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THE BERYLLIUM MOLECULE

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Abstract

The interaction of a normal Be atom with one which has an electronic configuration $2s2p$ has been studied by means of the Heitler-London method. Of the eight possible molecular states, two are calculated to be stable, namely ${}^1\Sigma A^N$ and ${}^1\Pi A^N$, and the ${}^1\Sigma$ state is the lower of the two. An attempt to obtain agreement with experiment in the case where a normal Li atom interacts with one in the $2p\,{}^2P$ state has not been successful, at least for the resulting Π states.

ONE cannot regard the problem of chemical valence as solved until the approximate validity of a few simple rules of wide applicability has been established by methods based on the quantum mechanics. Even for a diatomic molecule, where one must study the motion of a system of several elections in a field of two centers, no very powerful methods have as yet been developed, so that the degree of success to date is hardly commensurate with the effort expended.

One of the simplest cases, that of the interaction of two normal hydrogen atoms, has been studied by Heitler and London,[1] Sugiura,[2] Wang,[3] and Hylleraas.[4] For the heat of dissociation, Sugiura obtained 3.0 volts and Wang 3.6 volts, as compared with the experimental value of 4.4 volts. The preliminary work of Hylleraas still showed a discrepancy of 0.5 volt, and there appeared to be no convenient way to diminish this. However, Hylleraas was able to give an estimate of upper and lower limits to the heat of dissociation value. If one starts with an unperturbed system of two electrons moving independently of each other in a field of two centers, and introduces the electrostatic interaction between the two electrons as a perturbation, then it is possible to calculate the electronic energy as a function of the distance (leaving aside the $2/R$ term). The exact values for $R=0$ and $R=\infty$, respectively, are -5.8072 and -2.000. The values calculated with the above method are -5.6817 and -1.3932. The values found from the variation method are -5.6953 and -2.000. The assumption is made that the ratio of exact energy to the approximate value is a monotonic function of R. Accordingly, if we multiply values from the "separation" method by $5.8072/5.6817$, we shall find an upper limit for the electronic energy, and if we multiply values from the variation method by $5.8072/5.6953$, then we shall obtain a lower limit. The heat of dissociation then comes out to be $D=(4.37\pm 0.12)$ volts. This renders the assumption of monotone character plausible, but does not, of course, prove it.

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[1] W. Heitler u. F. London, Zeits. f. Physik **44**, 455 (1927).

[2] Y. Sugiura, Zeits. f. Physik **45**, 484 (1927).

[3] S. C. Wang, Phys. Rev. **31**, 579 (1928).

[4] E. Hylleraas, Zeits. f. Physik **71**, 739 (1931).

The status of the matter at present, then, is that there still remains at least 0.5 volt discrepancy between experimental and theoretical value. This agreement is not good, and apparently the only way to improve it is to employ a method similar to that used by Hylleraas[5] for helium, where the wave function contains as one of its arguments the distance between the two electrons.

Kemble and Zener,[6] and Zener and Guillemin[7] have attempted to calculate the heats of dissociation for some of the two-quantum states of the hydrogen molecule, and were unable to get good quantitative results. The first two writers considered only the Π states, assuming that most of the other states would be repulsive in character. This work thus gives us only limited information concerning the relative positions of the resulting energy levels. In the later paper,[7] it was shown how the earlier calculations of Sugiura could be simplified, but the quantitative results were not in good agreement with experiment. Hylleraas,[4] with the two-center wave functions as the unperturbed ones, has been able to improve on these results considerably. He obtains as heats of dissociation of the $p^1\Pi$, $p^3\Pi$ and $p^1\Sigma$ states the values 2.197 volts, 2.655 volts, and 3.185 volts, respectively, as against the experimental values 2.27, 2.84 and 3.37. The method breaks down for the $s\Sigma$ states, which probably need special consideration.

The present work was practically completed before the results of Hylleraas became known, and was based on the idea that though good quantitative agreement was not to be expected from the Heitler-London method, still the method should be capable of giving correctly the relative positions of the molecular energy levels. For small separations, however, one cannot hope for good results. If one wishes accuracy, then the procedure of Hylleraas should be adopted.

Since the atomic wave functions of Zener[8] gave good quantitative results[9] for Li_2, they will be used in the following calculations. When there are but two electrons on each atom, one can calculate rather readily the relative positions of the resulting energy levels. The mutual influence of the K-shells may be neglected, as Delbrück has shown[10] and so it is possible to ascertain whether or not beryllium molecules are stable. We have already shown[9] that two normal beryllium atoms repel each other, and shall now find out what happens when a normal beryllium atom interacts with one in the first excited state $(2s2p)$.

INTERACTION OF A NORMAL BE ATOM WITH AN EXCITED BE ATOM

Notation. For the most part, the notation will be that previously used.[8] However, to secure greater generality, some modifications must be made.[11] The wave function of electron 1 referred to nucleus a may now be written

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[5] E. A. Hylleraas, Zeits. f. Physik **54,** 347 (1929).

[6] E. C. Kemble and C. Zener, Phys. Rev. **33,** 512 (1929).

[7] C. Zener and V. Guillemin, Phys. Rev. **34,** 999 (1929).

[8] C. Zener, Phys. Rev. **36,** 51 (1930).

[9] J. H. Bartlett, Jr. and W. H. Furry, Phys. Rev. **38,** 1615 (1931).

[10] M. Delbrück, Ann. d. Physik **5,** 36 (1930).

[11] J. H. Bartlett, Jr., Phys. Rev. **37,** 507 (1931). The signs of i_5, i_6, and i_7 should be reversed. This means that on p. 530 the rôles of $^1\Pi$ and $^3\Pi$ will be interchanged.

$a_{\alpha n_1}(1)$ or $a_{\beta n_1}(1)$ where α and β denote the spin orientation and n_1 the orbital orientation.

Let

$$J(n_1n_2;\ n_3n_4) = \int H' a_{n_1}{}^*(1) a_{n_2}(1) b_{n_3}{}^*(2) b_{n_4}(2) dv$$

$$J'(n_1n_2;\ n_3n_4) = \int H' a_{n_1}{}^*(1) b_{n_2}(1) a_{n_3}(2) b_{n_4}{}^*(2) dv$$

$$J_a''(n_1n_2;\ n_3n_4) = \int H' a_{n_1}{}^*(1) a_{n_2}(1) a_{n_3}{}^*(2) b_{n_4}(2) dv$$

$$J_b''(n_1n_2;\ n_3n_4) = \int H' b_{n_1}{}^*(1) b_{n_2}(1) b_{n_3}{}^*(2) a_{n_4}(2) dv$$

$$S^{1/2}_{n_1n_2} = \int a_{n_1}{}^*(1) b_{n_2}(1) dv_1$$

$$S_{n_1n_2,n_3n_4} = S^{1/2}_{n_1n_2} S^{1/2}_{n_3n_4}.$$

The H' is to operate on the unstarred functions, and since the form of H' depends on the functions on which it operates, it follows that the order of the arguments in these integrals may not in general be changed without altering the values of the integral. For example,

$$J_a''(n_1n_2;\ n_3n_4) \neq J_a''(n_1n_2;\ n_4n_3).$$

The same is true for the S integrals, i.e., $S_{n1n2}{}^{1/2} \mp S_{n2n1}{}^{1/2}$, in general.

Instead of n_1n_2 etc., it proves convenient to use the letters s and p, where p takes on the value 0 or 1, according to the value of the magnetic quantum number. With this notation, one finds $S_{s0}{}^{1/2} = -S_{0s}{}^{1/2}$, illustrating the rule above. A further relation is that $J_a'' = (-)^m J_b''$, if m denotes the number of zeros occurring among the arguments n_1, n_2, n_3, n_4.

As before, small letters j, j', and j'' will refer to the contribution from the $(2/r)$ part of H' to the total integral.

If we define

$$I_a(n_1n_2) = \int a_{n_1}{}^* a_{n_2} (2/b) dv$$

$$I_b(n_1n_2) = \int b_{n_1}{}^* b_{n_2} (2/a) dv$$

$$I_a'(n_1n_2) = \int a_{n_1}{}^* b_{n_2} (2/b) dv$$

$$I_b'(n_1n_2) = \int a_{n_1}{}^* b_{n_2} (2/a) dv$$

then

$$J(n_1n_2;\ n_3n_4) = (2/R)\delta_{n_1n_2}\delta_{n_3n_4} + j(n_1n_2;\ n_3n_4)$$
$$- \delta_{n_1n_2} I_b(n_3n_4) - I_a(n_1n_2)\delta_{n_3n}$$

$$\begin{aligned} J'(n_1n_2;\, n_3n_4) &= (2/R)S_{n_1n_2,n_3n_4} + j'(n_1n_2;\, n_3n_4) \\ &\quad - S^{1/2}_{n_1n_2} I_a'(n_3n_4) - I_b'(n_1n_2)S^{1/2}_{n_3n_4} \\ J_a''(n_1n_2;\, n_3n_4) &= (2/R)\delta_{n_1n_2}S^{1/2}_{n_3n_4} + j_a''(n_1n_2;\, n_3n_4) \\ &\quad - \delta_{n_1n_2} I_b'(n_3n_4) - I_a(n_1n_2)S^{1/2}_{n_3n}. \end{aligned}$$

In particular,

$$\begin{aligned} I_a(s0) &= -\, I_b(s0) \\ I_a'(s0) &= -\, I_b'(0s) \\ I_a'(0s) &= -\, I_b'(s0) \\ I_a'(00) &= I_b'(00). \end{aligned}$$

Calculation of the energies. As unperturbed wave functions, we take

$$\begin{aligned} \Psi_1 &= (1/24)^{1/2} \sum_P (-)^{\sigma_P} P\{a_{\alpha p}(1)a_{\beta s}(2)b_{\alpha s}(3)b_{\beta s}(4)\} \\ \Psi_2 &= (1/24)^{1/2} \sum_P (-)^{\sigma_P} P\{a_{\alpha s}(1)a_{\beta p}(2)b_{\alpha s}(3)b_{\beta s}(4)\} \\ \Psi_3 &= (1/24)^{1/2} \sum_P (-)^{\sigma_P} P\{a_{\alpha s}(1)a_{\beta s}(2)b_{\alpha p}(3)b_{\beta s}(4)\} \\ \Psi_4 &= (1/24)^{1/2} \sum_P (-)^{\sigma_P} P\{a_{\alpha s}(1)a_{\beta s}(2)b_{\alpha s}(3)b_{\beta p}(4)\}. \end{aligned}$$

Here P denotes a permutation of the numbers (1234), and σ_P its order.

There will result, from the combination $(2s)^2$ and $2s2p$, states of Σ and Π types, of singlet or triplet character, and either symmetrical or antisymmetrical in the nuclei (S^N or A^N). That is, eight states are possible.

Forming linear combinations of the above functions, we obtain

$$\begin{aligned} u_1 &= \Psi_1 + \Psi_2 + \Psi_3 + \Psi_4 \quad (S^E\, S^N) \\ u_2 &= \Psi_1 - \Psi_2 + \Psi_3 - \Psi_4 \quad (A^E\, S^N) \\ u_3 &= \Psi_1 + \Psi_2 - \Psi_3 - \Psi_4 \quad (S^E\, A^N) \\ u_4 &= \Psi_1 - \Psi_2 - \Psi_3 + \Psi_4 \quad (A^E\, A^N). \end{aligned}$$

The symmetry types are indicated, S^E denoting a singlet, and A^E a triplet.

The energy is

$$E = \frac{\int u^* H u dv}{\int u^* u dv}$$

where

$$H = -\sum_{i=1}^{4} \Delta_i + (8/R) - \sum_{i=1}^{4}\left(\frac{4}{a_i} + \frac{4}{b_i}\right) + \sum_{i<j} 2/r_{ij}.$$

It is seen that H is symmetrical in the nuclei and in the electrons. Now let

$$H_{ij} = \int \Psi_i^* H \Psi_j dv$$

$$N_{ij} = \int \Psi_i^* \Psi_j dv.$$

The functions Ψ_1, Ψ_2, Ψ_3, and Ψ_4 are connected with each other by the transpositions $(\alpha\beta)$ and (ab).

$$(\alpha\beta)\Psi_1 = \Psi_2 \qquad (ab)\Psi_1 = \Psi_3 \qquad (\alpha\beta)(ab)\Psi_1 = \Psi_4$$

Accordingly

$$\begin{aligned} H_{11} &= H_{22} = H_{33} = H_{44} \\ H_{12} &= H_{21} = H_{34} = H_{43} \\ H_{13} &= H_{31} = H_{24} = H_{42} \\ H_{14} &= H_{41} = H_{23} = H_{32}. \end{aligned}$$

Similar relations hold for the N_{ij}'s.

As before H may be broken up into two parts, an unperturbed operator H_0 and a perturbing term H', the actual form of the H' depending upon the function upon which it operates. The unperturbed energy will depend only upon the symmetry in the electrons, so that for S^E, $H_0 u = E_a u$, and for A^E, $H_0 u = E_b u$, where $E_a - E_b$ equals the energy difference between the two levels ${}^1P$ and ${}^3P$ in the beryllium atom.

The energies are then:

$$\begin{aligned} E_1 &= E_a + (H_{11}' + H_{12}' + H_{13}' + H_{14}')/(N_{11} + N_{12} + N_{13} + N_{14}) \\ E_2 &= E_b + (H_{11}' - H_{12}' + H_{13}' - H_{14}')/(N_{11} - N_{12} + N_{13} - N_{14}) \\ E_3 &= E_a + (H_{11}' + H_{12}' - H_{13}' - H_{14}')/(N_{11} + N_{12} - N_{13} - N_{14}) \\ E_4 &= E_b + (H_{11}' - H_{12}' - H_{13}' + H_{14}')/(N_{11} - N_{12} - N_{13} + N_{14}). \end{aligned}$$

We may write

$$H_{ij} = \int \sum_P (-)^{\sigma P} [P a_{\alpha n_1}(1) a_{\beta n_2}(2) b_{\alpha n_3}(3) b_{\beta n_4}(4)]^* H \cdot [a_{\alpha n_1'}(1) a_{\beta n_2'}(2) b_{\alpha n_3'}(3) b_{\beta n_4}(4)] dv$$

and

$$H = H_0 + H'(14) + H'(24) + H'(13) + H'(23)$$

where

$$H'(kl) = (2/R) - (2/b_k) - (2/a_l) + (2/r_{kl})$$

$$\begin{aligned} H_{ij}'(13) &= (\delta_{n_2 n_2'} \delta_{n_4 n_4'} - S_{n_2' n_4, n_2 n_4'}) \{ J(n_1 n_1'; n_3 n_3') - J'(n_1 n_3'; n_1' n_3) \} \\ H_{ij}'(24) &= (\delta_{n_1 n_1'} \delta_{n_3 n_3'} - S_{n_1' n_3, n_1 n_3'}) \{ J(n_2 n_2'; n_4 n_4') - J'(n_2 n_4'; n_2' n_4) \} \\ H_{ij}'(14) &= \delta_{n_2 n_2'} \delta_{n_3 n_3'} J(n_1 n_1'; n_4 n_4') - \delta_{n_2 n_2'} S^{1/2}_{n_1 n_3'} J_b''(n_4 n_4'; n_3 n_1') \\ &\quad - \delta_{n_3 n_3'} S^{1/2}_{n_2' n_4} J_a''(n_1 n_1'; n_2 n_4') + S_{n_2' n_4, n_1 n_3'} J'(n_2 n_4'; n_1' n_3) \\ H_{ij}'(23) &= \delta_{n_1 n_1'} \delta_{n_4 n_4'} J(n_2 n_2'; n_3 n_3') - \delta_{n_1 n_1'} S^{1/2}_{n_2 n_4'} J_b''(n_3 n_3'; n_4 n_2') \\ &\quad - \delta_{n_4 n_4'} S^{1/2}_{n_1' n_3} J_a''(n_2 n_2'; n_1 n_3') + S_{n_1' n_3, n_2 n_4'} J'(n_1 n_3'; n_2' n_4). \end{aligned}$$

Let us calculate H'_{11}, H'_{21}, H'_{31}, and H'_{41}. For all these quantities $(n_1'n_2'n_3'n_4') = (psss)$.

For

$$\begin{aligned} H'_{11},\ (n_1n_2n_3n_4) &= (psss) \\ H'_{21},\ (n_1n_2n_3n_4) &= (spss) \\ H'_{31},\ (n_1n_2n_3n_4) &= (ssps) \\ H'_{41},\ (n_1n_2n_3n_4) &= (sssp) \end{aligned}$$

$$\begin{aligned} H_{11}'(13) &= (1 - S_{ss})\{J(pp;\ ss) - J'(ps;\ ps)\} \\ H_{21}'(13) &= \quad - S_{ss,ps}\{J(sp;\ ss) - J'(ss;\ ps)\} \\ H_{31}'(13) &= (1 - S_{ss})\{J(sp;\ ps) - J'(ss;\ pp)\} \\ H_{41}'(13) &= \quad S_{sp,ss}\{J(sp;\ ss) - J'(ss;\ ps)\} \\ H_{11}'(24) &= (1 - S_{ps})\{J(ss;\ ss) - J'(ss;\ ss)\} \\ H_{21}'(24) &= - S_{ps,ss}\{J(ps;\ ss) - J'(ps;\ ss)\} \\ H_{31}'(24) &= - S_{pp,ss}\{J(ss;\ ss) - J'(ss;\ ss)\} \\ H_{41}'(24) &= - S_{ps,ss}\{J(ss;\ ps) - J'(ss;\ sp)\} \end{aligned}$$

$$\begin{aligned} H_{11}'(14) &= J(pp;\ ss) - S_{ps}^{1/2}J_b''(ss;\ sp) - S_{ss}^{1/2}J_a''(pp;\ ss) + S_{ss,ps}J'(ss;\ ps) \\ H_{21}'(14) &= \qquad - S_{ss}^{1/2}J_a''(sp;\ ps) + S_{ss}J'(ps;\ ps) \\ H_{31}'(14) &= \qquad - S_{ss}^{1/2}J_b''(ss;\ pp) \qquad + S_{ss}J'(ss;\ pp) \\ H_{41}'(14) &= J(sp;\ ps) - S_{ss}^{1/2}J_b''(ps;\ sp) - S_{sp}^{1/2}J_a''(sp;\ ss) + S_{sp,ss}J'(ss;\ ps) \\ H_{11}'(23) &= J(ss;\ ss) - S_{ss}^{1/2}J_b''(ss;\ ss) - S_{ps}^{1/2}J_a''(ss;\ ps) + S_{ps,ss}J'(ps;\ ss) \\ H_{21}'(23) &= \qquad - S_{ps}^{1/2}J_a''(ps;\ ss) + S_{ps,ps}J'(ss;\ ss) \\ H_{31}'(23) &= \qquad - S_{pp}^{1/2}J_a''(ss;\ ss) + S_{pp,ss}J'(ss;\ ss) \\ H_{41}'(23) &= \qquad + S_{ps,ss}J'(ss;\ sp). \end{aligned}$$

For the terms in the denominators we have

$$\begin{aligned} N_{ij} &= \int \sum_P (-)^{\sigma P}[Pa_{\alpha n_1}(1)a_{\beta n_2}(2)b_{\alpha n_3}(3)b_{\beta n_4}(4)]^* \cdot a_{\alpha n_1'}(1)a_{\beta n_2'}(2)b_{\alpha n_3'}(3)b_{\beta n_4'}(4)dv \\ &= (\delta_{n_1n_1'}\delta_{n_3n_3'} - S_{n_1n_3',n_1'n_3})(\delta_{n_2n_2'}\delta_{n_4n_4'} - S_{n_2n_4',n_2'n_4}) \end{aligned}$$

$$\begin{aligned} N_{11} &= (1 - S_{ps})(1 - S_{ss}) \\ N_{21} &= S_{ss,ps} \cdot S_{ss,ps} = S_{ps} \cdot S_{ss} \\ N_{31} &= - S_{ss,pp}(1 - S_{ss}) \\ N_{41} &= S_{ss,ps} \cdot S_{ss,sp}. \end{aligned}$$

Three typical integrals will now be evaluated, and the others just tabulated.

$$\text{I.}\qquad j(s0;s0) = c^2 c_2^2 \int (2/r) a_1^2 b_2^2 \cos\theta_{a_1} \cos\theta_{b_2} e^{-\kappa(a_1+b_2)} dv_1 dv_2 .$$

If $(2/r)$ is expanded in terms of b_1, b_2, and P_n $(\cos\gamma)$, then one can integrate over dv_2, obtaining

$$j(s0;s0) = (8\pi c^2 c_2^2/3\kappa^4) \int a^2 \cos\theta_a \cos\theta_b \{\gamma_6(\kappa b)/(\kappa b)^2 + (\kappa b)\Gamma_3(\kappa b)\} \cdot e^{-\kappa a} dv .$$

This may be divided into two parts; one is conveniently integrated in the (a, b) coördinate system, while the (λ, μ) system is more suitable for the other. No difficulty is encountered, for the integrands do not give infinite contributions at any points of the regions involved. The result is:

$$\begin{aligned} j(s0;s0) = {} & (1/72)(\alpha/2)^3\kappa\{80[-240/\alpha^6 + 2A_5 + A_2] - 15(2A_0 + 14A_2/3) \\ & + 15(\alpha/2)(2A_3 + 2A_1) - (15/2)(\alpha/2)^2[-8A_2/5 + (\tfrac{2}{3})(A_4 - A_0)] \\ & - (9/4)(\alpha/2)^3[-12A_3/5 + (\tfrac{2}{3})(A_5 + A_1)] \\ & - (\tfrac{3}{8})(\alpha/2)^4[2A_6/3 - 14A_4/5 + 34A_2/21 - 2A_0/5]\}_{(1,\alpha)} \end{aligned}$$

$$\text{II.}\qquad j'(ss;s0) = c^3 c_2 \int (2/r) a_1 b_1 a_2 b_2 \cos\theta_{b_2} e^{-(\kappa/2)(a_1+a_2+b_1+b_2)} dv_{12} .$$

For the j' and j'' integrals, we make use of the Neumann expansion. The calculation was facilitated by grouping certain terms together. New symbols were introduced, definited as given below.

$$\begin{aligned} v_0(m,n,\alpha) &= \int_1^\infty \int_1^\infty Q_0\begin{pmatrix}\lambda_2\\ \lambda_1\end{pmatrix} \lambda_1^m \lambda_2^n e^{-(\alpha/2)(\lambda_1+\lambda_2)} d\lambda_1 d\lambda_2 \\ &= s_0(m,n,\alpha) + s_0(n,m,\alpha) \\ v_1(m,n,\alpha) &= \int_1^\infty \int_1^\infty Q_1\begin{pmatrix}\lambda_2\\ \lambda_1\end{pmatrix} P_1\begin{pmatrix}\lambda_1\\ \lambda_2\end{pmatrix} \lambda_1^m \lambda_2^n e^{-(\alpha/2)(\lambda_1+\lambda_2)} d\lambda_1 d\lambda_2 \\ &= s_1(m,n+1,\alpha) + s_1(n,m+1,\alpha) \\ v_2(m,n,\alpha) &= \int_1^\infty \int_1^\infty Q_2\begin{pmatrix}\lambda_2\\ \lambda_1\end{pmatrix} P_2\begin{pmatrix}\lambda_1\\ \lambda_2\end{pmatrix} \lambda_1^m \lambda_2^n e^{-(\alpha/2)(\lambda_1+\lambda_2)} d\lambda_1 d\lambda_2 \\ &= (3/2)s_2(m,n+2) - (\tfrac{1}{2})s_2(m,n) + (3/2)s_2(n,m+2) - (\tfrac{1}{2})s_2(n,m) \\ w_1(m,n,\alpha) &= \int_1^\infty \int_1^\infty \frac{dQ_1}{d\lambda}\begin{pmatrix}\lambda_2\\ \lambda_1\end{pmatrix} (\lambda_1^2-1)(\lambda_2^2-1)\lambda_1^m \lambda_2^n e^{-(\alpha/2)(\lambda_1+\lambda_2)} d\lambda_1 \lambda_2 d \end{aligned}$$

$$
\begin{aligned}
&= s_1(m+1, n+2) + s_1(n+1, m+2) - s_1(m+1, n) \\
&\quad - s_1(n+1, m) - s_0(m, n+2) - s_0(n, m+2) + s_0(m, n) \\
&\quad + s_0(n, m)
\end{aligned}
$$

$$
\begin{aligned}
w_2(m, n, \alpha) &= \int_1^\infty \int_1^\infty \frac{dQ_2}{d\lambda}\binom{\lambda_2}{\lambda_1} \frac{dP_2}{d\lambda}\binom{\lambda_1}{\lambda_2} \\
&\qquad (\lambda_1^2 - 1)(\lambda_2^2 - 1)\lambda_1^m \lambda_2^n e^{-(\alpha/2)(\lambda_1+\lambda_2)} d\lambda_1 d\lambda_2 \\
&= 6\{s_2(m+1, n+3) + s_2(n+1, m+3) - s_2(m+1, n+1) \\
&\quad - s_2(n+1, m+1) - s_1(m, n+3) - s_1(n, m+3) + s_1(m, n+1) \\
&\quad + s_1(n, m+1)\}
\end{aligned}
$$

$$
\begin{aligned}
\{\mathrm{I}, n\}_0 &= v_0(4, n) - (\tfrac{2}{3})v_0(2, n) + (\tfrac{1}{5})v_0(0, n) \\
\{\mathrm{II}, m, n\}_0 &= v_0(m, n) - (\tfrac{1}{5})v_0(m-2, n) \\
\{\mathrm{III}, n\}_0 &= (\tfrac{1}{3})v_0(4, n) - (6/5)v_0(2, n) + (\tfrac{1}{3})v_0(0, n) \\
\{\mathrm{I}, n\}_1 &= v_1(4, n) - (8/5)v_1(2, n) + (3/5)v_1(0, n) \\
\{\mathrm{II}, n\}_1 &= w_1(3, n) - (\tfrac{1}{5})w_1(1, n) \\
\{\mathrm{I}, n\}_2 &= (\tfrac{1}{3})v_2(2, n) - (1/7)v_2(0, n) \\
\{\mathrm{II}, m, n\}_2 &= v_2(m, n) + (1/7)v_2(m-2, n) \\
\{\mathrm{III}, n\}_2 &= (\tfrac{1}{3})v_2(4, n) - (2/7)v_2(2, n) + (\tfrac{1}{3})v_2(0, n) \\
\{\mathrm{IV}, n\}_2 &= (\tfrac{1}{3})w_2(2, n) - (1/7)w_2(0, n) \\
C_n(\alpha) &= (3/2)B_{n+2}(\alpha) - (\tfrac{1}{2})B_n(\alpha).
\end{aligned}
$$

With these symbols it becomes easy to write the resulting expressions for the integrals in question. For $\tau = 0$.

$$
\begin{aligned}
j'(ss; s0)^{(0)} &= (2\pi)^2 c^3 c_2 \int (2/r)(\lambda_1^2 - \mu_1^2)(\lambda_2 + \mu_2)(\lambda_2\mu_2 - 1)(R/2)^{10} \\
&\qquad e^{-\alpha(\lambda_1+\lambda_2)/2}(\lambda_1^2 - \mu_1^2)(\lambda_2^2 - \mu_2^2) d\lambda_1 d\lambda_2 d\mu_1 d\mu_2 \\
&= -\kappa(3^{1/2}/432)(\alpha/2)^9[\{\mathrm{I}, 3\}_0 - (\tfrac{1}{5})\{\mathrm{I}, 1\}_0]
\end{aligned}
$$

For $\tau = 2$,

$$
j'(ss; s0)^{(2)} = -\kappa(3^{1/2}/540)(\alpha/2)^9[\{\mathrm{I}, 3\}_2 + (\tfrac{1}{7})\{\mathrm{I}, 1\}_2]
$$

$$
\text{III. } j_a''(s0; ss) = c^3 c_2 \int (2/r) a_1^2 e^{-\kappa a_1} \cos\theta_{a_1} e^{-\kappa(a_2+b_2)/2} a_2 b_2 dv
$$

$$
\begin{aligned}
j_a''(s0; ss)^{(0)} &= \kappa(3^{1/2}/576)(\alpha/2)^9[B_1\{\mathrm{I}, 4\}_0 + (B_2 + B_0)\{\mathrm{I}, 3\}_0 \\
&\quad + (B_1 - B_3)\{\mathrm{I}, 2\}_0 - (B_4 + B_2)\{\mathrm{I}, 1\}_0 - B_3\{\mathrm{I}, 0\}_0] \\
j_a''(s0; ss)^{(1)} &= 0 \\
j_a''(s0; ss)^{(2)} &= -\kappa(3^{1/2}/144)(\alpha/2)^9[C_1\{\mathrm{I}, 4\}_2 + (C_2 + C_0)\{\mathrm{I}, 3\}_2 \\
&\quad + (C_1 - C_3)\{\mathrm{I}, 2\}_2 - (C_4 + C_2)\{\mathrm{I}, 1\}_2 - C_3\{\mathrm{I}, 0\}_2].
\end{aligned}
$$

The j'' integrals could be calculated directly without recourse to the Neumann expansion, but the formulation is much more awkward and does not enable one to obtain the result with reasonable speed. Both methods were used for $j''\ (ss;\, ss)$, giving results almost exactly the same, which indicated that the expansion converges rapidly. For the other integrals of this type a method due to Dr. A. S. Coolidge could be applied; it was used to calculate the values at $\alpha=3$ of those j'' integrals not having 1 as an argument, and a check was obtained in every case. This method consists of expanding functions referred to one atom in spherical harmonics of the other atom.[12]

The list of j, j', and j'' integrals follows.

$$
\begin{aligned}
p &= 0: \\
j(ss;\, ss) &= j \\
j(ss;\, s0) &= -I_a(s0) + \kappa(3^{1/2}/288)(\alpha/2)^4[24\{5A_2/3 + A_0/3\} \\
&\quad + 18(\alpha/2)\{4A_3/3 - 8A_1/15\} + 6(\alpha/2)^2\{A_4 - 2A_2/3 + A_0/5\} \\
&\quad + (\alpha/2)^3\{2A_5/3 - 4A_3/15 + 2A_1/35\}]_{(1,\alpha)} \\
j(ss;\, 00) &= (2i_3/3) + (i_9/3) = (k/192)\mathrm{II}c \\
j(s0;\, s0) &= \text{expression already given.} \\
j'(ss;\, ss) &= k \\
j'(ss;\, s0)^{(0)} &= \text{expression already given} \\
j'(ss;\, s0)^{(2)} &= \text{expression already given} \\
j'(ss;\, 00)^{(0)} &= (\kappa/96)(\alpha/2)^9[(\tfrac{1}{3})\{\mathrm{I}, 4\}_0 - (6/5)\{\mathrm{I}, 2\}_0 + (\tfrac{1}{3})\{\mathrm{I}, 0\}_0] \\
j'(ss;\, 00)^{(2)} &= -(\kappa/60)(\alpha/2)^9[(\tfrac{1}{3})\{\mathrm{III}, 2\}_2 - (1/7)\{\mathrm{III}, 0\}_2] \\
j'(s0;\, s0)^{(0)} &= +(\kappa/216)(\alpha/2)^9[\{\mathrm{II}, 3, 3\}_0 - (\tfrac{1}{5})\{\mathrm{II}, 3, 1\}_0] \\
j'(s0;\, s0)^{(1)} &= (\kappa/288)(\alpha/2)^9[\{\mathrm{I}, 4\}_1 - (8/5)\{\mathrm{I}, 2\}_1 + (3/5)\{\mathrm{I}, 0\}_1] \\
j'(s0;\, s0)^{(2)} &= (\kappa/1080)(\alpha/2)^9[\{\mathrm{II}, 3, 3\}_2 + (1/7)\{\mathrm{II}, 3, 1\}_2] \\
j''(ss;\, ss) &= j'' \\
j_a''(ss;\, s0)^{(0)} &= -\kappa(3^{1/2}/864)(\alpha/2)^9[B_0\{\mathrm{II}, 3, 4\}_0 + 2B_1\{\mathrm{II}, 3, 3\}_0 \\
&\quad - 2B_3\{\mathrm{II}, 3, 1\}_0 - B_4\{\mathrm{II}, 3, 0\}_0] \\
j_a''(ss;\, s0)^{(1)} &= \kappa(3^{1/2}/576)(\alpha/2)^9[B_1\{\mathrm{I}, 4\}_1 + 2B_2\{\mathrm{I}, 3\}_1 - 2B_4\{\mathrm{I}, 1\}_1 \\
&\quad - B_5\{\mathrm{I}, 0\}_1] \\
j_a''(ss;\, s0)^{(2)} &= \kappa(3^{1/2}/864)(\alpha/2)^9[C_0\{\mathrm{II}, 3, 4\}_2 + 2C_1\{\mathrm{II}, 3, 3\}_2 - 2C_3\{\mathrm{II}, 3, 1\}_2 \\
&\quad - C_4\{\mathrm{II}, 3, 0\}_2] \\
j''(ss;\, 00)^{(0)} &= (\kappa/192)(\alpha/2)^9[B_0\{\mathrm{III}, 4\}_0 + 2B_1\{\mathrm{III}, 3\}_0 - 2B_3\{\mathrm{III}, 1\}_0 \\
&\quad - B_4\{\mathrm{III}, 0\}_0]
\end{aligned}
$$

---

[12] We appreciate greatly the courtesy of Dr. Coolidge (Harvard University) in making us acquainted with his expansion method before publication.

$$\begin{aligned} j''(ss;\,00)^{(2)} &= (\kappa/96)(\alpha/2)^9[C_0\{\mathrm{III},4\}_2 + 2C_1\{\mathrm{III},3\}_2 - 2C_3\{\mathrm{III},1\}_2 \\ &\quad - C_4\{\mathrm{III},0\}_2] \end{aligned}$$

$$j_a''(ss;0s)^{(0)} = -\,j_a''(ss;\,s0)^{(0)} \qquad j''(s0;\,0s)^{(0)} = -\,j''(s0;\,s0)^{(0)}$$

$$j_a''(ss;0s)^{(1)} = j_a''(ss;\,s0)^{(1)} \qquad j''(s0;\,0s)^{(1)} = j''(s0;\,s0)^{(1)}$$

$$j_a''(ss;0s)^{(2)} = -\,j_a''(ss;\,s0)^{(2)} \qquad j''(s0;\,0s)^{(2)} = -\,j''(s0;\,s0)^{(2)}$$

$$\begin{aligned} j''(s0;\,s0)^{(0)} &= -\,(\kappa/288)(\alpha/2)^9[B_1\{\mathrm{II},3,4\}_0 + (B_2 + B_0)\{\mathrm{II},3,3\}_0 \\ &\quad + (B_1 - B_3)\{\mathrm{II},3,2\}_0 - (B_4 + B_2)\{\mathrm{II},3,1\}_0 - B_3\{\mathrm{II},3,0\}_0] \end{aligned}$$

$$\begin{aligned} j''(s0;\,s0)^{(1)} &= (\kappa/192)(\alpha/2)^9[B_2\{\mathrm{I},4\}_1 + (B_3 + B_1)\{\mathrm{I},3\}_1 + (B_2 - B_4)\}\mathrm{I},2\}_1 \\ &\quad - (B_5 + B_3)\{\mathrm{I},1\}_1 - B_4\{\mathrm{I},0\}_1] \end{aligned}$$

$$\begin{aligned} j''(s0;\,s0)^{(2)} &= (\kappa/288)(\alpha/2)^9[C_1\{\mathrm{II},3,4\}_2 + (C_2 + C_0)\{\mathrm{II},3,3\}_2 \\ &\quad + (C_1 - C_3)\{\mathrm{II},3,2\}_2 - (C_4 + C_2)\{\mathrm{II},3,1\}_2 - C_3\{\mathrm{II},3,0\}_2] \end{aligned}$$

$j_a''(s0;ss)^{(0)}$ = expression already given.

$j_a''(s0;ss)^{(2)}$ = expression already given.

$$\begin{aligned} j''(00;\,ss)^{(0)} &= (\kappa/192)(\alpha/2)^9[B_2\{\mathrm{I},4\}_0 + 2B_1\{\mathrm{I},3\}_0 + (B_0 - B_4)\{\mathrm{I},2\}_0 \\ &\quad - 2B_3\{\mathrm{I},1\}_0 - B_2\{\mathrm{I},0\}_0] \end{aligned}$$

$$\begin{aligned} j''(00;\,ss)^{(2)} &= -\,(\kappa/48)(\alpha/2)^9[C_2\{\mathrm{I},4\}_2 + 2C_1\{\mathrm{I},3\}_2 + (C_0 - C_4)\{\mathrm{I},2\}_2 \\ &\quad - 2C_3\{\mathrm{I},1\}_2 - C_2\{\mathrm{I},0\}_2] \end{aligned}$$

$$p = 1;$$

$$j(ss;\,11) = (2i_1/3) + (i_3/3) = (\kappa/384)Ic$$

$$\begin{aligned} j(s1;\,s1) &= (\kappa/1152)[(160/\alpha)\{(120/\alpha^2) + \alpha^4(A_2 - A_5)\} \\ &\quad - 320(\alpha/2)^3\cdot(A_0 - A_2) - 120(\alpha/2)^4(4A_3 - 4A_1) \\ &\quad - 60(\alpha/2)^5\cdot\{(4/3)(A_4 - A_2) + (4/15)(A_2 - A_0)\} \\ &\quad - 18(\alpha/2)^6\cdot\{(4/3)(A_5 - A_3) - (4/15)(A_3 - A_1)\} \\ &\quad - 3(\alpha/2)^7\cdot\{(4/3)(A_5 - A_4) - (8/15)(A_4 - A_2) + (4/35)(A_2 - A_0)\}]_{(1,\alpha)} \end{aligned}$$

$$j'(ss;\,11)^{(0)} = (\kappa/288)(\alpha/2)^9[\{\mathrm{I},4\}_0 - (6/5)\{\mathrm{I},2\}_0 + (\tfrac{1}{5})\{\mathrm{I},0\}_0]$$

$$j'(ss;\,11)^{(2)} = (\kappa/360)(\alpha/2)^9[\{\mathrm{I},4\}_2 - (6/7)\{\mathrm{I},2\}_2 - (1/7)\{\mathrm{I},0\}_2]$$

$$j'(s1;\,s1)^{(1)} = -\,(\kappa/576)(\alpha/2)^9[\{\mathrm{II},3\}_1 - (\tfrac{1}{5})\{\mathrm{II},1\}_1]$$

$$j'(s1;\,s1)^{(2)} = -\,(\kappa/960)(\alpha/2)^9[(\tfrac{1}{3})\{\mathrm{IV},2\}_2 - (1/7)\{\mathrm{IV},0\}_2]$$

$$\begin{aligned} j''(ss;\,11)^{(0)} &= (\kappa/576)(\alpha/2)^9[B_0(\{\mathrm{II},4,4\}_0 - \{\mathrm{II},2,4\}_0) \\ &\quad + 2B_1(\{\mathrm{II},4,3\}_0 - \{\mathrm{II},2,3\}_0) \\ &\quad - 2B_3(\{\mathrm{II},4,1\}_0 - \{\mathrm{II},2,1\}_0) - B_4(\{\mathrm{II},4,0\}_0 - \{\mathrm{II},2,0\}_0)] \end{aligned}$$

$$
\begin{aligned}
j''(ss;\,11)^{(2)} &= -(\kappa/576)(\alpha/2)^9[C_0(\{\mathrm{II},4,4\}_2-\{\mathrm{II},2,4\}_2)\\
&\quad +2C_1(\{\mathrm{II},4,3\}_2-\{\mathrm{II},2,3\}_2)\\
&\quad -2C_3(\{\mathrm{II},4,1\}_2-\{\mathrm{II},2,1\}_2)-C_4(\{\mathrm{II},4,0\}_2-\{\mathrm{II},2,0\}_2)]\\
j''(1s;\,s1)^{(1)} &= -(\kappa/768)(\alpha/2)^9[(B_0-B_2)\{\mathrm{II},3\}_1+(B_1-B_3)\{\mathrm{II},2\}_1\\
&\quad -(B_2-B_4)\{\mathrm{II},1\}_1-(B_3-B_5)\{\mathrm{II},0\}_1]\\
j''(1s;\,s1)^{(2)} &= -(\kappa/768)(\alpha/2)^9[(B_1-B_3)\{\mathrm{IV},3\}_2+(B_2-B_4)\{\mathrm{IV},2\}_2\\
&\quad -(B_3-B_5)\{\mathrm{IV},\mathrm{I}\}_2-(B_4-B_6)\{\mathrm{IV},0\}_2]\\
j''(s1;\,1s)^{(1)} &= j''(1s;\,s1)^{(1)} \qquad j''(s1;\,1s)^{(2)} = -j''(1s;\,s1)^{(2)}\\
j''(11;\,ss)^{(0)} &= (\kappa/384)(\alpha/2)^9[(B_0-B_2)(\{\mathrm{I},4\}_0-\{\mathrm{I},2\}_0)\\
&\quad -(B_2-B_4)(\{\mathrm{I},2\}_0-\{\mathrm{I},0\}_0)]\\
j''(11;\,ss)^{(2)} &= -(\kappa/96)(\alpha/2)^9[(C_0-C_2)(\{\mathrm{I},4\}_2-\{\mathrm{I},2\}_2)\\
&\quad -(C_2-C_4)(\{\mathrm{I},2\}_2-\{\mathrm{I},0\}_2)].
\end{aligned}
$$

In calculating the $s_\tau(m,n,\alpha)$ use was made of the following formulas in addition to those previously given.[11]

$$
\begin{aligned}
s_\tau(m,\,n+1,\,\alpha) &= (2/\alpha)(n+1)s_\tau(m,\,n,\,\alpha)+f_\tau(m,\,\alpha/2)A_0(1,\,\alpha/2)\\
&\quad -\sigma_\tau(m+n+1,\,0,\,\alpha)\\
s_2(m,\,n,\,\alpha) &= (3/2)s_1(m+1,\,n,\,\alpha)-(\tfrac{1}{2})s_0(m,\,n,\,\alpha).
\end{aligned}
$$

The following tables contain such necessary s_τ as have not been published previously. We then proceed to tabulate the resulting values of the integrals.

TABLE I. $s_0(m,\ n,\ \alpha)$.

α	$\alpha=3$	4	5	6	7	8	9	10
$s_0(0,1,\alpha)$	$0.0^{2}952$	$0.0^{2}2161$	$0.0^{3}547$	$0.0^{3}1481$	$0.0^{4}420$	$0.0^{4}1234$	$0.0^{5}3718$	$0.0^{5}1145$
$s_0(0,3,\alpha)$	0.01775	$0.0^{2}345$	$0.0^{3}793$	$0.0^{3}2019$	$0.0^{4}547$	$0.0^{4}1555$	$0.0^{5}457$	$0.0^{5}1375$
$s_0(0,5,\alpha)$	0.0449	$0.0^{2}672$	$0.0^{2}1310$	$0.0^{3}303$	$0.0^{4}764$	$0.0^{4}207$	$0.0^{5}582$	$0.0^{5}1715$
$s_0(0.6,\alpha)$	0.0832	0.01042	$0.0^{2}1800$	$0.0^{3}389$	$0.0^{4}937$	$0.0^{4}246$	$0.0^{5}670$	$0.0^{5}1952$
$s_0(1,0,\alpha)$	0.012998	$0.0^{2}2801$	$0.0^{3}6833$	$0.0^{3}1801$	$0.0^{4}5004$	$0.0^{4}1445$	$0.0^{5}430$	$0.0^{5}1307$
$s_0(1,1,\alpha)$	0.01708	$0.0^{2}3458$	$0.0^{3}8105$	$0.0^{3}2081$	$0.0^{4}5666$	$0.0^{4}1611$	$0.0^{5}474$	$0.0^{5}1427$
$s_0(1,2,\alpha)$	0.02381	$0.0^{2}4431$	$0.0^{3}986$	$0.0^{3}2447$	$0.0^{4}651$	$0.0^{4}1818$	$0.0^{5}527$	$0.0^{5}1570$
$s_0(1,3,\alpha)$	0.0358	$0.0^{2}5953$	$0.0^{2}1239$	$0.0^{3}2947$	$0.0^{4}760$	$0.0^{4}2078$	$0.0^{5}593$	$0.0^{5}1743$
$s_0(1,4,\alpha)$	0.0590	$0.0^{2}848$	$0.0^{2}1619$	$0.0^{3}3647$	$0.0^{4}907$	$0.0^{4}2413$	$0.0^{5}675$	$0.0^{5}1954$
$s_0(1,5,\alpha)$	0.1082	0.01301	$0.0^{2}222$	$0.0^{3}467$	$0.0^{3}1111$	$0.0^{4}2856$	$0.0^{5}780$	$0.0^{5}222$
$s_0(1,6,\alpha)$	0.225	0.0218	$0.0^{2}322$	$0.0^{3}625$	$0.0^{3}1401$	$0.0^{4}346$	$0.0^{5}918$	$0.0^{5}255$
$s_0(2,1,\alpha)$	0.03442	$0.0^{2}6019$	$0.0^{2}1281$	$0.0^{3}3073$	$0.0^{4}796$	$0.0^{4}2176$	$0.0^{5}6201$	$0.0^{5}1823$
$s_0(2,3,\alpha)$	0.0816	0.01126	$0.0^{2}2078$	$0.0^{3}4548$	$0.0^{3}1103$	$0.0^{4}2881$	$0.0^{5}793$	$0.0^{5}2266$
$s_0(2,5,\alpha)$	0.295	0.0279	$0.0^{2}408$	$0.0^{3}770$	$0.0^{3}1688$	$0.0^{4}411$	$0.0^{4}1074$	$0.0^{5}295$
$s_0(2,6,\alpha)$	0.673	0.0504	$0.0^{2}627$	$0.0^{2}1074$	$0.0^{3}2200$	$0.0^{4}510$	$0.0^{4}1287$	$0.0^{5}345$
$s_0(3,0,\alpha)$	0.05535	$0.0^{2}883$	$0.0^{2}1764$	$0.0^{3}4039$	$0.0^{3}1011$	$0.0^{4}2687$	$0.0^{5}749$	$0.0^{5}2164$
$s_0(3,1,\alpha)$	0.07936	0.01158	$0.0^{2}2188$	$0.0^{3}4825$	$0.0^{3}1176$	$0.0^{4}3062$	$0.0^{5}840$	$0.0^{5}2398$
$s_0(3,2,\alpha)$	0.1237	0.01603	$0.0^{2}2815$	$0.0^{3}5913$	$0.0^{3}1395$	$0.0^{4}3542$	$0.0^{5}954$	$0.0^{5}2684$
$s_0(3,3,\alpha)$	0.2136	0.02370	$0.0^{2}3786$	$0.0^{3}749$	$0.0^{3}1693$	$0.0^{4}4173$	$0.0^{4}1098$	$0.0^{5}3036$
$s_0(3,4,\alpha)$	0.4150	0.03801	$0.0^{2}5381$	$0.0^{3}985$	$0.0^{3}2115$	$0.0^{4}5024$	$0.0^{4}1287$	$0.0^{5}349$
$s_0(3,5,\alpha)$	0.916	0.0669	$0.0^{2}817$	$0.0^{2}1365$	$0.0^{3}2740$	$0.0^{4}6205$	$0.0^{4}1538$	$0.0^{5}406$
$s_0(3,6,\alpha)$	2.300	0.1305	0.01336	$0.0^{2}1983$	$0.0^{3}370$	$0.0^{4}791$	$0.0^{4}1881$	$0.0^{5}483$
$s_0(4,1,\alpha)$	0.2122	0.02502	$0.0^{2}4089$	$0.0^{3}8137$	$0.0^{3}1835$	$0.0^{4}4516$	$0.0^{4}1184$	$0.0^{5}3257$
$s_0(4,3,\alpha)$	0.6422	0.0559	$0.0^{2}7562$	$0.0^{2}1330$	$0.0^{3}2747$	$0.0^{4}635$	$0.0^{4}1589$	$0.0^{5}421$
$s_0(4,5,\alpha)$	3.218	0.1782	0.01798	$0.0^{2}2602$	$0.0^{3}470$	$0.0^{4}987$	$0.0^{4}2304$	$0.0^{5}580$
$s_0(4,6,\alpha)$	8.77	0.373	0.03121	$0.0^{2}398$	$0.0^{3}657$	$0.0^{3}1293$	$0.0^{4}2886$	$0.0^{5}702$

TABLE II. $s_1\ (m,\ n,\ \alpha)$.

α	$\alpha=3$	4	5	6	7	8	9	10
$s_1(0,0,\alpha)$	$0.0^{2}1936$	$0.0^{3}513$	$0.0^{3}1445$	$0.0^{4}4240$	$0.0^{4}1283$	$0.0^{5}3963$	$0.0^{5}1248$	$0.0^{6}3990$
$s_1(0,1,\alpha)$	$0.0^{2}2339$	$0.0^{3}597$	$0.0^{3}1641$	$0.0^{4}4730$	$0.0^{4}1412$	$0.0^{5}4319$	$0.0^{5}1349$	$0.0^{6}4279$
$s_1(0,2,\alpha)$	$0.0^{2}2930$	$0.0^{3}711$	$0.0^{3}1895$	$0.0^{4}5337$	$0.0^{4}1569$	$0.0^{5}4743$	$0.0^{5}1468$	$0.0^{6}4625$
$s_1(0,3,\alpha)$	$0.0^{2}3849$	$0.0^{3}874$	$0.0^{3}2233$	$0.0^{4}6122$	$0.0^{4}1766$	$0.0^{5}5258$	$0.0^{5}1609$	$0.0^{6}5028$
$s_1(0,4,\alpha)$	$0.0^{2}5385$	$0.0^{2}1117$	$0.0^{3}2705$	$0.0^{4}7151$	$0.0^{4}2015$	$0.0^{5}5891$	$0.0^{5}1778$	$0.0^{6}5495$
$s_1(0,5,\alpha)$	$0.0^{2}819$	$0.0^{2}1503$	$0.0^{3}3387$	$0.0^{4}854$	$0.0^{4}2336$	$0.0^{5}6685$	$0.0^{5}1985$	$0.0^{6}6068$
$s_1(0,6,\alpha)$	0.01392	$0.0^{2}2167$	$0.0^{3}4433$	$0.0^{3}1050$	$0.0^{4}2768$	$0.0^{5}7704$	$0.0^{5}2245$	$0.0^{6}658$
$s_1(1,1,\alpha)$	$0.0^{2}3695$	$0.0^{3}868$	$0.0^{3}2253$	$0.0^{4}623$	$0.0^{4}1805$	$0.0^{5}539$	$0.0^{5}1650$	$0.0^{6}5152$
$s_1(1,3,\alpha)$	$0.0^{2}669$	$0.0^{2}1353$	$0.0^{3}3201$	$0.0^{4}833$	$0.0^{4}2314$	$0.0^{5}670$	$0.0^{5}1998$	$0.0^{6}612$
$s_1(1,5,\alpha)$	0.01640	$0.0^{2}2560$	$0.0^{3}5155$	$0.0^{3}1218$	$0.0^{4}3169$	$0.0^{5}876$	$0.0^{5}2520$	$0.0^{6}753$
$s_1(2,0,\alpha)$	$0.0^{2}4964$	$0.0^{2}1106$	$0.0^{3}2772$	$0.0^{4}747$	$0.0^{4}2121$	$0.0^{5}6233$	$0.0^{5}1883$	$0.0^{6}582$
$s_1(2,1,\alpha)$	$0.0^{2}6451$	$0.0^{2}1352$	$0.0^{3}3259$	$0.0^{4}856$	$0.0^{4}2384$	$0.0^{5}691$	$0.0^{5}2063$	$0.0^{6}632$
$s_1(2,2,\alpha)$	$0.0^{2}888$	$0.0^{2}1712$	$0.0^{3}3926$	$0.0^{4}999$	$0.0^{4}2717$	$0.0^{5}774$	$0.0^{5}2281$	$0.0^{6}691$
$s_1(2,3,\alpha)$	0.01314	$0.0^{2}2271$	$0.0^{3}4878$	$0.0^{3}1190$	$0.0^{4}3145$	$0.0^{5}877$	$0.0^{5}2545$	$0.0^{6}762$
$s_1(2,4,\alpha)$	0.02135	$0.0^{2}3194$	$0.0^{3}6300$	$0.0^{3}1457$	$0.0^{4}3715$	$0.0^{4}1010$	$0.0^{5}2874$	$0.0^{6}850$
$s_1(2,5,\alpha)$	0.03872	$0.0^{2}4832$	$0.0^{3}853$	$0.0^{3}1844$	$0.0^{4}4490$	$0.0^{4}1184$	$0.0^{5}3290$	$0.0^{6}956$
$s_1(2,6,\alpha)$	0.07952	$0.0^{2}7991$	$0.0^{2}1228$	$0.0^{3}2431$	$0.0^{4}5592$	$0.0^{4}1418$	$0.0^{5}3828$	$0.0^{5}1093$
$s_1(3,1,\alpha)$	0.01262	$0.0^{2}2289$	$0.0^{3}5025$	$0.0^{3}1235$	$0.0^{4}3276$	$0.0^{5}915$	$0.0^{5}2652$	$0.0^{6}793$
$s_1(3,3,\alpha)$	0.02920	$0.0^{2}4176$	$0.0^{3}799$	$0.0^{3}1793$	$0.0^{4}4465$	$0.0^{4}1192$	$0.0^{5}3341$	$0.0^{6}975$
$s_1(3,5,\alpha)$	0.1027	0.01005	$0.0^{2}1530$	$0.0^{3}2964$	$0.0^{4}668$	$0.0^{4}1668$	$0.0^{5}4443$	$0.0^{5}1251$
$s_1(4,0,\alpha)$	0.01995	$0.0^{2}3298$	$0.0^{3}6792$	$0.0^{3}1596$	$0.0^{4}4087$	$0.0^{4}1111$	$0.0^{5}3159$	$0.0^{6}928$
$s_1(4,1,\alpha)$	0.02836	$0.0^{2}4290$	$0.0^{3}836$	$0.0^{3}1892$	$0.0^{4}4717$	$0.0^{4}1258$	$0.0^{5}3524$	$0.0^{5}1023$
$s_1(4,2,\alpha)$	0.04380	$0.0^{2}5880$	$0.0^{2}1065$	$0.0^{3}2299$	$0.0^{4}5550$	$0.0^{4}1445$	$0.0^{5}3975$	$0.0^{5}1138$
$s_1(4,3,\alpha)$	0.0748	$0.0^{2}860$	$0.0^{2}1419$	$0.0^{3}2883$	$0.0^{4}667$	$0.0^{4}1688$	$0.0^{5}4543$	$0.0^{5}1279$
$s_1(4,4,\alpha)$	0.1439	0.01364	$0.0^{2}1997$	$0.0^{3}3755$	$0.0^{4}826$	$0.0^{4}2013$	$0.0^{5}528$	$0.0^{5}1458$
$s_1(4,5,\alpha)$	0.3143	0.02376	$0.0^{2}3000$	$0.0^{3}5125$	$0.0^{3}1056$	$0.0^{4}2464$	$0.0^{5}625$	$0.0^{5}1685$
$s_1(4,6,\alpha)$	0.7803	0.04595	$0.0^{2}4821$	$0.0^{3}7393$	$0.0^{3}1406$	$0.0^{4}3102$	$0.0^{5}757$	$0.0^{5}1985$
$s_1(5,0,\alpha)$	0.0501	$0.0^{2}676$	$0.0^{2}1208$	$0.0^{3}2574$	$0.0^{4}6140$	$0.0^{4}1583$	$0.0^{5}4316$	$0.0^{5}1226$
$s_1(5,1,\alpha)$	0.0744	$0.0^{2}908$	$0.0^{2}1524$	$0.0^{3}3111$	$0.0^{4}7200$	$0.0^{4}1814$	$0.0^{5}4861$	$0.0^{5}1363$
$s_1)5,2,\alpha)$	0.1215	0.01299	$0.0^{2}2004$	$0.0^{3}3872$	$0.0^{4}8621$	$0.0^{4}2114$	$0.0^{5}5548$	$0.0^{5}1529$
$s_1(5,3,\alpha)$	0.2224	0.02002	$0.0^{2}2775$	$0.0^{3}4998$	$0.0^{3}1061$	$0.0^{4}2514$	$0.0^{5}643$	$0.0^{5}1741$
$s_1(5,4,\alpha)$	0.463	0.03381	$0.0^{2}4090$	$0.0^{3}674$	$0.0^{3}1348$	$0.0^{4}3061$	$0.0^{5}759$	$0.0^{5}2009$
$s_1(5,5,\alpha)$	1.101	0.0633	$0.0^{2}644$	$0.0^{3}960$	$0.0^{3}1781$	$0.0^{4}3839$	$0.0^{5}917$	$0.0^{5}2360$
$s_1(5,6,\alpha)$	2.984	0.1322	0.01099	$0.0^{2}1453$	$0.0^{3}2463$	$0.0^{4}4982$	$0.0^{4}1136$	$0.0^{5}2830$

TABLE III. $B_n(\alpha/2)$ *and* $C_n(\alpha/2)$.

α	$\alpha=3$	4	5	6	7	8	9	10
$B_0(\alpha/2)$	2.8390	3.6269	4.8402	6.6786	9.4531	13.645	20.001	29.681
$B_1(\alpha/2)$	−1.2439	−1.9488	−2.9698	−4.4858	−6.7694	−10.243	−15.561	−23.748
$B_2(\alpha/2)$	1.1806	1.6781	2.4644	3.6882	5.5849	8.524	13.085	20.182
$B_3(\alpha/2)$	−0.7754	−1.2451	−1.9485	−3.0238	−4.6832	−7.262	−11.283	−17.575
$B_4(\alpha/2)$	0.7713	1.1368	1.7226	2.6470	4.1009	6.384	9.972	15.621
$B_5(\alpha/2)$	−0.5656	−0.9203	−1.4606	−2.3003	−3.6118	−5.675	−8.926	−14.063
$B_6(\alpha/2)$	0.5766	0.8659	1.3348	2.0781	3.2614	5.132	8.100	12.805
$C_0(\alpha/2)$	0.3513	0.7037	1.2765	2.1930	3.6508	5.963	9.627	15.432
$C_1(\alpha/2)$	−0.5412	−0.8933	−1.4379	−2.2928	−3.6401	−5.771	−9.144	−14.489
$C_2(\alpha/2)$	0.5666	0.8662	1.3517	2.1264	3.3589	5.314	8.415	13.341
$C_3(\alpha/2)$	−0.4607	−0.7579	−1.2166	−1.9386	−3.0761	−4.882	−7.747	−12.307
$C_4(\alpha/2)$	0.4792	0.7305	1.1409	1.7937	2.8417	4.506	7.164	11.397

TABLE IV. *j, j', and j'' integrals for Σ states.*

α	$\alpha=3$	4	5	6	7	8	9	10
$j(ss;ss)/\kappa$	0.3367	0.3177	0.2969	0.2746	0.2527	0.2316	0.2121	0.1948
$j(ss;s0)/\kappa$	−0.0560	−0.0660	−0.0705	−0.0710	−0.0676	−0.0622	−0.0559	−0.0494
$j(s0;s0)/\kappa$	0.0386	0.0179	$0.0^{3}4$	−0.0117	−0.0189	−0.0218	−0.0219	−0.0204
$j(ss;00)/\kappa$	0.3458	0.3312	0.3140	0.2942	0.2734	0.2542	0.2302	0.2110
$j'(ss;ss)/\kappa$	0.2856	0.2379	0.1888	0.1432	0.1022	0.0714	0.0477	0.0302
$j'(ss;s0)^0/\kappa$	−0.1368	−0.1492	−0.1423	−0.1234	−0.0985	−0.0734	−0.0516	−0.0346
$j'(ss;s0)^2/\kappa$	$-0.0^{3}7$	$-0.0^{2}14$	$-0.0^{2}23$	$-0.0^{2}25$	$-0.0^{2}25$	$-0.0^{2}23$	$-0.0^{2}18$	$-0.0^{2}14$
$f'(ss;00)^0/\kappa$	0.1304	0.0361	−0.0287	−0.0608	−0.0693	−0.0629	−0.0502	−0.0369
$j'(ss;00)^2/\kappa$	$-0.0^{2}24$	$-0.0^{2}41$	$0.0^{2}54$	$-0.0^{2}50$	$-0.0^{2}49$	$-0.0^{2}42$	$-0.0^{2}33$	$-0.0^{2}25$
$j'(s0;s0)^0/\kappa$	0.0681	0.0964	0.1107	0.1097	0.0970	0.0779	0.0582	0.0410
$j'(s0;s0)^1/\kappa$	0.0479	0.0343	0.0225	0.0139	$0.0^{2}83$	$0.0^{2}47$	$0.0^{2}26$	$0.0^{2}14$
$j'(s0;s0)^2/\kappa$	$0.0^{2}14$	$0.0^{2}29$	$0.0^{2}41$	$0.0^{2}43$	$0.0^{2}42$	$0.0^{2}39$	$0.0^{2}32$	$0.0^{2}24$
$j''(ss;ss)/\kappa$	0.3155	0.2834	0.2482	0.2124	0.1762	0.1426	0.1132	0.0876
$j_a''(ss;s0)^0/\kappa$	−0.1508	−0.1771	−0.1860	−0.1816	−0.1667	−0.1466	−0.1257	−0.1038
$j_a''(ss;s0)^1/\kappa$	−0.0248	−0.0280	−0.0273	−0.0245	−0.0214	−0.0178	−0.0149	−0.0119
$j_a''(ss;s0)^2/\kappa$	$-0.0^{3}1$	$+0.0^{2}12$	$-0.0^{2}21$	$+0.0^{2}14$	$+0.^{3}9$	$+0.0^{3}7$	$+0.0^{3}7$	$+0.0^{2}18$
$j''(ss;00)^0/\kappa$	0.1459	0.0464	−0.0334	−0.0855	−0.1130	−0.1224	−0.1176	−0.1069
$j''(ss;00)^2/\kappa$	$0.0^{2}18$	$0.0^{2}70$	$-0.0^{2}56$	$-0.0^{3}1$	$0.0^{2}33$	$0.0^{2}17$	$-0.0^{2}17$	$0.0^{2}24$
$j''(s0;s0)^0/\kappa$	−0.0171	−0.0245	−0.0296	−0.0318	−0.0320	−0.0285	−0.0222	−0.0181
$j''(s0;s0)^1/\kappa$	0.0529	0.0411	0.0288	0.0195	0.0135	$0.0^{2}91$	$0.0^{2}70$	$0.0^{2}53$
$j''(s0;s0)^2/\kappa$	$-0.0^{2}33$	$-0.0^{2}98$	$-0.0^{2}55$	−0.0119	−0.0104	$-0.0^{2}86$	$-0.0^{2}65$	$-0.0^{2}68$
$j_a''(s0;ss)^0/\kappa$	0.0264	0.0308	0.0308	0.0290	0.0283	0.0222	0.0182	0.0161
$j_a''(s0;ss)^2/\kappa$	$0.0^{2}17$	$0.0^{2}40$	$0.0^{2}48$	$0.0^{2}48$	$0.0^{2}69$	$0.0^{2}62$	$0.0^{2}41$	$0.0^{2}14$
$j''(00;ss)^0/\kappa$	0.3189	0.2882	0.2541	0.2176	0.1777	0.1480	0.1178	0.0900
$j''(00;ss)^2/\kappa$	$-0.0^{2}17$	$-0.^{2}30$	$-0.0^{2}11$	$+0.0^{3}3$	$-0.0^{2}21$	$-0.0^{2}13$	$+0.0^{3}8$	$+0.0^{2}43$

TABLE V. j, j', and j'' integrals for Π states.

α	$\alpha=3$	4	5	6	7	8	9	10
$j(ss;11)/\kappa$	0.3313	0.3107	0.2878	0.2643	0.2424	0.2216	0.2028	0.1862
$j(s1;S1)/\kappa$	0.0651	0.0558	0.0464	0.0377	0.0300	0.0237	0.0187	0.0146
$j'(ss;11)^0/\kappa$	0.2539	0.1961	0.1420	0.0983	0.0644	0.0407	0.0243	0.0145
$j'(ss;11)^2/\kappa$	0.0^211	0.0^216	0.0^219	0.0^215	0.0^213	0.0^39	0.0^36	0.0^34
$j'(s1;s1)^1/\kappa$	0.0583	0.0456	0.0330	0.0232	0.0152	0.0^294	0.0^257	0.0^234
$j'(s1;s1)^2/\kappa$	0.0^38	0.0^38	0.0^37	0.0^37	0.0^35	0.0^33	0.0^32	0.0^32
$j''(ss;11)^0/\kappa$	0.2814	0.2350	0.1885	0.1480	0.1115	0.0840	0.0620	0.0450
$j''(ss;11)^2/\kappa$	-0.0^210	-0.0^239	$+0.0^227$	-0.0^33	-0.0^224	-0.0^220	$+0.0^37$	-0.0^229
$j''(s1;s1)^1/\kappa$	0.0651	0.0556	0.0452	0.0367	0.0283	0.0210	0.0156	0.0116
$j''(s1;s1)^2/\kappa$	-0.0^224	-0.0^217	-0.0^244	-0.0^230	-0.0^236	-0.0^230	-0.0^223	-0.0^225
$j''(11;ss)^0/\kappa$	0.3136	0.2816	0.2446	0.2088	0.1723	0.1402	0.1118	0.0872
$j''(11;ss)^2/\kappa$	0.0^39	0.0^212	0.0^39	0.0^34	-0.0^33	-0.0^35	-0.0^211	-0.0^218

The integrals $I_a(ss)$, $I_a(00)$, $I_a(11)$, $I_a'(ss)$, $S_{ss}^{1/2}$, $S_{00}^{1/2}$, and $S_{11}^{1/2}$ either have already been given or are readily obtainable from previous work.[11] No new procedure is involved in getting the formulations for the others integrals of this type, and we simply list the expressions. Numerical values are then tabulated.

$$I_a(ss) = \mathrm{I}. \quad I_a(00) = (\kappa/192)IIa. \quad I_a(11) = (\kappa/384)Ia$$

$$I_a(s0) = \kappa(3^{1/2}/36)\alpha^4\{120/\alpha^6 - A_5(1,\alpha) + A_2(1,\alpha)\}$$

$$I_a'(ss) = I'$$

$$I_a'(s0) = -\kappa(3^{1/2}/576)\alpha^4\{A_2(1,\alpha/2) + A_0(1,\alpha/2)\}$$

$$I_a'(0s) = \kappa(3^{1/2}/192)\alpha^4\{A_2(1,\alpha/2) - (\tfrac{1}{3})A_0(1,\alpha/2)\}$$

$$I_a'(00) = (\kappa/64)\alpha^4\{(\tfrac{1}{3})A_3(1,\alpha/2) - A_1(1,\alpha/2)\}$$

$$I_a'(11) = (\kappa/192)\alpha^4\{A_3(1,\alpha/2) - A_1(1,\alpha/2)\}$$

$$S_{ss}^{1/2} = S^{1/2}$$

$$S_{s0}^{1/2} = -(3^{1/2}/36)(\alpha/2)^5\{A_3(1,\alpha/2) - (\tfrac{1}{5})A_1(1,\alpha/2)\}$$

TABLE VI. I and I' integrals.

α	$\alpha=3$	4	5	6	7	8	9	10
$I_a(ss)/\kappa$	0.4468	0.4022	0.3564	0.3138	0.2772	0.2463	0.2206	0.1995
$I_a(s0)/\kappa$	0.1761	0.1692	0.1487	0.1247	0.1024	0.0835	0.0684	0.0565
$I_a(00)/\kappa$	0.5367	0.4928	0.4357	0.3782	0.3276	0.2846	0.2500	0.2218
$I_a(11)/\kappa$	0.4010	0.3568	0.3162	0.2813	0.2521	0.2268	0.2057	0.1878
$I_a'(ss)/\kappa$	0.4324	0.3835	0.3289	0.2738	0.2221	0.1761	0.1368	0.1045
$I_a'(s0)/\kappa$	−0.1530	−0.1823	−0.1925	−0.1869	−0.1704	−0.1480	−0.1239	−0.1005
$I_a'(0s)/\kappa$	0.3140	0.3386	0.3308	0.3018	0.2619	0.2185	0.1772	0.1394
$I_a'(00)/\kappa$	0.1534	0.0225	−0.0702	−0.1245	−0.1478	−0.1496	−0.1382	−0.1202
$I_a'(11)/\kappa$	0.3626	0.2932	0.2291	0.1744	0.1297	0.0946	0.0680	0.0483

TABLE VII. $S^{1/2}$ and S integrals.

α	$\alpha=3$	4	5	6	7	8	9	10
$S_{ss}^{1/2}$	0.8897	0.8149	0.7291	0.6373	0.5448	0.4562	0.3748	0.3024
S_{ss}	0.7916	0.6641	0.5316	0.4061	0.2968	0.2081	0.1405	0.0914
$S_{s0}^{1/2}$	−0.3865	−0.4636	−0.5036	−0.5088	−0.4859	−0.4441	−0.3911	−0.3339
S_{s0}	0.1494	0.2149	0.2536	0.2589	0.2361	0.1972	0.1530	0.1115
$S_{00}^{1/2}$	0.4825	0.2256	0.0^251	−0.1597	−0.2649	−0.3187	−0.3326	−0.3190
S_{00}	0.2328	0.0509	0.0^43	0.0256	0.0702	0.1016	0.1106	0.1017
$S_{11}^{1/2}$	0.8089	0.6947	0.5778	0.4679	0.3702	0.2871	0.2185	0.1641
S_{11}	0.6542	0.4826	0.3339	0.2189	0.1370	0.0824	0.0477	0.0269

TABKE VIII. J, J', and J'' integrals for Σ states.

α	$\alpha=3$	4	5	6	7	8	9	10
$J(ss;ss)/\kappa$	0.1098	0.0133	−0.0159	−0.0197	−0.0160	−0.0110	−0.0069	−0.0042
$J(00;ss)/\kappa$	0.0290	−0.0638	−0.0781	−0.0645	−0.0457	−0.0267	−0.0182	−0.0103
$J(0s;ss)/\kappa$	−0.1201	−0.1032	−0.0782	−0.0537	−0.0348	−0.0213	−0.0125	−0.0071
$J(s0;0s)/\kappa$	0.0386	0.0179	0.0004	−0.0117	−0.0189	−0.0218	−0.0219	−0.0204
$J'(ss;ss)/\kappa$	0.0439	−0.0550	−0.0782	−0.0704	−0.0550	−0.0373	−0.0236	−0.0147
$J'(ss;0s)/\kappa$	−0.0798	−0.1142	−0.1153	−0.0976	−0.0740	−0.0515	−0.0339	−0.0209
$J'(ss;s0)/\kappa$	−0.0635	−0.0131	0.0145	0.0244	0.0241	0.0193	0.0139	0.0091
$J'(ss;00)/\kappa$	0.0691	0.0191	0.0169	0.0233	0.0239	0.0208	0.0161	0.0109
$J'(0s;0s)/\kappa$	0.0365	−0.0004	−0.0249	−0.0345	−0.0331	−0.0269	−0.0198	−0.0130
$J''(ss;ss)/\kappa$	0.0787	−0.0204	−0.0489	−0.0490	−0.0413	−0.0318	−0.0230	−0.0167
$J_a''(ss;s0)/\kappa$	0.0533	0.0894	0.0935	0.0872	0.0706	0.0532	0.0367	0.0253
$J_a''(ss;0s)/\kappa$	0.0581	0.0109	−0.0098	−0.0213	−0.0219	−0.0183	−0.0132	−0.0102
$J_a''(s0;ss)/\kappa$	−0.1286	−0.1031	−0.0728	−0.0457	−0.0206	−0.0097	−0.0033	+0.0004
$J_a''(ss;00)/\kappa$	0.1004	0.0530	0.0314	0.0358	0.0358	0.0277	0.0184	0.0155
$J_a''(s0;\ 0)/\kappa$	0.1006	0.0852	0.0686	0.0392	0.0209	0.0091	0.0051	−0.0007
$J_a''(s0;0s)/\kappa$	0.0052	−0.0030	−0.0110	−0.0002	0.0061	0.0091	0.0089	0.0113
$J_a''(00;ss)/\kappa$	0.0004	−0.0924	−0.1020	−0.0845	−0.0692	−0.0451	−0.0286	−0.0168

TABLE IX. J, J', and J'' integrals for Π states.

α	$\alpha=3$	4	5	6	7	8	9	10
$J(11;ss)/\kappa$	0.1502	0.0517	0.0152	0.0025	−0.0012	−0.0015	−0.0013	−0.0011
$J(s1;s1)/\kappa$	0.0651	0.0558	0.0464	0.0377	0.0300	0.0237	0.0187	0.0146
$J'(ss;11)/\kappa$	0.0624	−0.0245	−0.0446	−0.0400	−0.0296	−0.0193	−0.0123	−0.0069
$J'(s1;S1)/\kappa$	0.0591	0.0464	0.0337	0.0239	0.0157	0.0097	0.0059	0.0036
$J''(ss;11)/\kappa$	0.0957	0.0058	−0.0127	−0.0175	−0.0174	−0.0115	−0.0049	−0.0061
$J''(1s;s1)/\kappa$	0.0627	0.0539	0.0408	0.0337	0.0247	0.0180	0.0133	0.0091
$J''(s1;1s)/\kappa$	0.0675	0.0573	0.0496	0.0397	0.0319	0.0240	0.0179	0.0141
$J''(11;ss)/\kappa$	0.1184	0.0160	−0.0222	−0.0315	−0.0317	−0.0258	−0.0199	−0.0154

TABLE X. H_{i1}' for Σ states.

α	$\alpha=3$	4	5	6	7	8		10
H_{11}'/κ	0.1155	0.0719	0.0421	0.0363	0.0384	0.0361	0.0223	0.0163
H_{21}'/κ	0.1575	0.0780	0.0215	−0.0136	−0.0237	−0.0185	−0.0117	−0.0077
H_{31}'/κ	−0.0884	−0.0490	−0.0219	−0.0296	−0.0399	−0.0429	−0.0399	−0.0350
H_{41}'/κ	−0.1720	−0.1009	−0.0484	−0.0157	−0.0067	−0.0102	−0.0148	−0.0155

TABLE XI. H_{i1}' for Π states.

α	$\alpha=3$	4	5	6	7	8	9	10
H_{11}'/κ	0.1696	0.1387	0.1048	0.0721	0.0497	0.0312	0.0184	0.0106
H_{21}'/κ	−0.0132	−0.0159	−0.0183	−0.0156	−0.0127	−0.0089	−0.0059	−0.0040
H_{31}'/κ	−0.1147	−0.0496	−0.0028	+0.0278	+0.0389	+0.0361	+0.0284	+0.0222
H_{41}'/κ	0.0093	0.0119	0.0167	0.0162	0.0165	0.0155	0.0137	0.0118

TABLE XII. N_{i1} for Σ states.

α	$\alpha=3$	4	5	6	7	8	9	10
N_{11}	0.1773	0.2637	0.3497	0.4401	0.5370	0.6356	0.7281	0.8073
N_{21}	0.1183	0.1427	0.1348	0.1052	0.0702	0.0411	0.0215	0.0102
N_{31}	−0.0895	−0.0617	−0.0017	+0.0604	+0.1015	+0.1151	+0.1072	+0.0877
N_{41}	−0.1183	−0.1427	−0.1348	−0.1052	−0.0702	−0.0411	−0.0215	− .0102

TABLE XIII. N_{i1} for Π states.

α	$\alpha=3$	4	5	6	7	8	9	10
N_{11}	0.2084	0.3359	0.4684	0.5938	0.7032	0.7918	0.8595	0.9086
N_{21}	0.0000	—	—	—	—	—	—	—
N_{31}	−0.1500	−0.1902	−0.1973	−0.1771	−0.1418	−0.1037	−0.0704	−0.0451
N_{41}	0.0000	—	—	—	—	—	—	—

TABLE XIV. *Energies.*

α	$\alpha=3$	4	5	6	7	8	9	10
$(1/\kappa)\,({}^1\Sigma S^N-E_a)$	0.1435	(0.0100)	−0.0193	−0.0452	−0.0500	(−0.0520)	−0.0528	−0.0468
$(1/\kappa)\,({}^3\Sigma S^N-E_b)$	0.4738	0.2267	0.1353	0.0719	0.0453	0.0292	0.0106	0.0050
$(1/\kappa)\,({}^1\Sigma A^N-E_a)$	1.0596	0.4908	0.2156	0.1152	0.1064	(0.1020)	0.0984	0.0799
$(1/\kappa)\,({}^3\Sigma A^N-E_b)$	−4.1589	−1.4500	−0.0721	+0.3768	+0.3229	+0.1992	+0.1023	+0.0622
$(1/\kappa)\,({}^1\Pi S^N-E_a)$	0.8733	0.5841	0.3703	0.2412	0.1646	0.1074	0.0692	0.0470
$(1/\kappa)\,({}^3\Pi S^N-E_b)$	1.0068	0.6390	0.3821	0.2383	0.1511	0.0882	0.0494	0.0290
$(1/\kappa)\,({}^1\Pi A^N-E_a)$	0.7305	0.3051	0.1091	0.0162	−0.0218	−0.0327	−0.0318	−0.0287
$(1/\kappa)\,({}^3\Pi A^N-E_b)$	0.8560	0.4108	0.2142	0.0987	0.0473	0.0218	(0.0136)	(0.0060)

DISCUSSION

The potential energy curves indicate that a stable beryllium molecule may be formed when a normal beryllium atom interacts with one in the $2s2p\ {}^1P$ state. There result two attractive states, ${}^1\Pi$ and ${}^1\Sigma$, of which the ${}^1\Sigma$ is the lower. This confirms the rule[11] that those states tend to lie lowest which have the smallest value of $\Sigma_i m_l(i)$, where $m_l(i)$ denotes the component of orbital angular momentum of the ith electron in the direction of the internuclear axis.

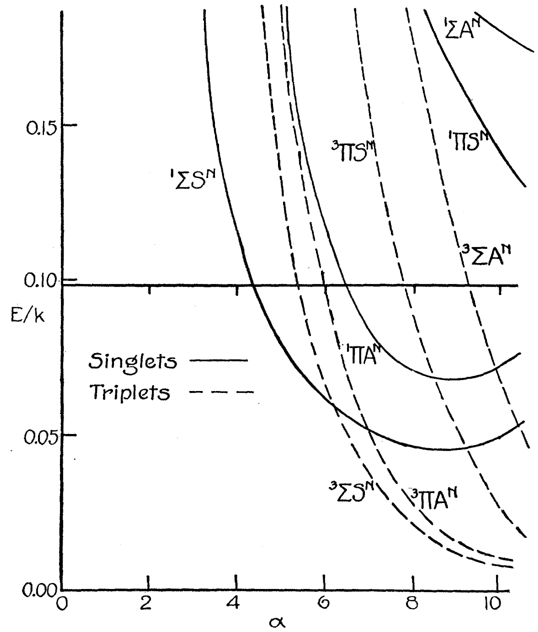

Fig. 1. Energy curves for Be_2.

For small values of the internuclear distance, the ${}^3\Sigma A^N$ curve, which indicates a repulsive state for large separations, behaves erratically. This probably means that the Heitler-London method is not applicable in this region.

An investigation has been made of the interaction of a normal lithium atom with one in the $2p\ {}^2P$ state. The integrals $J(pp,ss)$, $J'(pp,ss)$, $J(ps,ps)$, and $J'(ps,ps)$ occur in the energy expressions. It has not been possible to attain good agreement with experiment,[13] the most glaring discrepancy being

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[13] F. W. Loomis and R. E. Nusbaum, Phys. Rev. **38**, 1447 (1931).

for the $^1\Pi S^N$ state, which according to the calculations is repulsive, and according to experiment is attractive. We would accordingly not regard the results obtained for the $^1\Pi$ state in Be_2 as conclusive, but those for the $^1\Sigma$ state are probably more correct. The anomaly in Li_2 is being studied more closely, and it may be necessary to apply other methods to obtain agreement.

As has been seen, the energy expressions for Be_2 involve many terms, since the interaction process is quite complicated. If an attempt were to be made to extend the calculations to B_2, the degree of complication would increase to such an extent that it is quite doubtful whether or not the results would have much meaning. From the results obtained in this and previous articles, it seems reasonable to suppose that in order to have the most stable B_2 molecule, one of the atoms should have the electron configuration $2s2p^2$.

In conclusion, it appears that the general many-electron problem for homonuclear molecules is still far from solution, and that much more powerful methods than that of Heitler and London must be developed before progress can be made. For heteronuclear molecules. the situation is even less satisfactory.

Correction:—The Σ states in this article have been assigned the wrong symmetry in the nuclei. This error arises essentially because the wave function $a_p + b_p$ is of the character S^N for Π states, but A^N for Σ states.

For $p = 0$,

$$\int (a_p + b_p)(a_s + b_s) dv = S_{ps}^{1/2} + S_{sp}^{1/2} = 0.$$

The convention followed is that the directions $\Theta_a = 0$ and $\Theta_b = 0$ are to be the same, and not opposite to each other. This correction also applies to the Π states of a previous paper[11] by of the writers.