

## Quantum Mechanics of Beryllium Hydride

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The interaction of a normal hydrogen atom with a beryllium atom having the electronic configurations  $2s\ 2s$  and  $2s\ 2p$ , respectively, has been studied by the application of a modified Heitler-London method. It is shown that for beryllium in the  $^1S$  atomic state, the resulting  $^2\Sigma$  molecular state is repulsive. For beryllium in the  $^3P$  atomic state, the  $^4\Pi$  and  $^4\Sigma$  molecular states are repulsive, and the  $^2\Pi$  and  $^2\Sigma$  states are attractive. For beryllium in the  $^1P$  atomic

state both the  $^2\Pi$  and  $^2\Sigma$  molecular states are found to be repulsive. However, when the interaction between the  $^2\Sigma(^3P+^2S)$  and the  $^2\Sigma(^1S+^2S)$  molecular states is taken into account the lowest  $^2\Sigma$  state is found to be attractive. The calculated heats of dissociation for the attractive states are in poor agreement with the extrapolated values from the band system.

### INTRODUCTION

**I**N a recent series of papers,<sup>1, 2, 3, 4</sup> the Heitler-London method has been developed and applied to a study of the lithium and beryllium molecules. The results have not been encouraging, but before resorting to more elaborate and complicated methods of calculation, it seems to the point to ascertain whether or not the method, despite its limitations and imperfections, can be used with some success in other cases. If, in particular, one could arrive at a qualitative understanding of the formation of the hydrides, this would be at least a step toward a more perfect theory of valence. Hutchisson and Muskat<sup>5</sup> have made a beginning by calculating the heat of dissociation of lithium hydride. They found good agreement with the experimental value.

The purpose of the present paper is to study the next more complicated hydride, namely, beryllium hydride. The Heitler-London method has been applied to those states of BeH which dissociate into a normal hydrogen atom, and a beryllium atom in the  $^1S$ ,  $^3P$  and  $^1P$  atomic states, respectively.

The atomic wave functions used are similar to

<sup>1</sup> J. H. Bartlett, Jr., Phys. Rev. **37**, 507 (1931).

<sup>2</sup> J. H. Bartlett, Jr., and W. H. Furry, Phys. Rev. **38**, 1615 (1931).

<sup>3</sup> W. H. Furry and J. H. Bartlett, Jr., Phys. Rev. **39**, 210 (1932).

<sup>4</sup> W. H. Furry, Phys. Rev. **39**, 1015 (1932).

<sup>5</sup> E. Hutchisson and M. Muskat, Phys. Rev. **40**, 340 (1932).

those given by Zener<sup>6</sup> except that the coefficient in the exponent in the case of Be has been raised from 0.96 to unity. It has been shown<sup>4</sup> that the integrals arising in a calculation of this type are quite insensitive to small changes in the coefficient in the exponent, and this has been verified for a number of the integrals occurring in the present case. This change is made because of the great simplification which results in the calculation, since the tables of the previous papers<sup>1, 3</sup> can be used.

### NOTATION

The normalized atomic wave function for electron 1, on the beryllium nucleus, with quantum numbers  $(n, l, m)$  will be denoted by  $a(n, l, m/1)$ ; similarly for hydrogen,  $b(n, l, m/1)$ . For simplicity  $a(2, 0, 0/1)$  will be written  $a(s/1)$ ;  $b(1, 0, 0/1)$  will be written  $b(1)$ ; and both  $a(2, 1, 0/1)$  and  $a(2, 1, 1/1)$  will be written  $a(p/1)$ . Thus in the latter case the general formulation will hold for either  $\Pi$  or  $\Sigma$  states depending upon the value of  $m$ . The atomic wave functions are:

$$\begin{aligned} b(1) &= \pi^{-\frac{1}{2}} e^{-b_1}; & a(s/1) &= (3\pi)^{-\frac{1}{2}} a_1 e^{-a_1}, \\ a(p/1) &= \pi^{-\frac{1}{2}} a_1 \cos \theta_{a_1} e^{-a_1} \text{ for } m=0, \\ a(p/1) &= (2\pi)^{-\frac{1}{2}} a_1 \sin \theta_{a_1} e^{i\phi_1 - a_1} \text{ for } m=1. \end{aligned}$$

Let

$$S^{\frac{1}{2}} = \int a(s/1)b(1)dv,$$

$$S^{\frac{1}{2}}(p) = \int a(p/1)b(1)dv,$$

<sup>6</sup> Clarence Zener, Phys. Rev. **36**, 51 (1930).

$$J(s, s; b, b) = \int [a(s/1)]^2 H'(13) [b(3)]^2 dv,$$

$$K(s, b; s, b) = \int a(s/1) b(1) H'(13) a(s/3) b(3) dv,$$

$$J''(s, s; s, b) = \int [a(s/1)]^2 H'(13) a(s/3) b(3) dv,$$

$$J''(s, b; s, p^*) = \int a(s/1) b(1) H'(13) \\ \times a(s/3) a^*(p/3) dv.$$

The above examples are sufficient for the understanding of further integrals. All energies are to be measured relative to the energy of the separate atoms at infinite separation. Atomic units are used unless otherwise stated. A com-

plete tabulation of integrals is given in the appendix.

### I. INTERACTION OF NORMAL HYDROGEN WITH NORMAL BERYLLIUM

Assume the following as a suitable normalized molecular wave function:

$$\psi_a = [6(1-S)]^{-\frac{1}{2}} \sum_P (-1)^{\sigma_P} P [a_\alpha(s/1) a_\beta(s/2) b_\alpha(3)].$$

The total energy is given by

$$E = \int \psi_a^* H \psi_a dv.$$

Splitting off the unperturbed energy, say  $E_0$ , and substituting for  $\psi_a$ , results in

$$E - E_0 = E' = [6(1-S)]^{-1} \int \left[ \sum_P (-1)^{\sigma_P} P a_\alpha(s/1) a_\beta(s/2) b_\alpha(3) \right] H' \\ \cdot \left[ \sum_P (-1)^{\sigma_P} P a_\alpha(s/1) a_\beta(s/2) b_\alpha(3) \right] dv,$$

where the perturbative part of the Hamiltonian is

$$H' = H'(13) + H'(23)$$

and

$$H'(i3) = 2/R + 2/r_{i3} - 2/a_3 - 2/b_i.$$

Suppressing  $P$  in the second bracketed expression in the integral introduces a factor of 6. The perturbative part of the energy is

$$E' = \frac{2J(s, s; b, b) - K(s, b; s, b) - S^{\frac{1}{2}} J''(s, s; s, b)}{(1-S)}.$$

Table I gives the energy of the  ${}^2\Sigma(1S+2S)$  state as a function of the internuclear distance  $R$ .

TABLE I. Energy of the  ${}^2\Sigma(1S+2S)$  state.

$R$	$S^{\frac{1}{2}}$	$J(s, s; b, b)$	$K(s, b; s, b)$	$J''(s, s; s, b)$	$E'$
2.0	0.66801	-0.02427	-0.1984	-0.06526	0.349
2.5	0.57300	-0.03356	-0.1677	-0.07837	0.217
3.0	0.47704	-0.02549	-0.1172	-0.06617	0.126
4.0	0.30490	-0.023290	-0.04219	-0.03230	0.05012
5.0	0.18089	-0.021648	-0.01256	-0.01338	0.01208

### II. THE EXCITED STATES

One may write the following eight molecular wave functions, the first six arising from the  ${}^3P$  atomic state of beryllium and the last two from the  ${}^1P$  atomic state. Thus

$$\psi_1 = 0\{(\varphi_1 - \varphi_2)b(3)\alpha(1)\alpha(2)\alpha(3)\},$$

$$\psi_2 = 0\{(\varphi_1 - \varphi_2)b(3)\alpha(1)\alpha(2)\beta(3)\},$$

$$\psi_3 = 0\{(\varphi_1 - \varphi_2)b(3)[\alpha(1)\beta(2)\alpha(3) + \alpha(2)\beta(1)\alpha(3)]\},$$

$$\psi_4 = 0\{(\varphi_1 - \varphi_2)b(3)[\alpha(1)\beta(2)\beta(3) + \alpha(2)\beta(1)\beta(3)]\},$$

$$\psi_5 = 0\{(\varphi_1 - \varphi_2)b(3)\beta(1)\beta(2)\alpha(3)\},$$

$$\psi_6 = 0\{(\varphi_1 - \varphi_2)b(3)\beta(1)\beta(2)\beta(3)\},$$

$$\psi_7 = 0\{(\varphi_1 + \varphi_2)b(3)[\alpha(1)\beta(2)\alpha(3) - \alpha(2)\beta(1)\alpha(3)]\},$$

$$\psi_8 = 0\{(\varphi_1 + \varphi_2)b(3)[\alpha(1)\beta(2)\beta(3) - \alpha(2)\beta(1)\beta(3)]\},$$

where 0 stands for the operator  $\sum_p (-1)^{\sigma_P} P$  and

$$\varphi_1 = a(s/1)a(p/2); \quad \varphi_2 = a(s/2)a(p/1).$$

In order to get a molecular wave function which will give rise to  ${}^2\Pi$  or  ${}^2\Sigma$  states and whose atomic states are  ${}^3P$  for beryllium and  ${}^2S$  for hydrogen one will have to take a linear combination of the functions  $\psi_2$  and  $\psi_3$ , thus  $\psi_b = C_2\psi_2 + C_3\psi_3$ . The secular equation may be written as follows:

$$\begin{vmatrix} H_{22} - E & H_{23} - FE \\ H_{32} - FE & H_{33} - E \end{vmatrix} = 0,$$

where

$$H_{11}' = \{J(s, s; b, b) - K(s, b; s, b) - K(p, b; p^*, b) - S^{\frac{1}{2}}(p)[J''(s, s; p^*, b) - J''(s, p^*; s, b)] + S^{\frac{1}{2}}[J''(p, s; p^*, b) - J''(p^*, p; s, b)]\} \div [1 - S - S(p)],$$

$$H_{22}' = J(s, s; b, b) + J(p^*, p; b, b),$$

$$H_{33}' = \{2J(s, s; b, b) + 2J(p^*, p; b, b) - K(s, b; s, b) - K(p, b; p^*, b) - S^{\frac{1}{2}}(p)[J''(s, s; p^*, b) - J''(s, p^*; s, b)] + S^{\frac{1}{2}}[J''(p, s; p^*, b) - J''(p^*, p; s, b)]\} \div [2 - S - S(p)],$$

$$H_{23}' = \{-K(s, b; s, b) - K(p, b; p^*, b) - S^{\frac{1}{2}}(p)[J''(s, s; p^*, b) - J''(s, p^*; s, b)] + S^{\frac{1}{2}}[J''(p, s; p^*, b) - J''(p^*, p; s, b)]\} \div [2 - S - S(p)]^{\frac{1}{2}}.$$

Also

$$F = -[S + S(p)][2 - S - S(p)]^{-\frac{1}{2}}.$$

$$H_{ij} = \frac{\int \psi_i^* H \psi_j dv}{[\int |\psi_i|^2 dv \cdot \int |\psi_j|^2 dv]^{\frac{1}{2}}} = H_{ji}$$

and  $F = H_{ij}$  for  $H = 1$  and  $(ij) = (23)$ . The energies for both the doublet and quartet states are obtained from the secular equation, and a check can be made by solving for the energy of the quartet states directly by using  $\psi_1$  as the molecular wave function. Thus

$$(E - E_0) = \int \psi_1^* H' \psi_1 dv / \int \psi_1^* \psi_1 dv = H_{11}'.$$

The evaluation of the  $H'$ 's offers no difficulty, and so they will merely be listed:

The integrals are of the types dealt with in the previous papers.<sup>1-3</sup>

Table II gives the energies of the  ${}^2\Sigma({}^3P + {}^2S)$  and  ${}^4\Sigma({}^3P + {}^2S)$  states, together with the values

of new integrals arising in this connection and the values of the constants  $C_2$  and  $C_3$  (see Part III). Table III gives the corresponding information for the  $\Pi$ -states.

TABLE II. Energies of the  ${}^2\Sigma$  and  ${}^4\Sigma$  ( ${}^3P + {}^2S$ ) states.

R	2.0	2.5	3.0	4.0	5.0
$J(p^*p; bb)$	-0.08727	-0.07125	-0.05172	-0.01312	-0.02462
$K(p; p^*b)$	-0.1562	-0.1641	-0.1332	-0.06128	-0.02060
$J''(ps; p^*b)$	-0.03242	-0.02005	-0.02748	+0.01580	+0.02021
$J''(p^*p; sb)$	-0.1504	-0.1444	-0.1114	-0.07639	+0.04590
$J''(ss; pb)$	-0.01816	-0.05648	-0.06420	-0.06176	-0.04276
$J''(sp^*; sb)$	-0.06607	-0.02586	-0.0279	+0.01830	+0.01062
$S^{\frac{1}{2}}(p)$	0.58645	0.57288	0.52276	0.37851	0.24145
$H_{22}'$	-0.1115	-0.1048	-0.0772	-0.01641	-0.02627
$H_{23}'$	0.3685	0.3628	0.2721	0.1219	0.02996
$H_{33}'$	0.1506	0.1570	0.1192	0.07319	0.01512
$E'({}^2\Sigma)$	-0.2252	-0.2372	-0.1950	-0.08705	-0.02580
$H_{11}'({}^4\Sigma)$	1.400	0.9191	0.5128	0.1904	0.03864
$C_2$	0.6912	0.7085	0.7304	0.7723	0.7982
$C_3$	-0.3801	-0.4105	-0.4470	-0.5128	-0.5516

TABLE III. Energies of the  ${}^2\Pi$  and  ${}^4\Pi$  ( ${}^3P + {}^2S$ ) states.

R	2.0	2.5	3.0
$J(p^*, p; b, b)$	0.02518	0.0258	-0.02188
$K(p, b; p^*, b)$	0.05448	0.03427	0.02001
$J''(p, s; p^*, b)$	0.08316	0.06154	0.04517
$J''(p^*, p; s, b)$	-0.0264	-0.0432	-0.0442
$H_{22}'$	0.02916	-0.03098	-0.02737
$H_{23}'$	0.1634	0.1496	0.1050
$H_{33}'$	0.1323	0.07866	0.04879
$E'({}^2\Pi)$	-0.0825	-0.1097	-0.0871
$H_{11}'({}^4\Pi)$	0.3695	0.2419	0.1461

The energy arising from the interaction of a beryllium atom in the  $^1P$  atomic state and a hydrogen atom in the normal state is given by:

$$H_{77}' = \int \psi_i^* H' \psi_i dv / \int \psi_i^* \psi_i dv = \{2J(s, s; b, b) + 2J(p^*, p; b, b) - K(s, b; s, b) - K(p, b; p^*, b) - S^{\frac{1}{2}}(p)[J''(s, s; p^*, b) + J''(s, p^*; s, b)] - S^{\frac{1}{2}}[J''(p, s; p^*, b) + J''(p^*, p; s, b)]\} \div [2 - S - S(p)].$$

The energies are listed in Table IV.

TABLE IV. Energies of interaction between  $Be(^1P)$  and normal hydrogen.

R	2.0	2.5	3.0	4.0	5.0
$E'(^2\Sigma)$	0.2504	0.1962	0.1245	0.05987	0.0 <sup>2</sup> 8601
$E'(^2\Pi)$	0.06083	0.03646	0.02448	—	—

### III. THE GROUND STATE\*

Since the potential energy curve (see Fig. 1) for the  $^2\Sigma(^3P+^2S)$  molecular state crosses that of the  $^2\Sigma(^1S+^2S)$  state one would expect a considerable perturbing effect between these two states, and so as a suitable wave function for a ground state one assumes  $\psi = C_a\psi_a + C_b\psi_b$ . The constants  $C_2$  and  $C_3$  in  $\psi_b$  may be evaluated readily by first getting their ratio by using the  $H''$ 's and  $E'(^2\Sigma)$  in Table II, and then applying the normalization condition to  $\psi_b$ . The values so obtained are given

$$H_{ab}' = \frac{1}{3}(1-S)^{-\frac{1}{2}}[C_2 - C_3/w^{\frac{1}{2}}]\{S^{\frac{1}{2}}[2J''(s, p^*; s, b) - J''(s, s; p^*, b) + 2J''(s, b; s, p) - J''(p, b; s, s)] - S^{\frac{1}{2}}(p)[J''(s, s; s, b) + J''(s, b, s, s)] - K(s, b; p, b) - K(p, b; s, b)\}.$$

Also

$$\bar{F} = -(1-S)^{-\frac{1}{2}}[C_2 - C_3/w^{\frac{1}{2}}]S^{\frac{1}{2}}S^{\frac{1}{2}}(p),$$

where  $w^{\frac{1}{2}} = [2 - S - S(p)]^{\frac{1}{2}}$ .

In Table V are listed the values of new in-

\* As a further example of the perturbing effects of adjacent states see W. H. Furry's letter to the editor in this issue.

in Table II. Now if one measures the energy of the ground state relative to the  $^1S$  level of beryllium, and lets  $\epsilon (= 0.2008)$  denote the energy difference between the  $^1S$  and  $^3P$  levels one may write the secular equation for the ground state as follows:

$$\begin{vmatrix} H_{aa}' - E & H_{ab}' - \bar{F}(E - \epsilon) \\ H_{ba}' - \bar{F}E & H_{bb}' - (E - \epsilon) \end{vmatrix} = 0,$$

where  $H_{ij}' = \int \psi_i^* H' \psi_j dv$ , and  $\bar{F} = \int \psi_a^* \psi_b dv$ .

Clearly,  $H_{aa}'$  is the energy of the  $^2\Sigma(^1S+^2S)$  state relative to the  $^1S$  atomic level and  $H_{bb}'$  is the energy of the  $^2\Sigma(^3P+^2S)$  state relative to the  $^3P$  atomic level. The evaluation of  $H_{ab}'$  is rather laborious for in this case the permutations on both  $\psi_a$  and  $\psi_b$  must be carried out since the quantum numbers are not the same on both functions. The evaluation gives

integrals occurring in the calculation of the ground state together with the values of the energy  $E'$  of this state.  $E''$  represents the energy of the higher  $^2\Sigma$  molecular state which results from the perturbation in question. The energies  $E'$  are measured from the dissociated state  $^3P+^2S$  while the energies  $E''$  relate to the dissociated state  $^1S+^2S$ .

TABLE V.  $^2\Sigma$  (ground state).

R	$K(s, b; p, b)$	$J''(s, b; s, s)$	$K(p, b; s, b)$	$J''(s, b; s, p)$	$J''(p, b; s, s)$	$H_{ab}'$	$\bar{F}$	$E'$	$E''$
2.0	-0.0937	-0.4132	-0.3278	0.1600	-0.6741	+0.5989	-0.5457	-0.200	+1.307
2.5	-0.1091	-0.4478	-0.2662	0.1445	-0.6999	+0.5387	-0.4254	-0.255	+0.789
3.0	-0.0986	-0.4219	-0.1954	0.1182	-0.6570	+0.4174	-0.3102	-0.230	+0.441
4.0	-0.04077	-0.2998	-0.07254	0.06924	-0.4980	+0.1876	-0.1403	-0.0825	+0.0985
5.0	-0.01392	-0.1870	-0.02264	0.03107	-0.3227	+0.06739	-0.05316	-0.0 <sup>2</sup> 845	+0.0018

## IV. DISCUSSION

The analysis of the band systems of beryllium hydride<sup>7</sup> shows that the electronic transition in question is  ${}^2\Pi$  to  ${}^2\Sigma$  indicating that the normal state is  ${}^2\Sigma$ , dissociating into beryllium in the  ${}^1S$  state and hydrogen in the  ${}^2S$  state. Now it is to be observed from the potential energy curves for earth-alkali hydrides given by Mulliken<sup>8</sup> that, as the separation between the ground state and the first excited state increases, the ground state becomes less attractive. For HgH, the ground state is almost repulsive.

The calculation in Part I shows that a normal beryllium atom and a normal hydrogen atom will combine to give a repulsive molecular state. Mercury hydride would probably be similar, so that the theory seems to check the experimental results here. Accordingly, the reason that the ground state of BeH is, in fact, attractive, must be that the higher  ${}^2\Sigma$  states exert a considerable influence. This is verified by the calculation in Part III.

The calculation in Part II shows that a normal hydrogen atom and a beryllium atom in the  ${}^3P$  atomic state will combine to give an attractive  ${}^2\Pi$  state and to this approximation, an attractive  ${}^2\Sigma$  molecular state, and repulsive  ${}^4\Pi$  and  ${}^4\Sigma$  molecular states. The equilibrium distance is about the same for the attractive states, but the heat of dissociation of the  ${}^2\Sigma$  molecular state is about twice as great as that for the  ${}^2\Pi$  state. This is of no immediate physical interest, because of the perturbing effect of the nearby  ${}^2\Sigma$  state, but it may be helpful in the construction of a more complete theory of "directed" valence. One should note, however, that, of the states arising from  ${}^1P$  and  ${}^2S$ , the  ${}^2\Pi$  is the lower.

For the ground state and the first excited state the following molecular constants have been calculated: (the numbers in brackets refer to the work of Olsson<sup>7</sup>)

State	Internuclear distance (Angstroms)	Heat of dissociation (electron-volts per molecule)
${}^2\Sigma$	1.37 [1.34]	3.5 [2.13]
${}^2\Pi$	1.35 [1.33]	1.5 [2.22]

It is further seen from Fig. 1 that the  ${}^2\Sigma$  state arising from the interaction of a normal hydrogen atom with a  $2s\ 2p\ {}^1P$  beryllium atom is repulsive, which would indicate that the effect of spin valency is more important than that of orbital valency. It is not certain whether the  ${}^2\Pi$  state arising from this configuration is repulsive or slightly attractive at larger internuclear distances than calculated.

In conclusion, the writer wishes to express his indebtedness to Professor J. H. Bartlett, Jr. for suggesting the problem and for his constant interest. Thanks are also due to Dr. W. H. Furry for the use of certain unpublished tables.

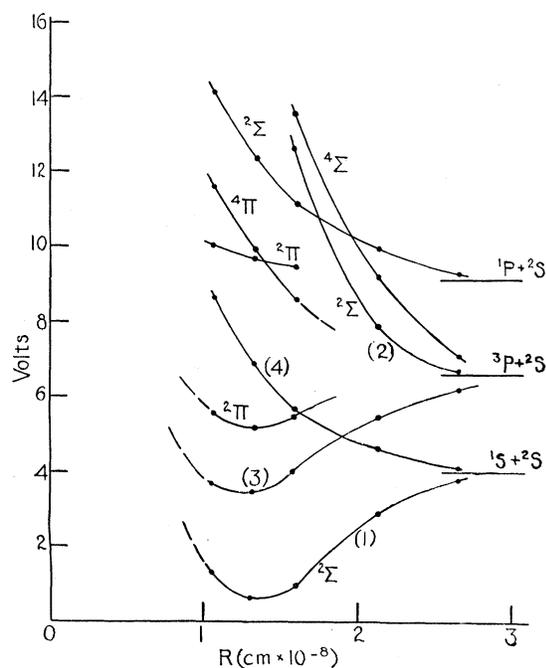


FIG. 1. Potential energy curves for BeH. (1) Ground state, resulting from perturbing effect of the  ${}^2\Sigma({}^1S+{}^2S)$  state on the  ${}^2\Sigma({}^3P+{}^2S)$  state. (2)  ${}^2\Sigma({}^1S+{}^2S)$  state after being perturbed by the  ${}^2\Sigma({}^3P+{}^2S)$  state. (3)  ${}^2\Sigma({}^3P+{}^2S)$  state, neglecting perturbation by other states. (4)  ${}^2\Sigma({}^1S+{}^2S)$  state, neglecting perturbation by other states.

<sup>7</sup> Ernst Olsson, Zeits. f. Physik 73, 732 (1932).

<sup>8</sup> R. S. Mulliken, Rev. Mod. Phys. 4, 8 (1932).

## APPENDIX: TABULATION OF INTEGRALS

I.  $\Sigma$  states

$$S^{\frac{1}{2}} = [R^4/4(3)^{\frac{1}{2}}][A_3(1, R) - \frac{1}{3}A_1(1, R)],$$

$$S^{\frac{1}{2}}(pb) = (3^{\frac{1}{2}}R/4)I_b(sb),$$

$$I_b(sb) = (R^3/3^{\frac{1}{2}})[A_2(1, R) - \frac{1}{3}A_0(1, R)],$$

$$I_b(bb) = 8R^2[A_2(0, 2R) - A_2(1, 2R)],$$

$$I_a(ss) = (8R^4/3)[A_4(0, 2R) - A_4(1, 2R) + A_3(1, 2R)],$$

$$I_a(sb) = (R^3/3^{\frac{1}{2}})[A_2(1, R) + \frac{1}{3}A_0(1, R)],$$

$$I_a(pp) = (8R^4/15)[2A_1(1, 2R) + 5A_3(1, 2R) + 5A_4(0, 2R) - 5A_4(1, 2R) + 2A_6(0, 2R) - 2A_6(1, 2R)],$$

$$I_a(pb) = (4R^3/3)A_1(1, R),$$

$$I_b(pb) = \frac{1}{2}I_a(pb),$$

$$I_a(ps) = (8R^4/3(3)^{\frac{1}{2}})[A_2(1, 2R) + A_5(0, 2R) - A_5(1, 2R)],$$

$$J(ss; bb) = 2/R + j(ss; bb) - I_b(bb) - I_a(ss),$$

$$K(sb; sb) = 2S/R + k(sb; sb) - S^{\frac{1}{2}}I_b(sb) - S^{\frac{1}{2}}I_a(sb),$$

$$J''(ss; sb) = 2S^{\frac{1}{2}}/R + j''(ss; sb) - I_b(sb) - S^{\frac{1}{2}}I_a(ss),$$

$$K(pb; pb) = 2S(p)/R + k(pb; pb) - S^{\frac{1}{2}}(p)[I_b(pb) + I_a(pb)],$$

$$J''(ps; pb) = j''(ps; pb) - S^{\frac{1}{2}}(p)I_a(ps),$$

$$J''(pp; sb) = 2S^{\frac{1}{2}}/R + j''(pp; sb) - I_b(sb) - S^{\frac{1}{2}}I_a(pp),$$

$$J''(ss; pb) = 2S^{\frac{1}{2}}(p)/R + j''(ss; pb) - I_b(pb) - S^{\frac{1}{2}}(p)I_a(ss),$$

$$J''(sp; sb) = j''(sp; sb) - S^{\frac{1}{2}}I_a(ps),$$

$$J''(sb; sp) = j''(sp; sb),$$

$$J''(pb; ss) = 2S^{\frac{1}{2}}(p)/R + j''(ss; pb) - S^{\frac{1}{2}}(p) - I_a(pb),$$

$$K(pb; sb) = 2S^{\frac{1}{2}}S^{\frac{1}{2}}(p)/R + k(pb; sb) - S^{\frac{1}{2}}(p)I_b(sb) - S^{\frac{1}{2}}I_a(pb),$$

$$K(sb; pb) = 2S^{\frac{1}{2}}S^{\frac{1}{2}}(p)/R + k(pb; sb) - S^{\frac{1}{2}}I_b(pb) - S^{\frac{1}{2}}(p)I_a(sb),$$

$$J''(sb; ss) = 2S^{\frac{1}{2}}/R + [j''(ss; sb) - I_b(sb)] + I_b(sb) - S^{\frac{1}{2}} - I_a(sb),$$

$$j(ss; bb) - I_a(ss) = (R^5/60)[A_0(1, 2R) - 5A_4(1, 2R)] - (R^4/6)[A_1(1, 2R) + A_3(1, 2R)],$$

$$k(sb; sb)^{(0)} = (R^7/12)[v_0(3, 3, 2R) - \frac{2}{3}v_0(3, 1, 2R) + (1/9)v_0(1, 1, 2R)],$$

$$k(sb; sb)^{(1)} = (R^7/4)[(1/9)v_1(2, 2, 2R) - (2/15)v_1(2, 0, 2R) + (1/25)v_1(0, 0, 2R)],$$

$$k(sb; sb)^{(2)} = (4R^7/135)v_2(2, 2, 2R),$$

$$\begin{aligned} j''(ss; sb) - I_b(sb) = & -[R^3/24(3)^{\frac{1}{2}}]\{(R^3/2)[B_0(R)A_5(1, 2R) + 3B_1(R)A_4(1, 2R) + 2B_2(R)A_3(1, 2R) \\ & - 2B_3(R)A_2(1, 2R) - 3B_4(R)A_1(1, 2R) - B_5(R)A_0(1, 2R)] + 3R^2[B_0(R)A_4(1, 2R) \\ & + 2B_1(R)A_3(1, 2R) - 2B_3(R)A_1(1, 2R) - B_4(R)A_0(1, 2R)] + 9R[B_0(R)A_3(1, 2R) \\ & + B_1(R)A_2(1, 2R) - B_2(R)A_1(1, 2R) - B_3(R)A_0(1, 2R)] + 12[B_0(R)A_2(1, 2R) - B_2(R)A_0(1, 2R)]\}, \end{aligned}$$

$$k(pb; pb)^{(0)} = (R^7/4)[v_0(2, 2, 2R) - \frac{2}{3}v_0(2, 0, 2R) + (1/9)v_0(0, 0, 2R)],$$

$$k(pb; pb)^{(1)} = (3R^7/4)[(1/9)v_1(3, 3, 2R) - (2/15)v_1(3, 1, 2R) + (1/25)v_1(1, 1, 2R)],$$

$$k(pb; pb)^{(2)} = (4R^7/45)v_2(0, 0, 2R),$$

$$\begin{aligned} j''(ps; pb)^{(0)} = & [R_3/16(3)^{\frac{1}{2}}][B_1(R)v_0(4, 2, 2R) + (B_0(R) + B_2(R))v_0(3, 2, 2R) \\ & + (B_1(R) - B_3(R))v_0(2, 2, 2R) - (B_2(R) + B_4(R))v_0(1, 2, 2R) - B_3(R)v_0(0, 2, 2R) \\ & - \frac{1}{3}B_1(R)v_0(4, 0, 2R) - \frac{1}{3}(B_0(R) + B_2(R))v_0(3, 0, 2R) - \frac{1}{3}(B_1(R) - B_3(R))v_0(2, 0, 2R) \\ & + \frac{1}{3}(B_2(R) + B_4(R))v_0(1, 0, 2R) + \frac{1}{3}B_3(R)v_0(0, 0, 2R)] \end{aligned}$$

$$\begin{aligned} j''(ps; pb)^{(1)} = & [3R^8/16(3)^{\frac{1}{2}}][\frac{1}{3}B_2(R)v_1(4, 3, 2R) + \frac{1}{3}(B_1(R) + B_3(R))v_1(3, 3, 2R) \\ & + \frac{1}{3}(B_2(R) - B_4(R))v_1(2, 3, 2R) - \frac{1}{3}(B_3(R) + B_5(R))v_1(1, 3, 2R) - \frac{1}{3}B_4(R)v_1(0, 3, 2R) \\ & - \frac{1}{5}B_2(R)v_1(4, 1, 2R) - \frac{1}{5}(B_1(R) + B_3(R))v_1(3, 1, 2R) - \frac{1}{5}(B_2(R) - B_4(R))v_1(2, 1, 2R) \\ & + \frac{1}{5}(B_3(R) + B_5(R))v_1(1, 1, 2R) + \frac{1}{5}B_4(R)v_1(0, 1, 2R)], \end{aligned}$$

$$\begin{aligned} j''(ps; pb)^{(2)} = & -[R^8/12(3)^{\frac{1}{2}}][C_1(R)v_2(4, 0, 2R) + (C_0(R) + C_2(R))v_2(3, 0, 2R) \\ & + (C_1(R) - C_3(R))v_2(2, 0, 2R) - (C_2(R) + C_4(R))v_2(1, 0, 2R) - C_3(R)v_2(0, 0, 2R)], \end{aligned}$$

$$\begin{aligned} j''(pp; sb)^{(0)} = & [R^8/16(3)^{\frac{1}{2}}][(B_0(R) - B_4(R))v_0(2, 3, 2R) + 2B_1(R)v_0(3, 3, 2R) - 2B_3(R)v_0(1, 3, 2R) \\ & + B_2(R)v_0(4, 3, 2R) - B_2(R)v_0(0, 3, 2R) - \frac{1}{3}(B_0(R) - B_4(R))v_0(2, 1, 2R) - \frac{2}{3}B_1(R)v_0(3, 1, 2R) \\ & + \frac{2}{3}B_3(R)v_0(1, 1, 2R) - \frac{1}{3}B_2(R)v_0(4, 1, 2R) + \frac{1}{3}B_2(R)v_0(0, 1, 2R)], \end{aligned}$$

$$\begin{aligned} j''(pp; sb)^{(1)} = & [3R^8/16(3)^{\frac{1}{2}}][\frac{1}{3}(B_1(R) - B_5(R))v_1(2, 2, 2R) + \frac{2}{3}B_2(R)v_1(3, 2, 2R) - \frac{2}{3}B_4(R)v_1(1, 2, 2R) \\ & + \frac{1}{3}B_3(R)v_1(4, 2, 2R) - \frac{1}{3}B_3(R)v_1(0, 2, 2R) - \frac{1}{5}(B_1(R) - B_5(R))v_1(2, 0, 2R) - \frac{2}{5}B_2(R)v_1(3, 0, 2R) \\ & + \frac{2}{5}B_4(R)v_1(1, 0, 2R) - \frac{1}{5}B_3(R)v_1(4, 0, 2R) + \frac{1}{5}B_3(R)v_1(0, 0, 2R)], \end{aligned}$$

$$\begin{aligned} j''(pp; sb)^{(2)} = & -[R^8/12(3)^{\frac{1}{2}}][(C_0(R) - C_4(R))v_2(2, 1, 2R) + 2C_1(R)v_2(3, 1, 2R) - 2C_3(R)v_2(1, 1, 2R) \\ & + C_2(R)(v_2(4, 1, 2R) - v_2(0, 1, 2R))], \end{aligned}$$

$$\begin{aligned} j''(ss; pb) - I_6(pb) = & -(R^8/6)\{(R^3/8)[(B_0(R) + 2B_2(R))A_4(1, 2R) + B_1(R)(2A_3(1, 2R) + A_5(1, 2R)) \\ & - B_4(R)(A_2(1, 2R) + A_0(1, 2R)) - (2B_3(R) + B_5(R))A_1(1, 2R)] + (3R^2/4)[B_1(R)A_4(1, 2R) \\ & + (B_0(R) + B_2(R))A_3(1, 2R) + (B_1(R) - B_3(R))A_2(1, 2R) - (B_2(R) + B_4(R))A_1(1, 2R) \\ & - B_3(R)A_0(1, 2R)] + (9R/4)[B_0(R)A_2(1, 2R) - B_2(R)A_0(1, 2R) + B_1(R)A_3(1, 2R) \\ & - B_3(R)A_1(1, 2R)] + 3B_0(R)A_1(1, 2R) + 3B_1(R)(A_2(1, 2R) - A_0(1, 2R)) - B_2(R)A_1(1, 2R)\}, \end{aligned}$$

$$\begin{aligned} j''(sp; sb)^{(0)} = & (R^8/48)\{B_1(R)v_0(4, 3, 2R) + [B_0(R) + B_2(R)]v_0(3, 3, 2R) + [B_1(R) - B_3(R)]v_0(2, 3, 2R) \\ & - [B_2(R) + B_4(R)]v_0(1, 3, 2R) - B_3(R)v_0(0, 3, 2R) - \frac{1}{3}[B_1(R)v_0(4, 1, 2R) \\ & + (B_0(R) + B_2(R))v_0(3, 1, 2R) + (B_1(R) - B_3(R))v_0(2, 1, 2R) - (B_2(R) + B_4(R))v_0(1, 1, 2R) \\ & - B_3(R)v_0(0, 1, 2R)]\}, \end{aligned}$$

$$\begin{aligned} j''(sp; sb)^{(1)} = & (R^8/16)\{B_2(R)v_1(4, 2, 2R) + (B_1(R) + B_3(R))v_1(3, 2, 2R) + (B_2(R) - B_4(R))v_1(2, 2, 2R) \\ & - (B_3(R) + B_5(R))v_1(1, 2, 2R) - B_4(R)v_1(0, 2, 2R) - \frac{1}{5}[B_2(R)v_1(4, 0, 2R) \\ & + (B_1(R) + B_3(R))v_1(3, 0, 2R) + (B_2(R) - B_4(R))v_1(2, 0, 2R) - (B_3(R) + B_5(R))v_1(1, 0, 2R) \\ & - B_4(R)v_1(0, 0, 2R)]\}, \end{aligned}$$

$$\begin{aligned} j''(sp; sb)^{(2)} = & -(R^8/36)[C_1(R)v_2(4, 1, 2R) + (C_0(R) + C_2(R))v_2(3, 1, 2R) \\ & + (C_1(R) - C_3(R))v_2(2, 1, 2R) - (C_2(R) + C_4(R))v_2(1, 1, 2R) - C_3(R)v_2(0, 1, 2R)], \end{aligned}$$

$$k(pb; sb)^{(0)} = [R^7/4(3)^{\frac{1}{2}}][v_0(2, 3, 2R) - \frac{1}{3}v_0(2, 1, 2R) - \frac{1}{3}v_0(0, 3, 2R) + (1/9)v_0(0, 1, 2R)],$$

$$k(pb; sb)^{(1)} = [3R^7/4(3)^{\frac{1}{2}}][\frac{1}{9}v_1(3, 2, 2R) - \frac{1}{15}v_1(3, 0, 2R) - \frac{1}{15}v_1(1, 2, 2R) \\ + \frac{1}{25}v_1(1, 0, 2R)],$$

$$k(pb; sb)^{(2)} = [R^7/45(3)^{\frac{1}{2}}]v_2(0, 1, 2R).$$

## II. II states

$$I_a(pp) = (R^4/8)\{[B_0(R) - B_2(R)][A_3(1, R) - A_1(1, R)] + [B_1(R) - B_3(R)][A_2(1, R) - A_0(1, R)]\},$$

$$j(p^*p; bb) - I_a(pp) = -(R^4/6)[A_3(1, 2R) - A_1(1, 2R)] - (R^5/60)[5A_4(1, 2R) \\ - 6A_2(1, 2R) + A_0(1, 2R)],$$

$$K(pb; p^*b) = -(R^7/60)[2.5w_1(2, 2, 2R) - w_1(2, 0, 2R) + \frac{1}{10}w_1(0, 0, 2R)],$$

$$J''(ps; p^*b) = -[R^8/320(3)^{\frac{1}{2}}]\{[B_0(R) - B_2(R)][5w_1(3, 2, 2R) - w_1(3, 0, 2R)] \\ + [B_1(R) - B_3(R)][5w_1(2, 2, 2R) - w_1(2, 0, 2R)] - [B_2(R) - B_4(R)][5w_1(1, 2, 2R) \\ - w_1(1, 0, 2R)] - [B_3(R) - B_5(R)][5w_1(0, 1, 2R) - w_1(0, 0, 2R)]\},$$

$$j''(p^*p; sb)^{(0)} = [R^8/32(3)^{\frac{1}{2}}]\{[B_0(R) - B_2(R)][v_0(4, 3, 2R) - \frac{1}{3}v_0(4, 1, 2R)] \\ - [B_0(R) - B_4(R)][v_0(2, 3, 2R) - \frac{1}{3}v_0(2, 1, 2R)] + [B_2(R) - B_4(R)][v_0(0, 3, 2R) - \frac{1}{3}v_0(0, 1, 2R)]\},$$

$$j''(p^*p; sb)^{(1)} = [3R^8/32(3)^{\frac{1}{2}}]\{[B_1(R) - B_3(R)][\frac{1}{3}v_1(4, 2, 2R) - \frac{1}{5}v_1(4, 0, 2R)] \\ - [B_1(R) - B_5(R)][\frac{1}{3}v_1(2, 2, 2R) - \frac{1}{5}v_1(2, 0, 2R)] \\ + [B_3(R) - B_5(R)][\frac{1}{3}v_1(0, 2, 2R) - \frac{1}{5}v_1(0, 0, 2R)]\},$$

$$j''(p^*p; sb)^{(2)} = -[R^8/24(3)^{\frac{1}{2}}]\{[C_0(R) - C_2(R)]v_2(4, 1, 2R) - [C_0(R) - C_4(R)]v_2(2, 1, 2R) \\ + [C_2(R) - C_4(R)]v_2(0, 1, 2R)\}.$$