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Accurate electronic energies of He_2^{++}

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Accurate adiabatic potential curves are calculated for the ground state and 11 excited states of He_2^{++} using the James-Coolidge method. The values are the best of all existing results for this system. The number of basis sets used was 75 for ${}^1\Sigma_g^+$ and 57 for ${}^1\Sigma_u^+$, ${}^3\Sigma_g^+$, and ${}^3\Sigma_u^+$. The ground-state energy curve has both a dip and a peak. A dip is also expected for the lowest ${}^1\Sigma_u^+$ state.

I. INTRODUCTION

Today we have many methods for studying particle-scattering problems in the low-energy region. Most of them require complete sets or isolated atomic states for bases. However, the use of precise adiabatic potentials and their corresponding wave functions may be, though cumbersome, a more powerful approach to such cross sections as charge transfer and excitation transfer in that they contain all the necessary information except for nonadiabatic effects. Thus the transition between two adiabatic states occurs due to these latter effects.

Meanwhile, the multicharge transfer process between heavy atoms has been spotlighted recently in connection with fundamental studies in nuclear fusion. Furthermore, there are experiments on He^{++}-He collisions,[1,2] such as

$$\begin{aligned} He^{++} + He &\to He + He^{++} \\ &\to He^{+} + He^{+} . \end{aligned}$$

For the theoretical analysis of these processes, precise potential curves are highly desirable.

Calculations for the ground state of He_2^{++} have been published by several authors.[3-5] Its excited states, however, have been given, to our knowledge, only by Browne,[6] who performed mixed basis-set calculations.

The purpose of this paper is to report the most accurate energies obtained so far for the ground and excited states of He_2^{++} using the James-Coolidge (JC) method.[7] Provided computer time is not a problem, the JC method for two-electron diatomic molecules yields energies to essentially any accuracy desired. Kotos and Roothaan,[3] using this method, calculated the ground state with 40 basis functions. Our calculation gives the "best" (lowest) ground-state energy of all existing works. We also calculated 11 excited states.

II. CALCULATION AND RESULTS

The ith-state electronic wave function ψ_i of He_2^{++} in the JC method is the linear combination of bases:

$$\psi_i = \sum_{n,m,j,k,p} C^i_{nmjkp}(\lambda_1^n \lambda_2^m \mu_1^j \mu_2^k \pm \lambda_1^m \lambda_2^n \mu_1^k \mu_2^j) \times \rho^p e^{-\alpha(\lambda_1+\lambda_2)} , \tag{1}$$

where C^i_{nmjkp} is a coefficient and the other arguments, using notations in Fig. 1, are

$$\begin{aligned} &\lambda_1 = (r_{a1} + r_{b1})/R , \quad \lambda_2 = (r_{a2} + r_{b2})/R , \\ &\mu_1 = (r_{a1} - r_{b1})/R , \quad \mu_2 = (r_{a2} - r_{b2})/R , \\ &\rho = 2r_{12}/R , \end{aligned} \tag{2}$$

and α is an orbital exponent. The sign + (−) indicates a singlet (triplet) state. The electronic Hamiltonian of He_2^{++} in atomic units (used throughout this paper) is

$$H = -\sum_{k=1,2}\left(\frac{\Delta_k}{2} + \frac{2}{r_{ak}} + \frac{2}{r_{bk}}\right) + \frac{1}{r_{12}} , \tag{3}$$

and then the ith energy state E_i is given by

$$E_i = \langle \psi_i | H | \psi_i \rangle + 4/R . \tag{4}$$

The summation of (1) over all positive integers n, m, j, k, and p is not allowed, but is subject to the restriction

$$m + n + j + k + p \geq 5 . \tag{5}$$

The number of bases under (5) is 75 for ${}^1\Sigma_g^+$ and 57

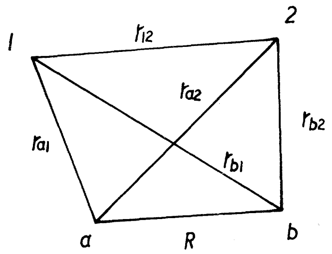

FIG. 1. Coordinate system for two helium atoms. The two nuclei and two electrons are at a, b, 1, and 2, respectively. The symbol alongside each interparticle line denotes distance.

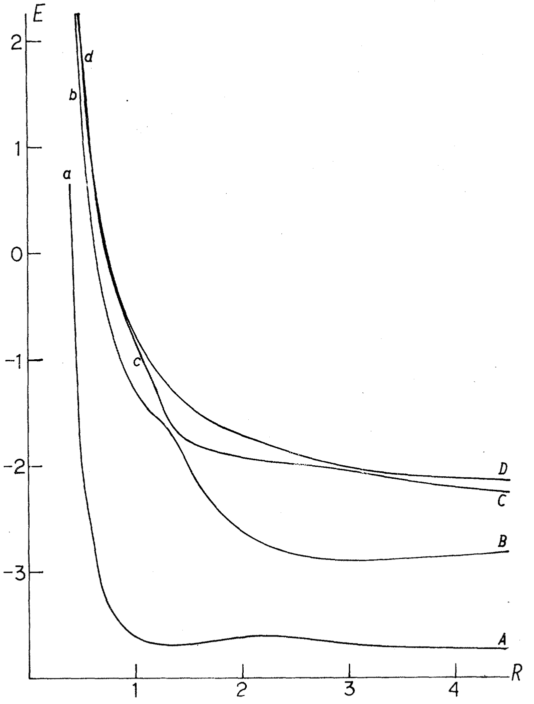

FIG. 2. Curves of the lowest $^1\Sigma_g^+$ adiabatic electronic potentials that were found: $E_1(^1\Sigma_g^+)$, $E_2(^1\Sigma_g^+)$, $E_3(^1\Sigma_g^+)$, and $E_4(^1\Sigma_g^+)$ of He_2^{++}.

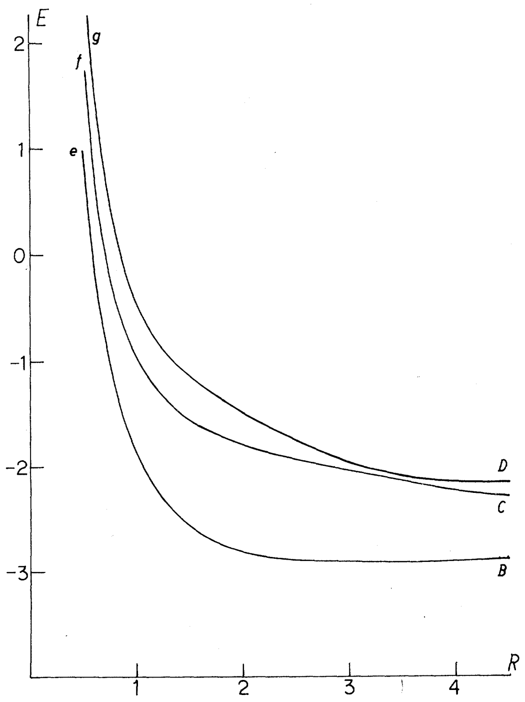

FIG. 3. Curves of the three lowest $^1\Sigma_u^+$ adiabatic electronic potentials $E_1(^1\Sigma_u^+)$, $E_2(^1\Sigma_u^+)$, and $E_3(^1\Sigma_u^+)$ of He_2^{++}.

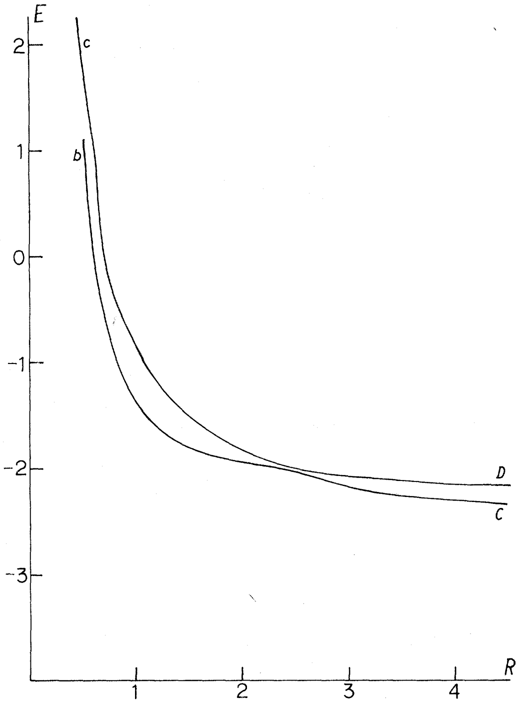

FIG. 4. Curves of the two lowest $^3\Sigma_g^+$ adiabatic electronic potentials $E_1(^3\Sigma_g^+)$ and $E_2(^3\Sigma_g^+)$ of He_2^{++}.

for $^1\Sigma_u^+$, $^3\Sigma_g^+$, and $^3\Sigma_u^+$. The exponent α is unknown, but is determined by trial and error so as to optimize (minimize) each level for each R.

First, we fix R and calculate each level as a function of α. Then, for the ith level, the best energy is the minimum of the energy functional for that level. This minimum point is decided generally by interpolation, because the function is discrete because of discrete choices for α. Iterating this procedure for various values of R and linking the minimum points of the level, the adiabatic potential curve is obtained.

We used a program[8] (see Appendix) which will soon be stored in the program library of the Computer Center at the University of Tokyo. The α values chosen are 0.50, 0.75, 1.00, 1.25, 1.50, 1.75, 2.00, 2.25, 2.50, 2.75, 3.00, and 3.50. The potential curves obtained are shown in Figs. 2, 3, 4, and 5 for the $^1\Sigma_g^+$, $^1\Sigma_u^+$, $^3\Sigma_g^+$, and $^3\Sigma_u^+$ states, respectively. Their values are listed in Tables I, II, III, and IV. In the figures, only 11 excited states are shown, because other higher states seem to be unreliable with such small basis sets. These states are assigned to (a) $\mathrm{He}^+(1s)+\mathrm{He}^+(1s)$, (b) $\mathrm{He}^{++}+\mathrm{He}(1s,1s)$, (c) $\mathrm{He}^+(1s)+\mathrm{He}^+(2s)$, and (d) $\mathrm{He}^+(1s)+\mathrm{He}^+(2p)$ at the infinitely-large-R limit, and their energies must converge to -4.0, -2.5, -2.5, and -2.903722, respectively.

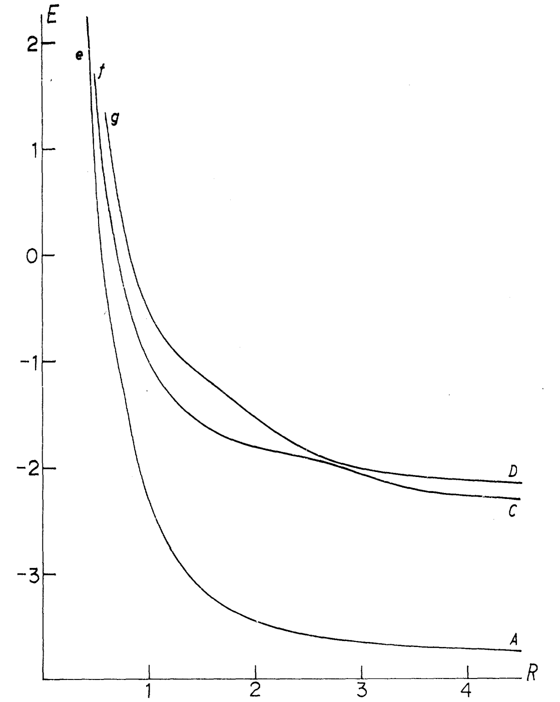

FIG. 5. Curves of the three lowest ${}^3\Sigma_u^+$ adiabatic electronic potentials $E_1({}^3\Sigma_u^+)$, $E_2({}^3\Sigma_u^+)$, and $E_3({}^3\Sigma_u^+)$ of He_2^{++}.

In the united-atom limit we obtain the states of He^{++}. All 12 states are assigned as follows: (a) $\mathrm{He}^{++}(1s,1s)$, (b) $\mathrm{He}^{++}(1s,2s)$, (c) $\mathrm{He}^{++}(1s,3s)$, (d) $\mathrm{He}^{++}(1s,3d)$, (e) $\mathrm{He}^{++}(1s,2p)$, (f) $\mathrm{He}^{++}(1s,3p)$, and (g) $\mathrm{He}^{++}(1s,4p)$.

The range of R is from 0.4 to 4.5. The present ground-state energy of −3.672960 at $R=1.2$, for example, is lower than Kotos and Roothaan's[3] −3.671966 and Mackrodt's[5] −3.56028. At $R=1.3$ our −3.681093 is lower than Kotos and Roothaan's −3.679636, Mackrodt's −3.553532 and Schwartz's[4] −3.60930. Our −3.643471 at $R=1.8$ is much better than Kotos and Roothaan's −3.6355 and Mackrodt's −3.408757. The difference between our results and those of Ref. 3 consists only in the different number of expansion terms, i.e., the addition of 35 terms to their 40 lowers the energies by 0.07–0.001. The ground state has at $R=1.33$ a dip of −3.681662 and at $R=2.17$ a peak of −3.626507 and may converge to −4.0 at $R\to\infty$. Also found are minima for $E_1({}^1\Sigma_u^+)$ and $E_2({}^1\Sigma_g^+)$. Those states are $\mathrm{He}^{++}+\mathrm{He}(1s, 1s)$, and the minima are expected[6] from the polarization effect due to bare and neutral helium atoms. The state $E_1({}^1\Sigma_u^+)$, from Table II and interpolation, has the minimum −2.916289 at $R=3.15$, which should be compared with Browne's −2.914722 at

TABLE I. The four lowest adiabatic potentials $E_1({}^1\Sigma_g^+)$, $E_2({}^1\Sigma_g^+)$, $E_3({}^1\Sigma_g^+)$, and $E_4({}^1\Sigma_g^+)$ of the ${}^1\Sigma_g^+$ state of He_2^{++}.

R	α	$-E_1({}^1\Sigma_g^+)$	α	$-E_2({}^1\Sigma_g^+)$	α	$-E_3({}^1\Sigma_g^+)$	α	$-E_4({}^1\Sigma_g^+)$
0.400	0.700	−0.642 899	0.427	−2.728 796			0.362	−3.466 142
0.500	0.879	1.948 626	0.476	−1.173 869	0.423	−1.806 515	0.444	−1.835 720
0.600	1.028	2.677 649	0.553	−0.229 844	0.479	−0.845 578	0.510	−0.833 808
0.700	1.210	3.103 879	0.638	0.382 217	0.571	−0.213 552	0.545	−0.192 274
0.800	1.250	3.358 481	0.738	0.796 131	0.656	0.290 513	0.584	0.249 266
0.900	1.375	3.510 705	0.750	1.087 210	0.745	0.623 259	0.616	0.576 791
1.000	1.425	3.599 729	0.751	1.297 034	0.815	0.876 838	0.639	0.792 640
1.100	1.531	3.648 961	0.890	1.452 087	0.865	1.082 482	0.718	0.960 330
1.200	1.635	3.672 96	0.972	1.569 138	0.982	1.303 976	0.863	1.140 221
1.300	1.699	3.681 096	1.060	1.665 448	1.114	1.566 746	0.973	1.277 585
1.400	1.748	3.679 574	1.252	1.831 235	1.107	1.712 347	1.052	1.380 147
1.500	1.892	3.672 587	1.366	2.031 251	1.124	1.771 580	1.112	1.461 988
1.600	1.964	3.663 016	1.500	2.201 377	1.197	1.814 441	1.189	1.528 498
1.700	2.070	3.652 854	1.625	2.343 232	1.279	1.849 488	1.272	1.587 132
1.800	2.159	3.643 471	1.847	2.460 550	1.336	1.878 409	1.350	1.638 919
1.900	2.250	3.635 764	1.875	2.557 002	1.369	1.902 799	1.432	1.685 294
2.000	2.323	3.630 249	2.067	2.635 618	1.425	1.923 088	1.515	1.727 911
2.100	2.439	3.627 189	2.170	2.699 137	1.501	1.941 419	1.600	1.767 459
2.200	2.504	3.626 565	2.265	2.749 857	1.572	1.955 097	1.684	1.804 542
2.300	2.645	3.628 211	2.398	2.789 897	1.614	1.973 563	1.765	1.839 542
2.400	2.742	3.631 831	2.489	2.821 028	1.683	1.987 629	1.849	1.872 695
2.500	2.851	3.637 001	2.545	2.844 848	1.756	2.001 540	1.931	1.904 189
2.700	3.052	3.650 655	2.817	2.875 915	1.866	2.028 640	2.086	1.962 048
3.000	3.614	3.675 582	3.091	2.895 327	2.089	2.070 237	2.266	2.033 368
3.500	3.949	3.711 879	3.546	2.892 370	2.685	2.154 309	2.728	2.081 873
4.000	4.499	3.739 927	3.581	2.871 353	3.056	2.222 012	2.771	2.136 854
4.500	4.943	3.757 366	4.480	2.837 039	3.658	2.265 611	3.084	2.158 740

TABLE II. The three lowest adiabatic total potentials $E_1(^1\Sigma_u^+)$, $E_2(^1\Sigma_u^+)$, and $E_3(^1\Sigma_u^+)$ of the $^1\Sigma_u^+$ state of He_2^{++}.

R	α	$-E_1(^1\Sigma_u^+)$	α	$-E_2(^1\Sigma_u^+)$	α	$-E_3(^1\Sigma_u^+)$
0.400	0.439	−2.612 773	0.351	−3.402 318		
0.500	0.523	−0.987 633	0.426	−1.760 513	0.360	−2.550 209
0.600	0.622	0.033 789	0.489	−0.745 736	0.422	−1.443 440
0.700	0.746	0.721 139	0.571	−0.067 513	0.479	−0.714 779
0.800	0.858	1.214 782	0.622	0.408 540	0.539	−0.192 495
0.900	0.902	1.581 159	0.703	0.727 838	0.588	0.185 451
1.000	1.051	1.861 723	0.784	0.977 735	0.628	0.446 406
1.100	1.122	2.080 402	0.835	1.167 388	0.680	0.656 000
1.200	1.244	2.252 656	0.868	1.312 792	0.748	0.820 297
1.300	1.353	2.389 681	0.937	1.418 189	0.771	0.951 162
1.400	1.442	2.499 092	1.008	1.507 887	0.806	1.056 921
1.500	1.556	2.586 769	1.067	1.580 595	0.838	1.144 855
1.600	1.632	2.657 107	1.115	1.640 363	0.872	1.223 350
1.700	1.735	2.713 556	1.186	1.688 939	0.964	1.293 253
1.800	1.820	2.758 827	1.257	1.731 924	1.054	1.373 001
1.900	1.893	2.795 035	1.324	1.769 685	1.112	1.447 883
2.000	1.896	2.823 956	1.389	1.803 207	1.247	1.512 537
2.100	2.061	2.846 884	1.418	1.834 244	1.293	1.570 635
2.200	2.128	2.864 977	1.544	1.863 194	1.355	1.619 991
2.300	2.217	2.879 157	1.619	1.890 467	1.454	1.661 638
2.400	2.293	2.890 143	1.695	1.916 135	1.614	1.702 209
2.500	2.360	2.898 526	1.770	1.940 371	1.792	1.752 664
2.700	2.520	2.909 304	1.911	1.984 385	1.970	1.858 066
3.000	2.728	2.915 515	2.296	2.041 136	2.226	1.987 987
3.500	3.175	2.912 056	2.511	2.140 199	2.437	2.110 899
4.000	3.560	2.898 994	3.093	2.230 944	2.709	2.140 969
4.500	4.047	2.882 364	3.493	2.285 724	2.996	2.163 957

TABLE III. The two lowest adiabatic total potentials $E_1(^3\Sigma_g^+)$ and $E_2(^3\Sigma_g^+)$ of the $3\Sigma_g^+$ state of He_2^{++}.

R	α	$-E_1(^3\Sigma_g^+)$	α	$-E_2(^3\Sigma_g^+)$
0.400	0.425	−2.634 818		
0.500	0.480	−1.085 034	0.396	−1.731 681
0.600	0.602	−0.144 815	0.438	−0.754 414
0.700	0.642	0.461 504	0.534	0.123 700
0.800	0.766	0.871 789	0.605	0.325 476
0.900	0.844	1.159 474	0.713	0.634 169
1.000	0.868	1.366 182	0.797	0.886 203
1.100	0.905	1.515 665	0.840	1.081 345
1.200	0.991	1.627 916	0.867	1.233 883
1.300	1.063	1.712 843	0.931	1.342 594
1.400	1.107	1.777 944	1.008	1.443 522
1.500	1.145	1.827 926	1.064	1.529 755
1.600	1.216	1.867 408	1.104	1.604 329
1.700	1.279	1.898 911	1.170	1.665 224
1.800	1.329	1.924 470	1.261	1.724 339
1.900	1.367	1.945 587	1.326	1.778 587
2.000	1.429	1.963 094	1.428	1.826 515
2.100	1.493	1.978 534	1.490	1.872 556
2.200	1.546	1.992 384	1.567	1.915 497
2.300	1.594	2.005 315	1.626	1.954 093
2.400	1.663	2.018 236	1.726	1.989 555
2.500	1.825	2.036 250	1.771	2.016 969
2.700	2.033	2.091 245	1.833	2.044 079
3.000	2.303	2.164 910	2.002	2.074 031
3.500	2.763	2.250 964	2.293	2.117 600
4.000	3.283	2.303 091	2.585	2.150 199
4.500	3.752	2.332 113	2.874	2.170 897

$R = 3.25$. The minimum of $E_2(^1\Sigma_g^+)$ at $R = 3.21$ is delicate. The value is −2.899464, higher than but close to the ultimately convergent −2.903722. Thus it must have a peak at least beyond $R = 4.5$. In contrast, Browne obtained −2.912783 at $R = 3.75$. His case need not necessarily have a peak. Finally, a slight difference still appears between the singlet and triplet state at $R = 4.5$, although it vanishes at $R \rightarrow \infty$. The difference between the u and g states with the same spin multiplicity is too small to be shown graphically.

What interests us most is the existence of vibrational levels in $E_1(^1\Sigma_g^+)$, $E_2(^1\Sigma_g^+)$, and $E_1^+(^1\Sigma_u^+)$ states. The frequency, depth of dip, and possible number N of the vibrational states of each electronic state are listed in Table 5. We expect that experiments will be able to observe the vibrational levels.

TABLE IV. The three lowest adiabatic total potentials $E_1(^3\Sigma_u^+)$, $E_2(^3\Sigma_u)$, and $E_3(^3\Sigma_u)$ of the $^3\Sigma_u$ state of He_2^{++}.

	Frequency (cm^{-1})	Depth (eV)	N
$E_1(^1\Sigma_g^+)$	2540	1.62	5
$E_2(^1\Sigma_g^+)$	1080	1.70	10
$E_1(^1\Sigma_u^+)$	680	0.80	10

TABLE V. The three lowest adiabatic total potentials $E_1(^3\Sigma_u^+)$, $E_2(^3\Sigma_u)$, and $E_3(^3\Sigma_u)$ of the $^3\Sigma_u$ state of He_2^{++}.

R	α	$-E_1(^3\Sigma_u^+)$	α	$-E_2(^3\Sigma_u^+)$	α	$-E_3(^3\Sigma_u^+)$
0.400	0.446	−2.456996				
0.500	0.571	−0.784698	0.428	−1.677479		
0.600	0.599	0.287247	0.496	−0.670890	0.409	−1.339295
0.700	0.843	1.031084	0.588	0.004666	0.454	−0.614913
0.800	0.884	1.575250	0.640	0.456146	0.527	−0.104246
0.900	1.031	1.987458	0.731	0.785848	0.583	0.269546
1.000	1.128	2.306840	0.806	1.030990	0.621	0.540613
1.100	1.231	2.557998	0.850	1.216234	0.686	0.704784
1.200	1.354	2.757710	0.872	1.358182	0.748	0.859939
1.300	1.506	2.917861	0.944	1.458113	0.794	0.982330
1.400	1.561	3.047253	1.020	1.544187	0.829	1.078014
1.500	1.636	3.152498	1.077	1.613924	0.857	1.152286
1.600	1.769	3.238677	1.112	1.671054	0.909	1.199896
1.700	1.861	3.309716	1.125	1.715219	1.056	1.275597
1.800	1.980	3.368668	1.248	1.754429	1.118	1.376021
1.900	2.083	3.417960	1.316	1.788840	1.237	1.463810
2.000	2.186	3.459471	1.362	1.819312	1.317	1.543482
2.100	2.300	3.494736	1.436	1.844977	1.345	1.613899
2.200	2.393	3.524918	1.518	1.870213	1.433	1.677617
2.300	2.512	3.550984	1.582	1.894204	1.559	1.740132
2.400	2.609	3.573683	1.637	1.916103	1.636	1.801204
2.500	2.725	3.593600	1.731	1.937964	1.768	1.859756
2.700	2.937	3.626937	1.862	1.979394	1.930	1.963198
3.000	3.263	3.665288	2.258	2.083598	2.080	2.032250
3.500	3.361	3.709587	2.711	2.211500	2.416	2.096260
4.000	4.443	3.737896	3.157	2.280687	2.746	2.135857
4.500	4.936	3.751768	3.585	2.315821	3.095	2.157984

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APPENDIX

The program used, "Householder's Method and QR Algorithm," is listed in Ref. 8 for general use. Moreover, the program will be stored very soon in the library of the Computer Center, University of Tokyo. The most characteristic feature of this program is the quadruple-precision calculation of multiple integrations of the matrix elements.

The Hamiltonian (3) is rewritten as

$$H = T/R^2 + U^{(1)}/R + U^{(12)}/R\ , \tag{A1}$$

where

$$T = -\tfrac{1}{2}(\Delta_1 + \Delta_2)R^2\ , \tag{A2}$$

$$U^{(1)} = \frac{4\lambda_1}{\mu_1^2 - \lambda_1^2} + \frac{4\lambda_2}{\mu_2^2 - \lambda_2^2}\ , \tag{A3}$$

$$U^{(2)} = 2/\rho\ . \tag{A4}$$

If we write

$$[m,n,j,k,p] = N_{mnjkp} \exp[-\alpha(\lambda_1 + \lambda_2)] \times (\lambda_1^m \lambda_2^n \mu_1^j \mu_2^k \pm \lambda_1^n \lambda_2^m \mu_1^k \mu_2^j)\rho^p \tag{A5}$$

(N_{mnjkp} is the normalization constant), then, for example, the matrix element of $U^{(1)}$ becomes

$$U_{fg}^{(1)} = 8\pi^2 N_f N_G (R/2)^6 [u^{(1)}(m_f n_f j_f k_f p_f, m_g n_g j_g k_g p_g; \alpha) \pm u^{(1)}(m_f n_f j_f k_f p_f, n_g m_g k_g j_g p_g; \alpha)]\ , \tag{A6}$$

where

$$u^{(1)}(m_f n_f j_f k_f p_f, m_g n_g j_g k_g p_g; \alpha) = -4[Z(12000) - Z(10020) + Z(21000) - Z(01200)]\ , \tag{A7}$$

$$\left.\begin{aligned} Z(12000) &= Z^0(m_f + m_g + 1, n_f + n_g + 2, j_f + j_g, k_f + k_g, p_f + p_g; 2\alpha)\ , \\ Z(10020) &= Z^0(m_f + m_g + 1, n_f + n_g, j_f + j_g, k_f + k_g + 2, p_f + p_g; 2\alpha)\ , \quad \text{etc.} \end{aligned}\right\} \tag{A8}$$

and

$$Z^{\nu}(m,n,j,k,p;2\alpha)=\frac{1}{4\pi^2}\int \exp[-2d(\lambda_1+\lambda_2)]\lambda_1^m\lambda_2^n\mu_1^j\mu_2^k\rho^p[(\lambda_1^2-1)(\lambda_2^2-1)(1-\mu_1^2)(1-\mu_2^2)]^{\nu/2}\cos^{\nu}(\phi_1-\phi_2)$$
$$\times d\lambda_1 d\lambda_2 d\mu_1 d\mu_2 d\phi_1 d\phi_2 . \quad \text{(A9)}$$

The auxiliary function Z^{ν} is calculated from the recurrence formula:

$$Z^{\nu}(m,n,j,k,p+2;2\alpha)=Z^{\nu}(m+2,n,j,k,p;2\alpha)+Z^{\nu}(m,n+2,j,k,p;2\alpha)$$
$$+Z^{\nu}(m,n,j+2,k,p;2\alpha)+Z^{\nu}(m,n,j,k+2,p;2\alpha)-2Z^{\nu}(m,n,j,k,p;2\alpha)$$
$$-2Z^{\nu}(m+1,n+1,j+1,k+1,p;2\alpha)-2Z^{\nu+1}(m,n,j,k,p;2\alpha) . \quad \text{(A10)}$$

Using (A9) we have

$$Z^0(m,n,j,k,0;2\alpha)=4A_m(2\alpha)A_n(2\alpha)/(j+1)(k+1) , \quad \text{(A11)}$$

$$Z^1(m,n,j,k,0;2\alpha)=0 , \quad \text{(A12)}$$

$$Z^2(m,n,j,k,0;2\alpha)=8[A_{m+2}(2\alpha)-A_m(2\alpha)]$$
$$\times\frac{A_{n+2}(2\alpha)-A_n(2\alpha)}{(j+1)(j+3)(k+1)(k+3)} , \quad \text{(A13)}$$

$$Z^3(m,n,j,k,0;2\alpha)=0 \quad \text{(A14)}$$

when j and k are both even; otherwise these vanish. The function $A_n(x)$ also has a recurrence property,

$$A_n(x)=\int_1^{\infty}\lambda^n e^{-x\lambda}d\lambda=(1/x)[e^{-x}+nA_{n-1}(x)] . \quad \text{(A15)}$$

By making a quadruple-precision calculation of this function, the matrix element $U_{fg}^{(1)}$ is obtained. Calculating other matrix elements is similar but more complicated.

This program is time consuming. To provide necessary auxiliary functions Z^{ν}, it takes about 2 min per one α value and 36 min for 18 α values by HITAC 8700/8800. The time for solving secular equations is 15 sec for a 75 × 75 matrix and 6 sec for a 57 × 57 matrix by the same machine. Thus total CPU time to provide all data from which we picked up adequate values and to optimize energies is about 4 h. The language used is FORTRAN IV.

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