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The normal mode, x, corresponds to an alternate expansion and contraction of the molecule without distortion. From the group theory point of view the displacement x is an eigenvector for the A_1 representation of the symmetry group C_{3v}. The normal modes y and z correspond to distortions of the molecule in which one angle remains 60° while one side is lengthened and the other shortened. They belong to the doubly degenerate E representation. In the special case of the equilateral triangle with equal masses, we see that the normal modes of vibration are independent of the values of the force constants. Substituting x, y and z into the Routh function, we easily obtain the equations of motion and from them the vibration frequencies:

$$\nu_x = \frac{1}{2\pi}\left(\frac{3(k_1+k_2)}{m_H}\right)^{\frac{1}{2}}, \quad \nu_y = \nu_z = \frac{1}{2\pi}\left(\frac{3(k_1-k_2)}{2m_H}\right)^{\frac{1}{2}}. \tag{50}$$

The real test whether or not the H_3^+ ion is an equilateral triangle would be a determination of its vibration spectrum. If H_3^+ has only two fundamental frequencies (ν_x and $\nu_y = \nu_z$) it is equilateral. If the degeneracy is removed, it is in some other configuration.

The force constants should be evaluated in the following manner. First set $\Delta\phi = 0$ and let $\Delta r_{ab} = \Delta r_{bc} = \Delta r$. Then $V = V_0 + (\frac{1}{2})(3k_1 + 6k_2)(\Delta r)^2$. This variation corresponds to Fig. 2. Second, we keep $\Delta r_{ab} = \Delta r_{bc} = 0$ and vary $\Delta\phi$. In this case,

$$V = V_0 + (\tfrac{1}{2})\frac{3r^2}{4}k_1(\Delta\phi)^2.$$

This variation of the potential energy with the angle is given in Fig. 4. Unfortunately, our calculations of the variation with angle is not sufficiently accurate for this purpose but as closely as we can tell, $k_2 = 0$ (agreeing with the central force approximation) and $k_1 = 4.8 \times 10^4$. From these force constants, it follows that

$$\nu_x = 1550 \text{ cm}^{-1}, \qquad \nu_y = \nu_z = 1100 \text{ cm}^{-1} \tag{51}$$

and the zero point energy of H_3^+ is

$$(\tfrac{1}{2})h\nu_x + (\tfrac{1}{2})h\nu_y + (\tfrac{1}{2})h\nu_z = 5.4 \text{ kcal.} \tag{52}$$

The z and y modes of vibration should be infra-red active and therefore susceptible to direct experimental observation.

Integrals Required for Computing the Energy of H_3 and of H_3^+

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Some of the difficult integrals required for the variational method calculation of the energy of the triatomic hydrogen molecule and positive ion were evaluated with the aid of the differential analyzer. The integral $\int_0^\pi \exp(-B(1 - A\cos\theta)^{\frac{1}{2}})d\theta$ is tabulated for a complete range of the parameters, A and B. The integral $K(c, ab) = (1/\pi)\int r_c^{-1}\exp(-r_a - r_b)d\tau$ is tabulated for many configurations of the three electrons or nuclei: a, b, and c. Numerical tables are given of all of the integrals occurring in the Sugiura treatment of the ground state of H_2. The values of all of the other integrals used in the calculation of the energy of H_3 and of H_3^+ are given. It is expected that these tables will be useful for many problems of molecular quantum mechanics.

THE success of a variational method calculation depends on the ability to evaluate the definite integrals which arise. At the present time we are very much limited in the types of charge distributions which we can consider because of the difficulties of integration. Machines such as the differential analyzer at the Moore School of Engineering at Philadelphia and at the Massachusetts Institute of Technology at Cambridge, make it possible to integrate with ease certain functions which would be extraordinarily difficult to handle by the more orthodox mathematical methods. In this work on the triatomic hydrogen ion and molecule we required the evaluation of a two-parameter family of definite integrals which were quite unmanageable from any analytical point of view. In a period of two weeks work on the differential analyzer, we were able to evaluate these integrals for over 200 values of the parameters with an accuracy which was well within the limits required for our present purposes. This shows that the differential analyzer can be used to good advantage in molecular quantum mechanics and should be extremely useful in improving the charge distributions which have been used heretofore.

The two integrals $L(aa, bc)$ and $L(ab, ac)$ (see Eqs. (27) and (28) of preceding article) were the ones which required special consideration. The integrations over the coordinates of the first electron gives:

$$L(aa, bc) = K(a, bc) - T(a, bc), \qquad (1)$$

where

$$T(a, bc) = \frac{1}{\pi} \int e^{-2r_{a2}-r_{b2}-r_{c2}} \left[1 + \frac{1}{r_{a2}} \right] d\tau \qquad (2)$$

and $K(a, bc)$ is defined as

$$K(a, bc) = \frac{1}{\pi} \int \frac{1}{r_a} e^{-r_b-r_c} d\tau. \qquad (3)$$

Similarly integrating $L(ab, bc)$ over the coordinates of the first electron,

$$L(ab, bc) = \frac{1}{\pi} \int K(2, ab) e^{-r_{b2}-r_{c2}} d\tau_2. \qquad (4)$$

Here,

$$K(2, ab) = \frac{1}{\pi} \int \frac{1}{r_{12}} e^{-r_{a1}-r_{b1}} d\tau_1. \qquad (5)$$

TABLE I. $K(c, ab) = (1/\pi) \int r_c^{-1} \exp(-r_a - r_b) d\tau = K_0(R, x) + \mu^2 K_2(R, x)$ where $x = R(\lambda - 1)/2$.

$K_0(R, x)$

x	$R=1.0$	$R=1.5$	$R=2.0$	$R=2.5$	$R=3.0$	$R=4.0$	$R=5.0$	$R=6.0$	$R=8.0$	$R=12.0$
0.0	.78245 5391	.61627 6976	.46460 541	.33941 6318	.24216 665	.11708 805	.05391 823	.02399 5317	.00443 1661	.00012 79176
0.25			.41379 6561	.30096 1124	.21413 066					
0.50	.63770 6403	.49354 2942	.36833 08	.26748 2122	.19017 84	.09168 849	.04221 922	.01881 202	.00348 8202	.00010 158319
0.75	.57007 1472	.44052 3495	.32867 1972	.23876 8881	.16880 800					
1.00	.50968 6841	.39424 0636	.29456 15	.21432 7444	.15273 62	.07399 680	.03423 458	.01532 147	.00286 2951	.00008 437508
1.25				.19357 4804						
1.50	.41156 9661	.32021 7155	.24058 18	.17593 8601	.12595 40	.06150 429	.02864 126	.01288 899	.00242 9807	.00007 250517
2.00	.33926 0520	.26602 4077	.20122 34	.14802 1433	.10651 15	.05245 363	.02459 248	.01112 862	.00211 6220	.00006 389365
2.25			.18559 96							
2.50		.22599 9	.17207 89	.12729 907						
2.75			.16030 65							
3.00	.24608 9478	.19583 1135	.14999 0	.11151 9340	.08099 023	.04049 475	.01921 476	.00878 053	.00169 5143	.00005 222460
4.00	.19154 9414	.15412 2753	.11916 05	.08931 7112	.06532 490	.03304 682	.01582 820	.00728 889	.00142 4175	.00004 459231
6.00	.13237 041	.10796 6230	.08447 10	.06398 0646	.04723 073	.02427 394	.01177 849	.00548 359	.00109 0301	.00003 497475
8.00			.06548 55		.03705 70	.01923 701	.00941 434	.00441 531	.00088 8598	.00002 900735

$-K_2(R, x)$

x	$R=1.0$	$R=1.5$	$R=2.0$	$R=2.5$	$R=3.0$	$R=4.0$	$R=5.0$	$R=6.0$	$R=8.0$	$R=12.0$
0.0	.04669 6505	.05845 1574	.05859 957	.05211 8824	.04301 838	.02550 986	.01349 055	.00664 4052	.00141 2498	.00004 80428
0.25			.03955 2640	.03586 8080	.03007 5405					
0.50	.01950 5634	.02599 0962	.02730 9	.02520 9253	.02145 2	.01334 46	.00731 673	.00370 893	.00082 3802	.00002 96750
0.75	.01316 441	.01798 054	.01927 291	.01808 583	.01560 513					
1.00	.00911 2644	.01272 4932	.01389 08	.01323 6898	.01157 15	.00751 69	.00426 372	.00222 115	.00051 4415	.00001 95827
1.25				.00987 6067						
1.50	.00468 0411	.00679 2965	.00766 05	.00750 4961	.00671 92	.00453 865	.00265 483	.00141 807	.00034 1352	.00001 36764
2.00	.00261 3074	.00391 8596	.00454 5	.00456 0118	.00416 87	.00291 44	.00175 21	.00095 705	.00023 8500	.00001 00063
2.25			.00358 71							
2.50		.00241 92	.00287 29	.00294 28						
2.75			.00233 28							
3.00	.00100 2710	.00158 2296	.00191 5	.00199 8320	.00188 84	.00139 55	.00087 717	.00049 705	.00013 1185	.00000 594563
4.00	.00047 472	.00077 620	.00096 88	.00103 8792	.00100 55	.00077 358	.00050 285	.00029 295	.00008 0793	.00000 388900
6.00	.00015 764	.00026 809	.00034 1	.00038 5637	.00038 61	.00031 22	.00021 223	.00012 847	.00003 7715	.00000 198486
8.00			.00016 2		.00018 84	.00015 71	.00010 959	.00006 803	.00002 0821	.00000 116630

The expression for $K(2, ab)$ was given in closed form in a previous paper,[1] but it requires considerable work to evaluate it for any particular configuration. This integral is required for many problems in molecular quantum mechanics and the tabulation of it, in Table I should be useful. The integration over the coordinates of the second electron in $T(a, bc)$ and $L(ab, bc)$ could not be carried out in closed form when the nuclei were fixed in a triangular configuration, and the rest of the integrations proceeded numerically. Introducing ellipsoidal coordinates with foci at a and at b:

$$d\tau_2 = (R_{ab}^3/8)(\lambda^2 - \mu^2)d\theta d\mu d\lambda,$$

$$r_{a2} = (R_{ab}/2)(\lambda + \mu), \quad r_{b2} = (R_{ab}/2)(\lambda - \mu),$$

$$r_{c2} = \frac{R_{ab}}{2}[(\lambda^2 + \mu^2 - 6\mu\lambda + 8) \quad (6)$$
$$+ 8(\sin^2 \phi/2)(\mu\lambda - 1) - 8\cos\theta\cos\phi/2$$
$$\times |\sin\phi/2|((\lambda^2-1)(1-\mu^2))^{\frac{1}{2}}]^{\frac{1}{2}}$$

where ϕ is defined as the angle abc. When a, b, c are in a line, $\phi = 0$ and for the equilateral triangle $\phi = 2\pi/3$. Thus in $T(a, bc)$ and $L(ab, bc)$ for the equilateral triangle:

$$r_{c2} = \frac{R_{ab}}{2}[(\lambda^2 + \mu^2 + 2)$$
$$- 2\sqrt{3}((\lambda^2-1)(1-\mu^2))^{\frac{1}{2}}\cos\theta]^{\frac{1}{2}}. \quad (7)$$

Now it is only in r_{c2} that the angle of rotation about the line a–b appears in these integrals.

[1] C. A. Coulson, Proc. Comb. Phil. Soc. **34**, 204 (1938).

The integration over θ has the form:

$$Q = \int_0^\pi \exp[-B(1-A\cos\theta)^{\frac{1}{2}}]d\theta, \quad (8)$$

where A and B are functions of λ and of μ. For a satisfactory numerical evaluation of $T(a, bc)$ and of $L(ab, bc)$ it is necessary to carry through the above integrations for a great many values of the parameters. A careful study of the function Q showed that it was a new type of transcendental function having some of the characteristics of Bessel functions and some properties of elliptical integrals. For small values of A an expansion of the integrand into a power series in $\cos\theta$ is useful, but for larger values of A this series does not converge sufficiently rapidly, if it converges at all. This family of integrals was evaluated on the differential analyzer of the Moore School of Electrical Engineering, in the following manner. The $(1-A\cos\theta)^{\frac{1}{2}}$ was plotted on a large sheet of graph paper for ten values of A. These curves were fed into the machine manually. A gear ratio multiplied them by the factor B. One integrater formed the exponential $\exp(-B(1-A\cos\theta)^{\frac{1}{2}}$ as the solution to a first-order differential equation. A second integrater performed the final integration over θ. The indefinite integral was obtained as a by-product and we should like to know some applications for it. Table II shows the values of the definite integrals which were obtained on the machine. These values will be useful in computing many of the exchange

TABLE II. $Q(A, B) = \int_0^\pi \exp[-B(1-A\cos\theta)^{\frac{1}{2}}]d\theta$.

A	$B=.5$	$B=1.0$	$B=1.5$	$B=2.0$	$B=2.25$	$B=2.44141$	$B=2.60417$	$B=2.88$	$B=3.0$	$B=3.33333$
1.0	2.0549	1.4146	1.0249	.7804	.6917	.6342	.5907	.5311	.5072	.4533
.95	2.0236	1.3555	.9456	.6853	.5907	.5292	.4838	.4183	.3937	.3349
.90	2.0053	1.3232	.9026	.6354	.5395	.4784	.4313	.3657	.3407	.2831
.80	1.9769	1.2753	.8412	.5687	.4706	.4088	.3642	.2994	.2752	.2199
.70	1.9583	1.2380	.8007	.5251	.4278	.3664	.3222	.2592	.2359	.1833
.60	1.9423	1.2168	.7705	.4948	.3974	.3371	.2932	.2322	.2098	.1593
.50	1.9283	1.1938	.7461	.4696	.3734	.3144	.2711	.2123	.1905	.1419
.40	1.9202	1.1800	.7291	.4531	.3576	.2983	.2560	.1980	.1780	.1300
.30	1.9124	1.1683	.7162	.4395	.3446	.2866	.2453	.1877	.1675	.12177
.20	1.9091	1.1615	.7076	.4315	.3372	.2793	.2377	.1809	.1611	.11613
.10				.4280					.1577	

A	$B=3.75$	$B=4.26667$	$B=5.33333$	$B=6.0$	$B=7.5$	$B=8.53333$	$B=10.0$	$B=12.0$	$B=13.33333$	$B=20.0$
1.0	.3993	.3484	.2727	.2423	.2031		.1501	.1231	.11136	.0740
.95	.2780	.2252	.1488	.1160	.07221		.03515			
.90	.2266	.1742	.1057	.07797	.04185		.015818			
.80	.1658	.1200	.06401	.04376	.01929		.005166			
.70	.1346	.09256	.04383	.02821	.01067	.005624				
.60	.1134	.07512	.03286	.01984	.006612	.003201				
.50	.09874	.06333	.02580	.01489	.004453					
.40	.08809	.05554	.02128	.011815	.003205					
.30	.08162	.05002	.01831	.009827	.002466					
.20	.07726	.04662	.01648	.008649	.002031					
.10										

integrals which arise in molecular quantum mechanics as well as in entirely different applications which we cannot foresee at the present time. For large values of B, the value of Q decreases inversely proportionally to B when A is unity and exponentially with B when A is small.

Using the values of Q computed on the differential analyzer, we evaluated the integrands of $T(a, bc)$ and of $L(ab, bc)$ for 230 values of λ and of μ for each nuclear configuration. The problem was then reduced to one of a double numerical integration. This numerical integration was carried out analytically. It has been the experience of practical workers such as the Statistical Laboratory at Edinburgh that greater accuracy can be obtained with less work in this way than by the use of graphical methods. Interpolation formulae were developed for fitting cubics to successive sequences of four points. These interpolation formulae were then integrated over the central segment of the regions which they fit and the total value of the integral was obtained by adding up all of these sub-integrals. Thus the integration of $T(a, bc)$ and of $L(ab, bc)$ over μ gives:

$$\int_{-1}^{1} I(\lambda, \mu) d\mu = \sum_i G(\mu_i) I(\lambda, \mu_i), \qquad (9)$$

where I is the value of the corresponding integrands and the $G(\mu_i)$ are numbers corresponding to the particular values of μ where the integrand was evaluated. For the values of μ_i which we considered $G(\mu) = G(-\mu)$ and:

$G(1.0)$	$= .018229,$	$G(.95)$	$= .046626,$
$G(.9)$	$= .069791,$	$G(.8)$	$= .165104,$
$G(.6)$	$= .165178,$	$G(.5)$	$= .086111,$
$G(.4)$	$= .098958,$	$G(.3)$	$= .100833,$
$G(.2)$	$= .099479,$	$G(.1)$	$= .084375,$
$G(.05)$	$= .040833,$	$G(0.0)$	$= .048958.$

These G's may be thought of as the coefficients in an improved Simpson's rule. The integration over λ (or $x = (\frac{1}{2})R(\lambda - 1)$) required even more care than that over μ because there were less points at which we knew the value of the function. Then too, the integration over λ or x is extended to infinity whereas the integration over μ is over finite limits. In the region between $x = 0$ and $x = 1$, the integrand of $L(ab, bc)$ passes through a flat maximum and looks like a parabola. Throughout this region, the integrand is fitted by cubics passing through sequences of four points and only the central segment of each

region is integrated. From $x = 1$ to infinity, the integrand of $L(ab, bc)$ behaves very nearly as $\exp(-1.5 x)$. For this reason we multiplied the integrand by $\exp(1.5 x)$ and fit cubics to every successive sequence of four points, multiplied these approximating cubics by $\exp(-1.5 x)$ and integrated over the central section of the region fitted. Adding up all of the sub-integrals, we obtained the value of $L(ab, bc)$:

$$L(ab, bc) = \frac{R^2}{4\pi} \sum_{i, j} k(x_j) G(\mu_i) l(x_j, \mu_i), \qquad (10)$$

where $l(x_j, u_1)$ is the value of

$$(\lambda^2 - \mu^2) K(2, ab) e^{-rb2} \int_0^{2\pi} e^{-rc2} d\theta$$

when $\lambda = 1 + 2x_j/R$ and $\mu = \mu_i$. For the values of x_j which we considered, the $k(x_j)$ are:

$k(0)$	$= .08333333,$	$k(.25)$	$= .32291667,$
$k(.50)$	$= .20572917,$	$k(1.0)$	$= .35858510,$
$k(1.5)$	$= .51497398,$	$k(2.0)$	$= .66439253,$
$k(4.0)$	$= 1.11010116,$	$k(6.0)$	$= 3.02627612,$
$k(.75)$	$= .24851861,$	$k(3.0)$	$= 1.17182926.$

Similarly, an improved Simpson's rule was obtained for the integration of $T(a, bc)$ over x. For this purpose we observe that the integrand of $T(a, bc)$ decreases as $\exp(-3.5 x)$ so that our best curve fitting is obtained by multiplying the integrand through by $\exp(3.5 x)$ and fitting cubics to successive sequences of four points, then these cubics are multiplied by $\exp(-3.5 x)$ and integrated over the central section of the region fitted. Adding up all of these sub-integrals we finally obtain for the value of $T(a, bc)$:

$$T(a, bc) = \frac{R^2}{4\pi} \sum_{i, j} p(x_j) G(\mu_1) t(x_j, \mu_1), \qquad (11)$$

where $t(x_j, \mu_1)$ is the value of

$$(\lambda^2 - \mu^2) e^{-2r_{a2} - rb2} \left[1 + \frac{1}{r_{a2}}\right] \int_0^{2\pi} e^{-rc2} d\theta$$

for the configuration of electron 2 corresponding to x_j, μ_1. Here the $p(x_j)$'s were the numbers:

$p(0)$	$= .0715969,$	$p(.25)$	$= .3874184,$
$p(.50)$	$= .0904707,$	$p(1.0)$	$= .4167317,$
$p(1.5)$	$= .4094224,$	$p(2.0)$	$= .7813404,$
$p(.75)$	$= .2956447,$	$p(3.0)$	$= 1.243573.$

It is interesting to note the differences in the values of the $k(x_j)$ from the corresponding $p(x_j)$ which are due to the difference in the method of curve fitting. If $l(x_j, u_1)$ were exactly a cubic from $x = 0$ to $x = 1$ and a cubic times $\exp(-1.5 x)$

TABLE III.

R/a_0	$I(R)$	$J(R)$	$G(R)$	$L(aa, bb)$	$L(ab, ab)$	$L(aa, ab)$
1.0	.85838 53627	.73575 88e^2/a_0	.72932 94e^2/a_0	.55452 13e^2/a_0	.43665 1e^2/a_0	.50704 485
1.5	.72517 30203	.55782 55	.58368 82	.49033 75	.29683 5	.40536 896
2.0	.58645 28938	.40600 59	.47252 65	.42597 43	.18415 6	.30803 646
2.5	.45830 79088	.28729 75	.39056 69	.36838 78	.10662 2	.22559 548
3.0	.34850 948	.19914 83	.33002 83	.31980 35	.05850 83	.16074 246
4.0	.18926 160	.09157 820	.24958 067	.24755 392	.01562 72	.07698 167
5.0	.09657 7238	.04042 768	.19994 552	.19956 908	.00371 704	.03495 3043
6.0	.04709 6292	.01735 126	.16665 949	.16659 267	.00081 4027	.01531 1456
8.0	.01017 5699	.00301 91637	.12499 987	.12499 7955	.00003 28959	.00273 87379
12.0	.00037 47970	.00007 9874761	.08333 333	.08333 3331	.00000 00354836	.00007 4658581

$$I(R) = \frac{1}{\pi} \int \exp(-r_a - r_b) d\tau \qquad L(aa, bb) = \frac{1}{\pi^2} \int\int \frac{1}{r_{12}} \exp(-2r_{a1} - 2r_{b2}) d\tau_1 d\tau_2$$

$$J(R) = \frac{1}{\pi} \int \frac{1}{r_a} \exp(-r_a - r_b) d\tau \qquad L(ab, ab) = \frac{1}{\pi^2} \int\int \frac{1}{r_{12}} \exp(-r_{a1} - r_{b1} - r_{a2} - r_{b2}) d\tau_1 d\tau_2$$

$$G(R) = \frac{1}{\pi} \int \frac{1}{r_a} \exp(-2r_b) d\tau \qquad L(aa, ab) = \frac{1}{\pi^2} \int\int \frac{1}{r_{12}} \exp(-2r_{a1} - r_{a2} - r_{b2}) d\tau_1 d\tau_2.$$

from $x=1$ to infinity, the $k(x_j)$'s would make (62) exactly true. Similarly, if $t(x_j, u_1)$ were really a cubic times $\exp(-3.5 x)$, the $p(x_j)$ would make (63) exactly true. So it is evident that the method of curve fitting makes a considerable amount of difference in the result which we obtain. The careless use of interpolation formulae could easily result in an error of one to two percent in the final answer. We believe that our method of integration should give the values of the integrals to within a half of one percent.

In this way we obtained the values for the equilateral triangular configuration:

R/a_0	$L(ab, bc)$	$L(aa, bc)$	$K(a, bc)$
2.0	.169845 e^2a_0	.258356 e^2/a_0	.294562 e^2/a_0
2.5	.095383	.177685	.193575
3.0	.050862	.119193	.125954

Comparing the values of $L(aa, bc)$ with the corresponding $K(a, bc)$ we see that the difference $T(a, bc)$, is small and therefore requires less accuracy in the computations than does the $L(ab, bc)$. The last two figures of $L(ab, bc)$ and of $L(aa, bc)$ are probably not significant. These integrals are given in units of e^2/a_0 or 627.4 kcal. per mole so that an error of 0.001 (which is certainly larger than any which we have made in these computations) would still give the values of these integrals to within 0.6 kcal. and would be sufficiently accurate for the purposes of this problem.

The other integrals which occur in this problem are integrals involving the distances of the electrons to only two nuclei. These integrals arise in a consideration of H_2 as well as in the triatomic molecule and ion. In spite of the fact that they have been used in many computations, we do not believe that they have ever been published in a tabular form. Table III gives the values of these integrals for many internuclear separations, R.

Next, we wish to discuss the dependence of the three center integrals on the angle between the nuclei. For the internuclear separation corresponding to $R = 2.0$, Stevenson and Hirschfelder[2] have computed the second derivatives of the integrals with respect to the angle of bending, ϕ. In addition, we know the values of the integrals for $\phi = 0$, i.e., when the three nuclei are in a line; the values for $\phi = \pi$, when nucleus a coincides with nucleus c to make these integrals equal to the two center integrals which we have tabulated; and the values for $\phi = 2\pi/3$, which is the equilateral triangle model which we have just been considering. With these four pieces of information we can express the angle dependence of the integrals in the form:

$$L = L_0 + L_1 \cos \phi + L_2 \cos^2 \phi + L_3 \cos^3 \phi$$

and evaluate the four constants L_0, L_1, L_2, L_3 to agree with the facts at our disposal. Thus or $R = 2.0 \, a_0$

$L(ab, bc) = .155966 - .025373 \cos \phi$
$\qquad + .006715 \cos^2 \phi + .003898 \cos^3 \phi,$
$L(ab, ac) = .098042 - .094281 \cos \phi$
$\qquad + .081583 \cos^2 \phi - .034130 \cos^3 \phi,$
$L(bb, ac) = .165902 - .128456 \cos \phi$
$\qquad + .094192 \cos^2 \phi - .037424 \cos^3 \phi,$
$L(aa, bc) = .225658 - .052216 \cos \phi$
$\qquad + .022556 \cos^2 \phi - .007606 \cos^3 \phi.$

For $R = 2.5$ and $R = 3.0$, we do not know the derivatives of ϕ as we depart from a straight line, but from the values of the integrals for $\phi = 0$, π, and $2\pi/3$ we could evaluate three constants.