.0001)590,590,585
  585 R=R-CORR
      CALL POTEN(R,V,DV,DDV)
      GO TO 580
  590 RMAX=R
      EMAX=V
      WRITE(NW,903) RINF,EINF,RMAX,EMAX
  600 CONTINUE
  900 FORMAT(8E10.4)
  901 FORMAT('1',25X,15H  PROGRAM SCAN )
  902 FORMAT(' ',4X,3HR1=,E14.5,7H    R2=,E12.5,7H    R3=,E12.5,
     1       /4X,5HEMIN=,E12.5,7H    RC=,E12.5,7H    EC=,E12.5,/)
  903 FORMAT(' ',3X,34H POTENTIAL HAS A SPURIOUS MAXIMUM ,
     1       /4X,5HRINF=,E12.5,7H  EINF=,E12.5,
     2       /4X,5HRMAX=,E12.5,7H  EMAX=,E12.5)
  904 FORMAT('-',/17X,32H RESULTS IN UNITS OF EMIN AND R1 )
  906 FORMAT('-',17X,31H RESULTS IN UNITS USED IN POTEN )
  910 FORMAT(' ',3X,35H POTENTIAL HAS NO SPURIOUS MAXIMUM  ,
     1       /3X,16H FOR E LESS THAN ,E15.5,
   2      /3X,19H AND R GREATER THAN ,E12.5)
911 FORMAT(20A4)
912 FORMAT('0',20X,33HINTERMOLECULAR POTENTIAL FUNCTION,//
   125X,6HV(R) =,//12X,1HR,17X,4HV(R),15X,5HDV(R),12X,6HDDV(R),//)
914 FORMAT('0',12X,17A4)
915 FORMAT (I2)
704 CONTINUE
    RETURN
    END
```

Appendix B

IBM 3090 Job Control Language and Input Files

THIS IS THE JCL (JOB CONTROL LANGUAGE) CODE TO COMPILE AND LINK THE PROGRAM

```
//HURLJJ21  JOB   (8604,CC18),HURLJJ,MSGLEVEL=(1,1),CLASS=A,            0001009
//       MSGCLASS=T,NOTIFY=HURLJJ,                                      0002009
//       REGION=6M,TIME=1440                                            0003009
//*
//SCALAR EXEC  VSF2CL,FVTERM='SYSOUT=*',FVLNSPC='3200,(400,50)',        0006009
// PARM.FORT='XREF',                                                    0006009
//             COND.FORT=(8,LT),
//        PARM.LKED='LIST,LET,NOMAP,AMODE=31,RMODE=ANY',                0006109
//             COND.LKED=(4,LT)
//FORT.SYSPRINT DD SYSOUT=*
//*FORT.SYSPRINT DD DSN=&&LIST,DCB=(RECFM=VBA,LRECL=137,BLKSIZE=3429),  0006200
//*         DISP=(NEW,PASS),UNIT=SYSDA,SPACE=(CYL,(5,2))                0006300
//FORT.SYSIN DD DSN=HURLJJ.MLM1.PDS(QCOLL),DISP=SHR
//****************************************************************
//LKED.SYSPRINT DD SYSOUT=*
//LKED.SYSLIB DD  DSN=SYS1.VSF2MATH,DISP=SHR                            0009000
//            DD  DSN=SYS1.VSF2FORT,DISP=SHR                            0009000
//            DD  DSN=SYS1.VSF2LINK,DISP=SHR
//LKED.SYSUT1 DD  UNIT=VIO,SPACE=(1024,(1500,100))                      0012003
//LKED.SYSLMOD DD  DSN=HURLJJ.MLMLIB(QCOLL),DISP=SHR                    0012003
//*
```

THIS IS THE JCL CODE TO RUN THE PROGRAM

```
//HURLJJ23 JOB   (8604,CC18),PHILMR,MSGLEVEL=(1,1),CLASS=A,             0001009
//       MSGCLASS=T,NOTIFY=HURLJJ,                                      0002009
//       REGION=6M,TIME=1440,PRTY=1                                     0003009
//*
//TARTS    EXEC  PGM=QCOLL
//STEPLIB  DD DSN=HURLJJ.MLMLIB,DISP=SHR
//FT10F001 DD DSN=HURLJJ.MLM1.PDS(LUQUAD),DISP=SHR
//FT11F001 DD DSN=HURLJJ.MLM1.PDS(INPUT),DISP=SHR
//FT06F001 DD SYSOUT=*
//FT04F001 DD SYSOUT=*
//FT08F001 DD SYSOUT=*
//FT20F001 DD DSN=HURLJJ.LUPH002.OUT,DISP=(NEW,KEEP),
//           DCB=(LRECL=80,BLKSIZE=8000,RECFM=FB,DSORG=PS),
//           SPACE=(TRK,(20,5)),
//           UNIT=3380,VOL=SER=SCTCH2
//FT21F001 DD DSN=HURLJJ.LUCS002.OUT,DISP=(NEW,KEEP),
//           DCB=(LRECL=80,BLKSIZE=8000,RECFM=FB,DSORG=PS),
//           SPACE=(TRK,(20,5)),
//           UNIT=3380,VOL=SER=SCTCH2
//FT22F001 DD DSN=HURLJJ.LUCI002.OUT,DISP=(NEW,KEEP),
//           DCB=(LRECL=80,BLKSIZE=8000,RECFM=FB,DSORG=PS),
//           SPACE=(TRK,(20,5)),
//           UNIT=3380,VOL=SER=SCTCH2
//FT09F001 DD DUMMY
//*GO.FT11F001 DD DSN=&&TEMP,DISP=(NEW,DELETE),DCB=(LRECL=80,
//*         BLKSIZE=3200),SPACE=(CYL,(2,1)),UNIT=SYSDA
```

THIS IS THE INPUT FILE LUQUAD

```
 40
+.998238E+00          +.452128E-02
+.990726E+00          +.104983E-01
+.977260E+00          +.164211E-01
+.957917E+00          +.222458E-01
+.932813E+00          +.279370E-01
+.902099E+00          +.334602E-01
+.865959E+00          +.387822E-01
+.824612E+00          +.438709E-01
+.778306E+00          +.486958E-01
+.727318E+00          +.532278E-01
+.671957E+00          +.574398E-01
+.612554E+00          +.613062E-01
+.549467E+00          +.648040E-01
+.483076E+00          +.679120E-01
+.413779E+00          +.706116E-01
+.341994E+00          +.728865E-01
+.268152E+00          +.747231E-01
+.192698E+00          +.761102E-01
+.116084E+00          +.770398E-01
+.387724E-01          +.775059E-01
 28
+.507346E-01          +.123779E+00
+.267487E+00          +.232279E+00
+.658137E+00          +.247512E+00
+.122397E+01          +.192307E+00
+.196677E+01          +.116405E+00
+.288888E+01          +.563459E-01
+.399331E+01          +.220664E-01
+.528374E+01          +.702589E-02
+.676460E+01          +.182061E-02
+.844122E+01          +.383344E-03
+.103198E+02          +.653509E-04
+.124079E+02          +.897136E-05
+.147141E+02          +.984701E-06
+.172487E+02          +.856407E-07
+.200238E+02          +.583684E-08
+.230539E+02          +.307564E-09
+.263563E+02          +.123259E-10
+.299520E+02          +.368217E-12
+.338666E+02          +.799879E-14
+.381322E+02          +.122492E-15
+.427897E+02          +.127112E-17
+.478921E+02          +.848859E-20
+.535113E+02          +.340245E-22
+.597488E+02          +.742015E-25
+.667570E+02          +.760041E-28
+.747868E+02          +.287391E-31
+.843178E+02          +.254182E-35
+.965824E+02          +.166138E-40
```

Sample QCOLL.INP file.

```
HFD-B(HE) Potential: Mol. Phys. 61(6), 1487 (1987).
10.948 2.9630    1   64
.10,      .20,      .30,      .40,      .50
.60,      .70,      .80,      .90,      1.00
1.20,     1.40,     1.60,     2.00,     2.40
2.80,     3.20,     3.60,     4.00,     4.50
5.00,     5.50,     6.00,     7.00,     8.00
9.00,     10.00,    12.00,    14.00,    16.00
20.00,    25.00,    30.00,    35.00,    40.00
45.00,    50.00,    60.00,    70.00,    80.00
90.00,    100.0,    120.0,    140.0,    160.0
180.0,    200.0,    250.0,    300.0,    350.0
400.0,    500.0,    600.0,    700.0,    800.0
900.0,    1000.,    1200.,    1400.,    1600.
1800.,    2000.,    2200.,    2500.,
 4.0026   4.0026   1.00D0
 1.0E-06  0.4      5.0     1.0Q-50    1.0Q-50    40
```

Appendix C

Sample Output for HFD–B(HE) Potential

```
                            4He-4He Phase Shifts
  HFD-B(HE) Potential: Mol. Phys. 61(6), 1487 (1987).
    0.0100    4    1
    1.8479    0.0010    0.0000    0.0000
    0.0800    5    1
    1.4085    0.0204    0.0003    0.0000    0.0000
    0.1500    6    1
    1.2608    0.0507    0.0012    0.0001    0.0000    0.0000
    0.2200    6    1
    1.1583    0.0876    0.0026    0.0003    0.0001    0.0000
    0.2900    6    1
    1.0764    0.1291    0.0044    0.0004    0.0001    0.0000
    0.3600    6    1
    1.0068    0.1736    0.0067    0.0007    0.0002    0.0001
    0.4300    6    1
    0.9454    0.2197    0.0094    0.0010    0.0002    0.0001
    0.5000    7    1
    0.8901    0.2662    0.0126    0.0013    0.0003    0.0001    0.0000
    0.5700    7    1
    0.8395    0.3119    0.0163    0.0017    0.0004    0.0001    0.0001
    0.6400    7    1
    0.7926    0.3561    0.0203    0.0022    0.0005    0.0002    0.0001
    0.7100    7    1
    0.7488    0.3980    0.0248    0.0027    0.0006    0.0002    0.0001
         -         -         -         -         -         -         -
         -         -         -         -         -         -         -
         -         -         -         -         -         -         -
         -         -         -         -         -         -         -
         -         -         -         -         -         -         -
         -         -         -         -         -         -         -
         -         -         -         -         -         -         -
         -         -         -         -         -         -         -
         -         -         -         -         -         -         -

  900.0 00  270    1
  -16.5065  -15.0049  -13.5727  -12.2099  -10.9169   -9.6940   -8.5406   -7.4601
   -6.4501   -5.5123   -4.6474   -3.8560   -3.1390   -2.4969   -1.9302   -1.4392
   -1.0234   -0.6815   -0.4108   -0.2068   -0.0625    0.0313    0.0853    0.1108
    0.1175    0.1134    0.1038    0.0921    0.0802    0.0691    0.0592    0.0505
    0.0431    0.0369    0.0315    0.0271    0.0233    0.0200    0.0173    0.0150
    0.0131    0.0114    0.0100    0.0096    0.0085    0.0076    0.0068    0.0061
    0.0055    0.0049    0.0044    0.0040    0.0036    0.0033    0.0030    0.0027
    0.0025    0.0023    0.0021    0.0019    0.0018    0.0016    0.0015    0.0014
    0.0013    0.0012    0.0011    0.0010    0.0009    0.0009    0.0008    0.0008
    0.0007    0.0007    0.0006    0.0006    0.0005    0.0005    0.0005    0.0004
    0.0004    0.0004    0.0004    0.0003    0.0003    0.0003    0.0003    0.0003
    0.0003    0.0002    0.0002    0.0002    0.0002    0.0002    0.0002    ------

  950.0000  276   -1
  -16.8902  -15.3873  -13.9523  -12.5854  -11.2869  -10.0569   -8.8960   -7.8045
   -6.7830   -5.8320   -4.9522   -4.1443   -3.4088   -2.7465   -2.1578   -1.6429
   -1.2016   -0.8329   -0.5348   -0.3036   -0.1337   -0.0171    0.0557    0.0954
    0.1121    0.1142    0.1081    0.0981    0.0868    0.0756    0.0653    0.0561
    0.0481    0.0412    0.0354    0.0304    0.0262    0.0226    0.0195    0.0170
    0.0147    0.0129    0.0113    0.0099    0.0095    0.0085    0.0076    0.0068
    0.0061    0.0055    0.0050    0.0045    0.0041    0.0037    0.0033    0.0030
    0.0028    0.0025    0.0023    0.0021    0.0020    0.0018    0.0017    0.0015
    0.0014    0.0013    0.0012    0.0011    0.0010    0.0010    0.0009    0.0008
    0.0008    0.0007    0.0007    0.0006    0.0006    0.0006    0.0005    0.0005
    0.0005    0.0004    0.0004    0.0004    0.0004    0.0003    0.0003    0.0003
    0.0003    0.0003    0.0003    0.0002    0.0002    0.0002    0.0002    ------
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4He-4He Cross Sections

HFD-B(HE) Potential: Mol. Phys. 61(6), 1487 (1987).

0.010000	681.678079	681.307225	681.529112	681.306723
0.080000	89.051963	89.673998	89.313379	89.683435
0.150000	43.101167	44.605143	43.744089	44.636400
0.220000	26.019370	28.261387	26.997114	28.323051
0.290000	17.130919	19.961423	18.391571	20.059953
0.360000	11.770391	15.033685	13.256718	15.173455
0.430000	8.292816	11.832524	9.944437	12.015759
0.500000	5.959570	9.626529	7.716232	9.853347
0.570000	4.379282	8.039359	6.184320	8.308009
0.640000	3.317068	6.857174	5.120315	7.164375
0.710000	2.618505	5.949918	4.378220	6.291303
0.780000	2.175860	5.234758	3.859535	5.605319
0.850000	1.911570	4.657303	3.495759	5.051791
0.920000	1.769196	4.181088	3.238633	4.594322
0.990000	1.707800	3.781290	3.054132	4.208384
1.060000	1.698037	3.440778	2.918421	3.877264
1.130000	1.719233	3.147551	2.814986	3.589447
1.200000	1.757143	2.893063	2.732559	3.336883
1.340000	1.848250	2.477019	2.603091	2.916098
1.480000	1.929623	2.159062	2.496103	2.584639
1.620000	1.987408	1.918493	2.398534	2.324374
1.760000	2.020345	1.740982	2.306537	2.122888
1.900000	2.032138	1.615609	2.219939	1.970672
2.040000	2.027847	1.533455	2.139714	1.859867
2.180000	2.012334	1.486906	2.066911	1.783681
2.320000	1.989683	1.469299	2.002262	1.736108
2.460000	1.963075	1.474737	1.946087	1.711792
2.600000	1.934831	1.497986	1.898315	1.705952
2.740000	1.906550	1.534419	1.858557	1.714339
2.880000	1.879242	1.579981	1.826187	1.733212
3.020000	1.853464	1.631176	1.807416	1.759326
-	-	-	-	-
-	-	-	-	-
-	-	-	-	-
-	-	-	-	-
-	-	-	-	-
-	-	-	-	-
-	-	-	-	-
650.000000	0.471724	0.578996	0.537576	0.607371
700.000000	0.464799	0.571732	0.530472	0.599984
750.000000	0.458377	0.564977	0.523874	0.593119
800.000000	0.452392	0.558665	0.517718	0.586707
850.000000	0.446788	0.552742	0.511947	0.580692
900.000000	0.441523	0.547163	0.506517	0.575028
950.000000	0.436558	0.541892	0.501392	0.569678
1000.000000	0.432068	0.537233	0.496525	0.563857
1400.000000	0.401519	0.504428	0.464862	0.530873
1960.000000	0.371688	0.472031	0.433718	0.498215
2744.000000	0.342605	0.440074	0.403117	0.465896
3841.600000	0.314311	0.408619	0.373111	0.433978
5378.240000	0.286854	0.377735	0.343763	0.402539
7529.536000	0.260289	0.347495	0.315144	0.371662
10541.350400	0.234670	0.317971	0.287323	0.341428
14757.890560	0.210057	0.289231	0.260367	0.311913
20661.046784	0.186514	0.261344	0.234347	0.283192
28925.465498	0.164109	0.234382	0.209333	0.255340
40495.651697	0.142911	0.208428	0.185396	0.228437
56693.912375	0.122986	0.183570	0.162609	0.202569
79371.477325	0.104395	0.159900	0.141048	0.177826
111120.068256	0.087188	0.137504	0.120782	0.154300
155568.095558	0.071413	0.116458	0.101877	0.132073
217795.333781	0.057116	0.096830	0.084392	0.111222
304913.467293	0.044341	0.078689	0.068383	0.091817

4He-4He Collision Integrals

HFD-B(HE) Potential: Mol. Phys. 61(6), 1487 (1987).

0.10	30.88096	16.32928	10.17694	6.81921	4.79657	3.55700	2.80582	19.23484
0.20	11.17769	5.43487	3.32027	2.45108	2.10711	1.98681	1.95335	7.96784
0.30	6.03894	3.14968	2.28189	2.02336	1.94825	1.91746	1.88947	4.71035
0.40	3.98348	2.43277	2.03524	1.92437	1.87260	1.82474	1.77220	3.29713
0.50	3.16899	2.16089	1.93106	1.84757	1.78250	1.71485	1.64445	2.62631
0.60	2.76631	2.02341	1.85469	1.76753	1.68585	1.60218	1.51845	2.28653
0.70	2.47789	1.92804	1.78350	1.68519	1.58895	1.49347	1.40161	2.10286
0.80	2.28955	1.85307	1.71388	1.60347	1.49610	1.39357	1.29924	2.00113
0.90	2.15236	1.78729	1.64574	1.52487	1.41032	1.30547	1.21354	1.93961
1.00	2.04620	1.72667	1.57993	1.45124	1.33338	1.23022	1.14413	1.89718
1.20	1.88611	1.61577	1.45865	1.32284	1.20782	1.11581	1.04600	1.83168
1.40	1.76440	1.51684	1.35434	1.22086	1.11645	1.03966	0.98593	1.76929
1.60	1.66505	1.42982	1.26766	1.14241	1.05147	0.98918	0.94799	1.70429
2.00	1.50974	1.28962	1.13987	1.03737	0.97122	0.92952	0.90223	1.57385
2.40	1.39209	1.18705	1.05611	0.97464	0.92522	0.89377	0.87122	1.45652
2.80	1.30104	1.11198	0.99954	0.93371	0.89394	0.86690	0.84565	1.35910
3.20	1.22838	1.05612	0.95930	0.90413	0.86964	0.84449	0.82375	1.28104
3.60	1.16979	1.01347	0.92900	0.88088	0.84934	0.82520	0.80504	1.21913
4.00	1.12233	0.97992	0.90497	0.86156	0.83184	0.80850	0.78904	1.16979
4.50	1.07450	0.94670	0.88061	0.84113	0.81299	0.79061	0.77211	1.12138
5.00	1.03609	0.92019	0.86054	0.82373	0.79683	0.77540	0.75779	1.08364
5.50	1.00463	0.89836	0.84349	0.80866	0.78282	0.76226	0.74539	1.05344
6.00	0.97829	0.87989	0.82868	0.79542	0.77053	0.75073	0.73446	1.02873
7.00	0.93645	0.84996	0.80399	0.77314	0.74983	0.73121	0.71580	0.99023
8.00	0.90436	0.82640	0.78399	0.75495	0.73284	0.71506	0.70021	0.96109
9.00	0.87859	0.80715	0.76730	0.73965	0.71844	0.70128	0.68684	0.93784
10.00	0.85707	0.79091	0.75304	0.72646	0.70595	0.68924	0.67513	0.91847
12.00	0.82249	0.76448	0.72961	0.70460	0.68507	0.66900	0.65534	0.88753
14.00	0.79600	0.74348	0.71074	0.68684	0.66797	0.65235	0.63900	0.86371
16.00	0.77541	0.72631	0.69504	0.67192	0.65353	0.63822	0.62509	0.84480
20.00	0.74452	0.69930	0.66984	0.64773	0.62996	0.61507	0.60225	0.81526
25.00	0.71579	0.67367	0.64562	0.62427	0.60697	0.59241	0.57983	0.78756
30.00	0.69350	0.65357	0.62638	0.60552	0.58853	0.57419	0.56177	0.76631
35.00	0.67534	0.63705	0.61044	0.58991	0.57314	0.55895	0.54666	0.74906
40.00	0.65997	0.62299	0.59683	0.57654	0.55994	0.54587	0.53367	0.73456
45.00	0.64670	0.61073	0.58495	0.56486	0.54838	0.53441	0.52230	0.72200
50.00	0.63516	0.59986	0.57441	0.55448	0.53811	0.52423	0.51218	0.71090
60.00	0.61607	0.58138	0.55634	0.53667	0.52049	0.50675	0.49482	0.69182
70.00	0.60052	0.56608	0.54126	0.52177	0.50572	0.49210	0.48028	0.67595
80.00	0.58703	0.55293	0.52831	0.50896	0.49304	0.47952	0.46778	0.66250
90.00	0.57503	0.54137	0.51695	0.49774	0.48192	0.46849	0.45683	0.65074
100.00	0.56435	0.53110	0.50687	0.48778	0.47206	0.45872	0.44714	0.64023
120.00	0.54623	0.51352	0.48956	0.47068	0.45512	0.44191	0.43044	0.62205
140.00	0.53119	0.49880	0.47505	0.45632	0.44089	0.42780	0.41642	0.60677
160.00	0.51829	0.48618	0.46262	0.44404	0.42873	0.41572	0.40443	0.59364
180.00	0.50698	0.47509	0.45168	0.43322	0.41801	0.40509	0.39388	0.58205
200.00	0.49695	0.46529	0.44202	0.42367	0.40854	0.39569	0.38455	0.57178
250.00	0.47588	0.44464	0.42166	0.40354	0.38861	0.37595	0.36497	0.55000
300.00	0.45887	0.42797	0.40523	0.38731	0.37256	0.36006	0.34923	0.53228
350.00	0.44466	0.41401	0.39148	0.37373	0.35914	0.34679	0.33610	0.51735
400.00	0.43244	0.40204	0.37970	0.36211	0.34766	0.33543	0.32486	0.50449
500.00	0.41220	0.38222	0.36022	0.34292	0.32873	0.31674	0.30637	0.48301
600.00	0.39593	0.36630	0.34458	0.32752	0.31355	0.30174	0.29154	0.46567
700.00	0.38226	0.35296	0.33151	0.31468	0.30089	0.28925	0.27920	0.45102
800.00	0.37059	0.34157	0.32034	0.30370	0.29008	0.27859	0.26867	0.43845
900.00	0.36041	0.33163	0.31060	0.29413	0.28066	0.26930	0.25950	0.42745
1000.00	0.35134	0.32280	0.30196	0.28566	0.27233	0.26109	0.25140	0.41764
1200.00	0.33583	0.30772	0.28723	0.27121	0.25812	0.24710	0.23760	0.40078
1400.00	0.32291	0.29517	0.27497	0.25920	0.24633	0.23549	0.22617	0.38667
1600.00	0.31188	0.28446	0.26452	0.24896	0.23628	0.22561	0.21644	0.37456
1800.00	0.30225	0.27512	0.25542	0.24006	0.22755	0.21703	0.20799	0.36396
2000.00	0.29371	0.26686	0.24737	0.23220	0.21984	0.20947	0.20055	0.35454
2200.00	0.28606	0.25947	0.24018	0.22517	0.21296	0.20271	0.19391	0.34609
2500.00	0.27593	0.24968	0.23066	0.21588	0.20387	0.19379	0.18515	0.33484

4He-4He Collision Integrals (cont.)

0.10	13.28796	9.93871	7.77342	6.28488	11.69400	8.39757	6.36718	10.20299
0.20	5.36785	3.94209	3.07771	2.52576	4.56602	3.48838	2.92599	4.32311
0.30	3.19296	2.43234	2.03323	1.83257	3.04234	2.53789	2.27218	2.76968
0.40	2.36757	1.96681	1.81189	1.77650	2.47413	2.17063	2.00231	2.22109
0.50	2.04130	1.84536	1.80646	1.82297	2.19053	1.97959	1.85931	2.02322
0.60	1.91640	1.82824	1.82744	1.83751	2.02303	1.86261	1.76661	1.94871
0.70	1.86916	1.82819	1.82424	1.80584	1.91109	1.77891	1.69221	1.91017
0.80	1.84699	1.81744	1.79243	1.74243	1.82808	1.71004	1.62379	1.87589
0.90	1.82803	1.79084	1.73995	1.66323	1.76048	1.64791	1.55785	1.83643
1.00	1.80444	1.75096	1.67585	1.57965	1.70147	1.58942	1.49429	1.79075
1.20	1.73911	1.64860	1.53890	1.42393	1.59750	1.48073	1.37777	1.68795
1.40	1.65787	1.53885	1.41366	1.29882	1.50559	1.38422	1.27950	1.58305
1.60	1.57244	1.43719	1.31042	1.20564	1.42396	1.30143	1.20028	1.48615
2.00	1.41649	1.27694	1.16774	1.09112	1.29025	1.17515	1.08926	1.33006
2.40	1.29507	1.17038	1.08530	1.03200	1.19134	1.09033	1.02136	1.22220
2.80	1.20629	1.10121	1.03621	0.99750	1.11915	1.03310	0.97807	1.15004
3.20	1.14215	1.05500	1.00402	0.97316	1.06613	0.99325	0.94844	1.10130
3.60	1.09517	1.02233	0.98032	0.95328	1.02641	0.96419	0.92644	1.06725
4.00	1.05972	0.99761	0.96109	0.93580	0.99588	0.94190	0.90886	1.04218
4.50	1.02605	0.97331	0.94070	0.91640	0.96641	0.91995	0.89060	1.01841
5.00	0.99998	0.95344	0.92302	0.89936	0.94336	0.90213	0.87494	0.99956
5.50	0.97882	0.93646	0.90743	0.88437	0.92460	0.88698	0.86110	0.98362
6.00	0.96104	0.92159	0.89359	0.87119	0.90880	0.87369	0.84865	0.96960
7.00	0.93215	0.89647	0.87015	0.84909	0.88303	0.85104	0.82703	0.94529
8.00	0.90915	0.87591	0.85099	0.83113	0.86230	0.83211	0.80886	0.92455
9.00	0.89018	0.85876	0.83506	0.81615	0.84488	0.81590	0.79333	0.90653
10.00	0.87404	0.84407	0.82136	0.80321	0.82989	0.80184	0.77987	0.89073
12.00	0.84781	0.82011	0.79890	0.78179	0.80499	0.77839	0.75748	0.86435
14.00	0.82701	0.80098	0.78083	0.76441	0.78492	0.75943	0.73933	0.84307
16.00	0.81003	0.78513	0.76571	0.74978	0.76821	0.74358	0.72411	0.82543
20.00	0.78319	0.75981	0.74134	0.72603	0.74146	0.71812	0.69951	0.79746
25.00	0.75779	0.73557	0.71779	0.70291	0.71600	0.69367	0.67573	0.77102
30.00	0.73786	0.71635	0.69897	0.68434	0.69596	0.67429	0.65679	0.75031
35.00	0.72145	0.70040	0.68327	0.66880	0.67944	0.65824	0.64103	0.73329
40.00	0.70749	0.68675	0.66980	0.65544	0.66541	0.64454	0.62755	0.71885
45.00	0.69535	0.67481	0.65799	0.64370	0.65320	0.63259	0.61576	0.70631
50.00	0.68460	0.66421	0.64747	0.63324	0.64239	0.62199	0.60529	0.69522
60.00	0.66614	0.64598	0.62937	0.61521	0.62393	0.60382	0.58732	0.67626
70.00	0.65063	0.63065	0.61412	0.60003	0.60854	0.58863	0.57225	0.66041
80.00	0.63732	0.61743	0.60097	0.58692	0.59529	0.57555	0.55927	0.64679
90.00	0.62564	0.60581	0.58939	0.57538	0.58369	0.56407	0.54789	0.63486
100.00	0.61523	0.59546	0.57910	0.56513	0.57338	0.55386	0.53774	0.62417
120.00	0.59726	0.57760	0.56131	0.54739	0.55567	0.53630	0.52029	0.60577
140.00	0.58210	0.56251	0.54625	0.53237	0.54078	0.52154	0.50562	0.59038
160.00	0.56908	0.54955	0.53334	0.51948	0.52796	0.50882	0.49298	0.57692
180.00	0.55754	0.53805	0.52187	0.50804	0.51671	0.49765	0.48189	0.56530
200.00	0.54734	0.52789	0.51173	0.49791	0.50669	0.48771	0.47202	0.55473
250.00	0.52566	0.50628	0.49019	0.47646	0.48561	0.46680	0.45126	0.53282
300.00	0.50803	0.48873	0.47273	0.45908	0.46853	0.44987	0.43446	0.51502
350.00	0.49317	0.47395	0.45803	0.44447	0.45420	0.43567	0.42038	0.50011
400.00	0.48040	0.46125	0.44540	0.43192	0.44187	0.42347	0.40828	0.48720
500.00	0.45909	0.44013	0.42445	0.41111	0.42146	0.40327	0.38828	0.46589
600.00	0.44189	0.42306	0.40751	0.39431	0.40496	0.38696	0.37214	0.44854
700.00	0.42742	0.40874	0.39332	0.38023	0.39115	0.37332	0.35864	0.43402
800.00	0.41499	0.39643	0.38113	0.36815	0.37929	0.36161	0.34707	0.42151
900.00	0.40410	0.38566	0.37047	0.35758	0.36892	0.35138	0.33695	0.41054
1000.00	0.39442	0.37609	0.36099	0.34819	0.35971	0.34230	0.32799	0.40078
1200.00	0.37780	0.35967	0.34476	0.33212	0.34394	0.32675	0.31264	0.38403
1400.00	0.36390	0.34595	0.33120	0.31870	0.33077	0.31379	0.29986	0.37001
1600.00	0.35197	0.33419	0.31958	0.30721	0.31949	0.30269	0.28892	0.35798
1800.00	0.34154	0.32391	0.30943	0.29718	0.30965	0.29301	0.27939	0.34745
2000.00	0.33229	0.31480	0.30044	0.28830	0.30092	0.28444	0.27095	0.33810
2200.00	0.32398	0.30662	0.29237	0.28033	0.29310	0.27676	0.26340	0.32971
2500.00	0.31294	0.29575	0.28166	0.26976	0.28272	0.26658	0.25338	0.31855

Distribution

EXTERNAL

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