

Tables Useful for the Calculation of the Molecular Integrals IX

Eiichi Ishiguro (石黒英一)

Department of Physics, Faculty of Science,
Ochanomizu University, Tokyo

Tadashi Arai and Michiko Sakamoto

(荒井 正・坂本三知子)

Department of Physics, Faculty of Science,
Kyoto University, Kyoto

In Part IX we give the numerical table for the molecular integrals in the case of homonuclear diatomic molecule including $1s$, $2s$, $2p$ atomic orbitals (AO's). For convenience, we shall explain briefly the conventions here adopted.

(1) Units. We shall use the following atomic units: lengths in units of the Bohr radius $a_0 = 0.5293 \text{ \AA}$; energies in units of $e^2/a_0 = 27.204 \text{ ev}$.

(2) Atomic orbitals. Let α_a, β_a, \dots be the atomic orbitals with their centers at A, and $\gamma_b, \delta_b, \dots$ be those with their centers at B. Their explicit forms are:

$$h_a(1) = (1s)_a = \sqrt{\frac{\delta_1^3}{\pi}} e^{-\delta_1 \gamma_{a1}} \quad (1s \text{ orbital}),$$

$$s_a^o(1) = (2s^o)_a = c_1 h_a(1) + c_2 s_a(1), \quad c_2 > 0 \quad (\text{orthogonalized } 2s \text{ orbital}),$$

where $s_a(1) = (2s)_a = \sqrt{\frac{\delta_2^5}{3\pi}} r_{a1} e^{-\delta_2 \gamma_{a1}} \quad (\text{Slater } 2s \text{ orbital}),$

$$\sigma_a(1) = (2p\sigma)_a = \sqrt{\frac{\delta_2^5}{\pi}} r_{a1} \cos \theta_{a1} e^{-\delta_2 \gamma_{a1}} \quad (2p\sigma \text{ orbital}),$$

$$\pi_a(1) = (2p\pi)_a = \sqrt{\frac{\delta_2^5}{\pi}} r_{a1} \sin \theta_{a1} \cos \varphi_1 e^{-\delta_2 \gamma_{a1}} \quad (2p\pi \text{ orbital}),$$

$$\pi'_a(1) = (2p\pi')_a = \sqrt{\frac{\delta_2^5}{\pi}} r_{a1} \sin \theta_{a1} \sin \varphi_1 e^{-\delta_2 \gamma_{a1}} \quad (2p\pi' \text{ orbital}),$$

$$\pi_a^+(1) = (2p\pi^+)_a = \sqrt{\frac{\delta_2^5}{2\pi}} r_{a1} \sin \theta_{a1} e^{i\varphi_1} \cdot e^{-\delta_2 \gamma_{a1}} = \frac{1}{\sqrt{2}} [\pi_a(1) + i\pi'_a(1)]$$

$$\pi_a^-(1) = (2p\pi^-)_a = \sqrt{\frac{\delta_2^5}{2\pi}} r_{a1} \sin \theta_{a1} e^{-i\varphi_1} \cdot e^{-\delta_2 \gamma_{a1}} = \frac{1}{\sqrt{2}} [\pi_a(1) - i\pi'_a(1)]$$

In the above, the coordinate system is chosen as follows; the position of electron is denoted by P, $r_{a1} = \overline{AP}$, $r_{b1} = \overline{BP}$, $\theta_{a1} = \angle \overline{BAP}$, $\theta_{b1} = \angle \overline{ABP}$.

c_1, c_2 are the constants determined by the orthonormality conditions;

$$\int s_a^o(1)^2 d\tau_1 = 1, \quad \int h_a(1) s_a^o(1) d\tau_1 = 0.$$

(3) Molecular integrals

Integrals	Notations	Definitions
Mononuclear	$J_{\alpha\beta}^o$ $(\alpha_a \frac{1}{r_a} \beta_a)$	$\int \alpha_a(1)^* \left(\frac{1}{r_{a1}}\right) \beta_a(1) d\tau_1$
	$T_{\alpha\beta}^o$ $(\alpha_a -\frac{1}{2} \Delta \beta_a)$	$\int \alpha_a(1)^* \left(-\frac{1}{2} \Delta_1\right) \beta_a(1) d\tau_1$
	$D_{\alpha\beta\gamma\delta}^o$ $(\alpha_a \gamma_a; \beta_a \delta_a)$	$\int \alpha_a(1)^* \gamma_a(1) \left(\frac{1}{r_{12}}\right) \beta_a(2)^* \delta_a(2) d\tau_1 d\tau_2$
Overlap	$S_{\alpha\beta}$ $(\alpha_a \beta_b)$	$\int \alpha_a(1)^* \beta_b(1) d\tau$
Kinetic	$T_{\alpha\beta}$ $(\alpha_a -\frac{1}{2} \Delta \beta_b)$	$\int \alpha_a(1)^* \left(-\frac{1}{2} \Delta_1\right) \beta_b(1) d\tau_1$
Nuclear Attraction	$K_{\alpha\beta}$ $(\alpha_a \frac{1}{r_b} \beta_a)$	$\int \alpha_a(1)^* \left(\frac{1}{r_{b1}}\right) \beta_a(1) d\tau_1$
Resonance	$J_{\alpha\beta}$ $(\alpha_b \frac{1}{r_b} \beta_a)$	$\int \alpha_b(1)^* \left(\frac{1}{r_{b1}}\right) \beta_a(1) d\tau_1$
Coulomb	$D_{\alpha\beta\gamma\delta}$ $(\alpha_a \gamma_a; \beta_b \delta_b)$	$\int \alpha_a(1)^* \gamma_a(1) \left(\frac{1}{r_{12}}\right) \beta_b(2)^* \delta_b(2) d\tau_1 d\tau_2$
Exchange	$C_{\alpha\beta\gamma\delta}$ $(\alpha_a \gamma_b; \beta_b \delta_a)$	$\int \alpha_a(1)^* \gamma_b(1) \left(\frac{1}{r_{12}}\right) \beta_b(2)^* \delta_a(2) d\tau_1 d\tau_2$
Ionic	$L_{\alpha\beta\gamma\delta}$ $(\alpha_a \gamma_a; \beta_a \delta_b)$	$\int \alpha_a(1)^* \gamma_a(1) \left(\frac{1}{r_{12}}\right) \beta_a(2)^* \delta_b(2) d\tau_1 d\tau_2$

(4) Parameters. As parameters we put $\alpha = \delta_1 R$, $\beta = \delta_2 R$, where R is the internuclear distance \overline{AB} .

In table XXVIII we tabulated the molecular integrals for 4 sets of parameters α, β .

Set	I	II	III	IV
α	14.00	13.25	14.00	17.75
β	3.00	3.25	3.50	5.25

Two differences should be mentioned of this table as compared to the table given by Kotani, Amemiya, Ishiguro and Kimura⁽¹⁾, namely,

- (i) here we considered $(2s)^o$ AO instead of $(2s)$ AO.

(ii) the definition of θ_{v1} is different by 180° .

(5) Coefficients C_1, C_2 are found to be

Set	I	II	III	IV
C_1	-0.13673 271	-0.17427 870	-0.18021 926	-0.24051 759
C_2	1.00930 463	1.01507 294	1.01610 973	1.02851 773

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$$L_{\alpha\beta\gamma\delta} = \dots = \int \alpha_a(1)^* \beta_a(2)^* \frac{1}{r_{12}} \gamma_a(1) \delta_b(2) d\tau_1 d\tau_2,$$

References

(1) M. Kotani, A. Amemiya, E. Ishiguro and T. Kimura: Table of Molecular Integrals, Maruzen Co. Ltd., (1955) page 226-230.

(2) E. Ishiguro, T. Arai, M. Sakamoto and K. Takayanagi: Natural Science Rep. Ochanomizu Univ. **6**, 157 (1955).

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Table XXVIII

		$\alpha; \beta$			
		14.00; 3.00	13.25; 3.25	14.00; 3.50	17.75; 5.25
<i>S</i>	hh	0.00006 68	0.00012 81	0.00006 68	0.00000 24
	hs^0	0.06822 09	0.07115 47	0.06193 42	0.22142 23
	$h\sigma$	0.11457 13	0.11848 78	0.10327 44	0.03676 16
	s^0s^0	0.63053 16	0.58397 90	0.54022 37	0.27500 81
	$s^0\sigma$	0.49784 74	0.48731 41	0.47535 05	0.30530 76
	$\sigma\sigma$	0.15931 86	0.21916 52	0.26485 62	0.30528 67
	$\pi\pi$	0.46799 84	0.41734 78	0.37016 96	0.14127 30
<i>J⁰R</i>	hh	14.00000 00	13.25000 00	14.00000 00	17.75000 00
	hs^0	-1.13943 92	-1.35065 99	-1.47179 06	-2.42521 91
	s^0s^0	1.57789 93	1.74269 56	1.88262 25	2.91665 39
	$\sigma\sigma$	1.50000 00	1.62500 00	1.75000 00	2.62500 00
	$\pi\pi$				
<i>JR</i>	hh	0.00017 46	0.00033 24	0.00017 46	0.00000 65
	hs^0	0.48066 83	0.47371 05	0.43403 86	0.19176 30
	s^0h	0.07098 40	0.07479 63	0.06514 06	0.02343 39
	$h\sigma$	0.81620 39	0.79876 64	0.73197 66	0.32071 30
	σh	0.11907 25	0.12437 14	0.10847 72	0.03887 37
	s^0s^0				
	$s^0\sigma$	0.76141 28	0.73271 39	0.71254 56	0.45209 91
	σs^0	0.80227 74	0.79336 72	0.79943 04	0.58579 75
	σs^0	0.54945 36	0.57087 25	0.58627 78	0.47465 51
	$\sigma\sigma$	0.37340 30	0.45319 88	0.51744 47	0.57832 37
	$\pi\pi$	0.52276 42	0.48962 53	0.45358 99	0.21264 75
	<i>KR</i>	hh	1.00000 00	1.00000 00	1.00000 00
hs^0		-0.00000 04	-0.00000 07	-0.00000 03	-0.00000 00
$h\sigma$		0.01840 29	0.02402 93	0.02340 52	0.02348 05
s^0s^0		0.94066 04	0.95681 09	0.96912 68	0.99753 36
$s^0\sigma$		0.37499 46	0.36905 49	0.35980 40	0.27288 46
	$\sigma\sigma$	1.13544 63	1.14417 25	1.14656 59	1.10155 97
	$\pi\pi$	0.84490 08	0.86503 94	0.88186 38	0.94572 28

		$\alpha; \beta$				
		14.00; 3.00	13.25; 3.25	14.00; 3.50	17.75; 5.25	
$T^0 R^2$	hh	98.00000 00	87.78125 00	98.00000 00	157.53125 00	
	hs^0	-15.95214 88	-17.89624 38	-20.60506 83	-43.04763 80	
	$s^0 s^0$	4.05821 31	5.38556 85	6.35189 80	16.45394 11	
	$\sigma\sigma$	4.50000 00	5.28125 00	6.12500 00	13.78125 00	
	$\pi\pi$					
	$(h_a -4/2 h_a) R^2$					
	$(h_a -4/2 s_a^0) R^2$					
	$(s_a^0 -4/2 s_a^0) R^2$					
	$(\sigma_a -4/2 \sigma_a) R^2$					
	$(\pi_a -4/2 \pi_a) R^2$					
TR^2	hh	-0.00410 17	-0.00684 10	-0.00410 17	-0.00026 58	
	hs^0	0.04370 62	0.03061 26	0.00699 14	-0.08430 06	
	hs	0.19886 41	0.18265 05	0.12678 51	-0.09844 70	
	$s^0 s^0$	0.56630 83	0.57012 45	0.55698 53	0.13844 42	
	$s^0 \sigma$	1.05640 83	1.13704 35	1.19242 27	0.77635 74	
	$\sigma\sigma$	1.52348 43	1.78832 62	1.99986 89	1.86516 64	
	$\pi\pi$	1.03059 23	0.97844 67	0.90784 03	0.28587 95	
	$(h_a -4/2 h_b) R^2$					
	$(h_a -4/2 s_b^0) R^2$					
	$(h_a -4/2 \sigma_b) R^2$					
$D^0 R$	$hhhh$	8.75000 00	8.28125 00	8.75000 00	11.09375 00	
	$hhhs^0$	-0.50235 62	-0.58893 31	-0.64066 51	-1.03834 64	
	$hs^0 hs^0$	1.49790 95	1.62153 83	1.74605 11	2.61540 11	
	$hs^0 h\sigma$	1.49614 93	1.61862 57	1.74272 00	2.60687 48	
	$hs^0 s^0$					
	$hs^0 s^0 s^0$					
	$hs^0 \sigma$	0.04662 44	0.06859 82	0.07698 36	0.16263 29	
	$hs^0 \pi\pi$	-0.00745 87	-0.01349 35	-0.01557 86	-0.04192 86	
	$hs^0 \sigma\sigma$	-0.00402 53	-0.00725 06	-0.00836 72	-0.02246 39	
	$hs^0 \pi\sigma$	0.01516 65	0.02364 36	0.02676 05	0.06114 11	
$h\sigma\sigma$	$hs^0 \sigma\sigma$	0.02465 91	0.03538 09	0.03955 80	0.08059 73	
	$hs^0 \pi\pi$	1.07763 75	1.16087 43	1.24899 76	1.85504 47	
	$s^0 s^0 s^0 s^0$	1.08334 84	1.16988 91	1.25919 50	1.87755 88	
	$s^0 \sigma s^0$					
	$\pi s^0 \pi s^0$					
	$\sigma s^0 s^0 \sigma$	0.23836 20	0.25583 49	0.27503 33	0.40362 85	
	$\pi s^0 s^0 \pi$	1.17421 88	1.27207 03	1.36992 19	2.05488 28	
	$\sigma\sigma\sigma$	1.04765 63	1.13495 09	1.22226 56	1.83339 84	
	$\pi\pi\pi\pi$					
	$\sigma\pi\sigma\pi$					

<i>DR</i>	$\pi\sigma\pi\pi$ $\pi\pi'\pi'\pi$ ++ ++ ++ +- -+ -+	$(\pi_a\sigma_a; \pi_a\sigma_a)R$ $(\pi_a\pi_a'; \pi_a\pi_a')R$ $(\pi_a^+\pi_a^+; \pi_a^+\pi_a^+)R$ $(\pi_a^+\pi_a^-; \pi_a^-\pi_a^+)R$	0.06328 13 1.11093 75 0.12656 25	0.06855 47 1.20351 56 0.13710 94	0.07382 81 1.29609 38 0.14765 63	0.11074 22 1.94414 06 0.22148 44
<i>hhhh</i>	<i>hhhs</i>	$(h_a h_a; h_b h_b)R$	1.00000 00	1.00000 00	1.00000 00	1.00000 00
<i>hhhs</i>	<i>hhhs</i>	$(h_a h_a; h_b s_b^0)R$	-0.00000 07	-0.00000 14	-0.00000 06	-0.00000 00
<i>hhhs</i>	<i>hhhs</i>	$(h_a h_a; h_b \sigma_b)R$	0.01840 23	0.02402 81	0.02340 47	0.02348 04
<i>hshs</i>	<i>hshs</i>	$(h_a h_a; s_b^0 s_b^0)R$	0.93855 04	0.95463 75	0.96740 39	0.99727 15
<i>hshs</i>	<i>hshs</i>	$(h_a h_a; s_b^0 \sigma_b)R$	0.37138 80	0.36536 27	0.35687 88	0.27244 45
<i>hs</i>	<i>hs</i>	$(h_a h_a; \sigma_b \sigma_b)R$	1.12928 13	1.13789 99	1.14159 95	1.10082 05
<i>hs</i>	<i>hs</i>	$(h_a h_a; \pi_b \pi_b)R$	0.84487 64	0.86501 13	0.88184 38	0.94572 09
<i>hhs</i>	<i>hhs</i>	$(h_a s_a^0; h_b s_b^0)R$	-0.00000 11	-0.00000 25	-0.00000 13	-0.00000 00
<i>hhs</i>	<i>hhs</i>	$(h_a s_a^0; s_b^0 \sigma_b)R$	-0.00000 18	-0.00000 42	-0.00000 21	-0.00000 01
<i>hhs</i>	<i>hhs</i>	$(h_a s_a^0; s_b^0 s_b^0)R$	-0.00104 93	-0.00131 92	-0.00108 95	-0.00022 71
<i>hs</i>	<i>hs</i>	$(h_a s_a^0; s_b^0 \sigma_b)R$	-0.00176 55	-0.00220 29	-0.00182 14	-0.00037 78
<i>hs</i>	<i>hs</i>	$(h_a s_a^0; \sigma_b \sigma_b)R$	-0.00297 31	-0.00368 24	-0.00304 74	-0.00062 86
<i>hs</i>	<i>hs</i>	$(h_a s_a^0; \pi_b \pi_b)R$	-0.00005 89	-0.00008 06	-0.00005 99	-0.00000 78
<i>hs</i>	<i>hs</i>	$(h_a \sigma_a; h_b \sigma_b)R$	0.00067 43	0.00114 77	0.00109 20	0.00110 26
<i>hs</i>	<i>hs</i>	$(h_a \sigma_a; s_b^0 s_b^0)R$	0.01244 06	0.01759 22	0.01844 53	0.02274 79
<i>hs</i>	<i>hs</i>	$(h_a \sigma_a; s_b^0 \sigma_b)R$	0.00678 35	0.00983 58	0.01055 62	0.01176 28
<i>hs</i>	<i>hs</i>	$(h_a \sigma_a; \sigma_b \sigma_b)R$	0.01636 10	0.02336 75	0.02469 19	0.02900 83
<i>hs</i>	<i>hs</i>	$(h_a \sigma_a; \pi_b \pi_b)R$	0.01064 37	0.01498 70	0.01555 49	0.01967 78
<i>hs</i>	<i>hs</i>	$(h_a \pi_a; h_b \pi_b)R$	0.00033 85	0.00057 69	0.00054 76	0.00055 13
<i>hs</i>	<i>hs</i>	$(h_a \pi_a; s_b^0 \pi_b)R$	0.00662 78	0.00851 59	0.00814 77	0.00636 53
<i>hs</i>	<i>hs</i>	$(h_a \pi_a; \sigma_b \pi_b)R$	0.00489 19	0.00612 56	0.00574 26	0.00358 96
<i>hs</i>	<i>hs</i>	$(s_a^0 s_a^0; s_b^0 s_b^0)R$	0.82038 94	0.85159 62	0.87959 41	0.97730 61
<i>hs</i>	<i>hs</i>	$(s_a^0 s_a^0; s_b^0 \sigma_b)R$	0.21043 12	0.22300 23	0.23381 64	0.24290 04
<i>hs</i>	<i>hs</i>	$(s_a^0 s_a^0; \sigma_b s_b^0)R$	0.03395 18	0.04965 14	0.06415 32	0.10158 44
<i>hs</i>	<i>hs</i>	$(s_a \sigma_a; \sigma_b s_b^0)R$	0.20895 99	0.23067 02	0.24944 68	0.28487 71
<i>hs</i>	<i>hs</i>	$(s_a \sigma_a; \sigma_b \sigma_b)R$	0.79356 53	0.82250 01	0.84744 62	0.93996 38
<i>hs</i>	<i>hs</i>	$(\pi_a s_a^0; \pi_b s_b^0)R$	0.11331 51	0.10988 85	0.10565 11	0.06913 78
<i>hs</i>	<i>hs</i>	$(\pi_a \sigma_a; \pi_b s_b^0)R$	0.05378 60	0.05360 01	0.05265 01	0.03419 87
<i>hs</i>	<i>hs</i>	$(\pi_a \sigma_a; \pi_b \sigma_b)R$	0.01916 82	0.02183 83	0.02361 20	0.01949 35
<i>hs</i>	<i>hs</i>	$(\pi_a \pi_a; \sigma_b \sigma_b)R$	0.85341 52	0.88817 97	0.91707 25	1.00790 86

		$\alpha; \beta$				17.75; 5.25
		14.00; 3.00	13.25; 3.25	14.00; 3.50	17.75; 5.25	
CR	s^0s^0	0.87969 84	0.91756 19	0.95103 56	1.05495 64	
	$\pi\sigma\pi s^0$	0.21488 70	0.22434 53	0.23085 43	0.22407 77	
	s^0s^0	0.94361 21	0.99207 44	1.03375 42	1.15571 89	
	$\pi\pi\pi\pi$	0.78468 35	0.80950 78	0.83054 47	0.91330 28	
	$\pi\pi'\pi\pi'$	0.74537 47	0.77349 06	0.79790 48	0.89961 38	
	$\pi\pi\pi'\pi'$	0.01965 44	0.01800 86	0.01631 99	0.00684 45	
	$++$	0.76502 91	0.79149 92	0.81422 47	0.90645 83	
	$+-$	0.03930 88	0.03601 72	0.03263 98	0.01368 91	
	$+-$	0.00000 00	0.00000 01	0.00000 00	0.00000 00	
	$++$	0.00001 32	0.00002 63	0.00001 22	0.00000 01	
	$hhhh$	$(h_a h_b; h_b h_a)R$	0.00002 24	0.00004 40	0.00002 05	0.00000 02
	$hhhs^0$	$(h_a h_b; h_b s_a^0)R$	0.00005 88	0.00011 11	0.00005 72	0.00000 14
	$hshs^0$	$(h_a h_b; s_b^0 s_a^0)R$	0.00005 73	0.00011 33	0.00006 08	0.00000 18
	hs^0hs^0	$(h_a h_b; s_b^0 s_a^0)R$	0.00004 41	0.00009 85	0.00005 72	0.00000 22
	hs^0s^0	$(h_a h_b; \pi_b \pi_a)R$	0.00003 80	0.00006 89	0.00003 36	0.00000 06
hs^0s^0	$(h_a s_b^0; h_b s_a^0)R$	0.00503 75	0.00559 86	0.00424 63	0.00054 92	
hs^0s^0	$(h_a s_b^0; s_b^0 h_a)R$	0.02069 92	0.02135 51	0.01704 19	0.00270 94	
hs^0s^0	$(h_a s_b^0; h_b s_a)R$	0.00845 02	0.00931 00	0.00707 15	0.00091 10	
hs^0s^0	$(h_a s_b^0; s_b h_a)R$	0.03499 32	0.03582 87	0.02861 00	0.00451 80	
hs^0s^0	$(h_a s_b^0; s_b^0 s_a^0)R$	0.05368 78	0.05449 09	0.04624 25	0.01071 73	
hs^0s^0	$(h_a s_b^0; s_b^0 s_a)R$	0.03940 10	0.04313 71	0.03863 68	0.01137 49	
hs^0s^0	$(h_a s_b^0; s_b s_a^0)R$	0.05694 89	0.05951 19	0.05229 85	0.01397 64	
hs^0s^0	$(h_a s_b^0; s_b s_a)R$	0.02764 53	0.03516 77	0.03484 67	0.01399 72	
hs^0s^0	$(h_a s_b^0; \pi_b \pi_a)R$	0.03609 56	0.03540 04	0.02861 19	0.00487 54	
hs^0s^0	$(h_a s_b; h_b s_a)R$	0.01417 50	0.01548 17	0.01177 64	0.00151 12	
hs^0s^0	$(h_a s_b; s_b h_a)R$	0.05916 11	0.06011 59	0.04803 32	0.00753 39	
hs^0s^0	$(h_a s_b; s_b^0 s_a^0)R$	0.09013 92	0.09070 76	0.07708 31	0.01778 82	
hs^0s^0	$(h_a s_b; s_b^0 s_a)R$	0.06608 53	0.07173 23	0.06435 14	0.01887 50	
hs^0s^0	$(h_a s_b; s_b s_a^0)R$	0.09564 98	0.09911 08	0.08720 92	0.02320 04	
hs^0s^0	$(h_a s_b; s_b s_a)R$	0.04635 44	0.05848 24	0.05804 37	0.02322 85	
hs^0s^0	$(h_a s_b; \pi_b \pi_a)R$	0.06059 21	0.05891 72	0.04768 56	0.00809 12	
hs^0s^0	$(h_a \pi_b; h_b \pi_a)R$	0.00000 96	0.00001 44	0.00000 88	0.00000 05	
hs^0s^0	$(h_a \pi_b; \pi_b h_a)R$	0.00014 68	0.00016 83	0.00012 07	0.00001 21	

<i>LR</i>	$\alpha; \beta$	14.00; 3.00	13.25; 3.25	14.00; 3.50	17.75; 5.25
$hhs\bar{h}$	$(h_a s_a^0; h_a h_b)R$	-0.00000 23	-0.00000 57	-0.00000 29	0.00000 01
$hhs\bar{s}^0$	$(h_a s_a^0; h_a s_b^0)R$	-0.01511 28	-0.01827 67	-0.01718 63	-0.00945 74
$hs^0s^0\bar{h}$	$(h_a s_a^0; s_a^0 h_b)R$	-0.00000 10	-0.00000 23	-0.00000 12	-0.00000 00
$hhs^0\bar{s}$	$(h_a s_a^0; h_a s_b)R$	-0.02580 05	-0.03100 93	-0.02914 66	-0.01587 70
$hhs^0\bar{h}$	$(h_a s_a^0; \sigma_a h_b)R$	-0.00000 19	-0.00000 45	-0.00000 24	-0.00000 01
$hs^0s^0\bar{s}^0$	$(h_a s_a^0; s_a^0 s_b^0)R$	0.00011 65	0.00024 93	0.00023 89	0.00018 27
$hs^0s^0\bar{\sigma}$	$(h_a s_a^0; s_a^0 \sigma_b)R$	0.00025 18	0.00050 35	0.00047 45	0.00033 41
$hhs^0\bar{s}^0$	$(h_a s_a^0; \sigma_a s_b^0)R$	-0.00047 73	-0.00081 48	-0.00083 16	-0.00077 11
$hhs^0\bar{\sigma}$	$(h_a s_a^0; \sigma_a \sigma_b)R$	-0.00078 87	-0.00134 04	-0.00137 42	-0.00128 02
$h\pi s\bar{\sigma}\bar{\pi}$	$(h_a s_a^0; \pi_a \sigma_b)R$	-0.00041 70	-0.00062 99	-0.00057 66	-0.00030 84
$hhs\bar{h}$	$(h_a \sigma_a; h_a h_b)R$	0.00000 46	0.00001 11	0.00000 60	0.00000 03
$hhs\bar{s}^0$	$(h_a \sigma_a; h_a s_b^0)R$	0.00164 52	0.00245 49	0.00245 74	0.00197 33
$hs^0s^0\bar{h}$	$(h_a \sigma_a; s_a^0 h_b)R$	0.00135 85	0.00188 72	0.00160 37	0.00058 38
$hhs\bar{\sigma}$	$(h_a \sigma_a; h_a \sigma_b)R$	0.00274 39	0.00406 65	0.00408 36	0.00328 02
$hhs\bar{h}$	$(h_a \sigma_a; \sigma_a h_b)R$	0.00227 86	0.00313 82	0.00267 02	0.00096 79
$hs^0s^0\bar{s}^0$	$(h_a \sigma_a; s_a^0 s_b^0)R$	0.00744 39	0.01048 72	0.01105 80	0.01143 74
$hs^0s^0\bar{\sigma}$	$(h_a \sigma_a; s_a^0 \sigma_b)R$	0.00722 14	0.01099 64	0.01238 60	0.01565 43
$hhs\bar{s}^0$	$(h_a \sigma_a; \sigma_a s_b^0)R$	0.01545 57	0.02083 85	0.02123 03	0.01922 60
$hhs\bar{\sigma}$	$(h_a \sigma_a; \sigma_a \sigma_b)R$	0.01873 87	0.02596 31	0.02719 12	0.02734 05
$h\pi s\bar{\sigma}\bar{\pi}$	$(h_a \sigma_a; \pi_a \sigma_b)R$	0.00458 07	0.00609 05	0.00597 05	0.00419 92
$hhs\bar{\pi}$	$(h_a \pi_a; h_a \pi_b)R$	0.00143 14	0.00189 12	0.00169 90	0.00078 86
$h\pi s\bar{h}$	$(h_a \pi_a; \pi_a h_b)R$	0.00005 65	0.00009 07	0.00006 89	0.00001 57
$hs^0\pi\bar{\pi}$	$(h_a \pi_a; s_a^0 \pi_b)R$	0.00707 64	0.00892 62	0.00844 25	0.00497 94
$h\pi s\bar{s}^0$	$(h_a \pi_a; \pi_a s_b^0)R$	0.01182 11	0.01527 56	0.01489 42	0.01039 12
$hhs\bar{\sigma}$	$(h_a \pi_a; \sigma_a \pi_b)R$	0.00458 07	0.00609 05	0.00597 05	0.00419 92
$h\pi s\bar{\pi}$	$(h_a \pi_a; \pi_a \sigma_b)R$	0.01633 21	0.02129 04	0.02109 92	0.01561 46
$s^0hs^0\bar{h}$	$(s_a^0 s_a^0; h_a h_b)R$	0.00008 49	0.00017 11	0.00009 37	0.00000 43
$s^0hs^0\bar{s}^0$	$(s_a^0 s_a^0; h_a s_b^0)R$	0.09909 93	0.11060 31	0.10342 57	0.05409 85
$s^0s^0s^0\bar{h}$	$(s_a^0 s_a^0; s_a^0 h_b)R$	0.06537 96	0.06997 85	0.06197 85	0.02328 34
$s^0hs^0\bar{\sigma}$	$(s_a^0 s_a^0; s_a^0 \sigma_b)R$	0.16659 09	0.18444 78	0.17270 04	0.08993 31
$s^0s^0\bar{h}$	$(s_a^0 s_a^0; \sigma_a h_b)R$	0.10972 76	0.11642 21	0.10325 58	0.03862 72
$s^0s^0s^0\bar{s}^0$	$(s_a^0 s_a^0; s_a^0 s_b^0)R$	0.62126 11	0.61155 88	0.60014 14	0.40416 18
$s^0s^0s^0\bar{\sigma}$	$(s_a^0 s_a^0; s_a^0 \sigma_b)R$	0.59887 43	0.61684 12	0.63262 49	0.51047 77
$s^0s^0s^0\bar{h}$	$(s_a^0 s_a^0; \sigma_a h_b)R$	0.46009 45	0.48076 76	0.49802 87	0.42459 09
$s^0s^0\bar{s}^0$	$(s_a^0 s_a^0; \sigma_a s_b)R$	0.25235 89	0.32563 81	0.38864 58	0.49877 64

$s^0\pi s^0\bar{\pi}$	0.43953 60	0.41561 68	0.38898 81	0.19208 82
$s^0h^0\bar{h}$	0.00009 71	0.00019 62	0.00010 77	0.00000 49
s^0hs^0	0.10062 96	0.11291 92	0.10571 35	0.05586 45
$s^0s^0\bar{h}$	0.07813 24	0.08295 07	0.07293 53	0.02587 86
s^0hs^0	0.16920 16	0.18835 68	0.17656 12	0.09288 59
$ss^0\bar{h}$	0.13119 61	0.13808 69	0.12156 40	0.04293 45
ss^0s^0	0.64003 05	0.63335 69	0.62392 97	0.42825 96
ss^0s^0	0.60638 93	0.63167 89	0.65253 56	0.54248 50
ss^0s^0	0.49968 76	0.52346 85	0.54333 66	0.46565 05
ss^0s^0	0.27508 36	0.35847 15	0.42942 13	0.55370 71
$s\pi s\bar{\pi}$	0.44185 97	0.41975 23	0.39396 06	0.19711 73
$\pi h^0\bar{h}$	0.00008 01	0.00016 19	0.00008 86	0.00000 40
πh^0s^0	0.10029 02	0.11233 47	0.10508 94	0.05520 70
$\pi s^0\bar{h}$	0.05915 71	0.06370 44	0.05664 87	0.02199 81
πh^0s^0	0.16856 01	0.18729 26	0.17544 18	0.09176 26
$\pi s\pi\bar{h}$	0.09924 98	0.10593 88	0.09434 67	0.03649 37
$\pi s^0\pi s^0$	0.61604 69	0.60667 02	0.59420 59	0.39668 77
$\pi s^0\pi s^0$	0.60127 30	0.61838 19	0.63169 14	0.50175 25
$\pi s^0\pi s^0$	0.44255 64	0.46296 48	0.47907 89	0.40760 70
$\pi s^0\pi s^0$	0.24399 55	0.31414 27	0.37357 46	0.47690 47
$\pi s\pi\bar{h}$	0.46133 58	0.43569 12	0.40671 17	0.19809 85
$\pi s\pi\bar{h}$	0.41964 29	0.39727 73	0.37175 11	0.18397 35
$\pi s\pi\bar{h}$	0.02084 64	0.01920 69	0.01748 03	0.00706 25
$s^0h^0\bar{h}$	0.00002 67	0.00005 38	0.00002 99	0.00000 14
$s^0h^0s^0$	0.00331 18	0.00465 32	0.00465 04	0.00355 84
$s^0s^0\bar{h}$	0.02554 91	0.02656 36	0.02287 07	0.00663 49
$s^0h^0s^0$	0.00537 32	0.00749 83	0.00754 86	0.00585 00
$s^0s^0\bar{h}$	0.04292 44	0.04425 09	0.03813 73	0.01100 59
$s^0s^0s^0$	0.10053 35	0.10488 44	0.10834 14	0.08868 40
$s^0s^0s^0$	0.06214 11	0.07891 64	0.09329 97	0.11172 80
$s^0s^0s^0$	0.17433 93	0.17630 11	0.17792 92	0.13468 02
$s^0s^0s^0$	0.14394 35	0.16118 42	0.17560 03	0.17403 09
$s^0\pi s\bar{\pi}$	0.07112 60	0.06979 43	0.06732 74	0.03686 80
$s^0\pi s\bar{\pi}$	0.00291 71	0.00363 40	0.00325 41	0.00143 22
$s^0\pi s\bar{\pi}$	0.00096 35	0.00114 38	0.00089 41	0.00017 28

LR

		$\alpha; \beta$					
		14.00; 3.00	13.25; 3.25	14.00; 3.50	17.75; 5.25		
$s^0 s^0 \pi \pi$ $s^0 \pi \pi \bar{s}^0$ $s^0 \sigma \pi \pi$ $s^0 \pi \pi \sigma$ $\sigma h \pi \pi$	$(s_a^0 \pi_a; s_a^0 \pi_b) R$ $(s_a^0 \pi_a; \pi_a s_b^0) R$ $(s_a^0 \pi_a; \sigma_a \pi_b) R$ $(s_a^0 \pi_a; \pi_a \sigma_b) R$ $(\sigma_a \pi_a; h_a \pi_b) R$	0.09711 41 0.11852 84 0.07112 60 0.13704 86 0.00037 30	0.09150 11 0.11438 66 0.06979 43 0.13649 73 0.00054 92	0.08511 31 0.10895 54 0.06732 74 0.13416 22 0.00050 71	0.03967 14 0.05937 09 0.03686 80 0.08284 69 0.00027 92		
	$\sigma \pi \bar{h}$ $\sigma s^0 \pi \pi$ $\sigma \pi \bar{s}^0$ $\sigma \sigma \pi \pi$ $\sigma \pi \pi \sigma$	$(\sigma_a \pi_a; \pi_a h_b) R$ $(\sigma_a \pi_a; s_a^0 \pi_b) R$ $(\sigma_a \pi_a; \pi_a s_b^0) R$ $(\sigma_a \pi_a; \sigma_a \pi_b) R$ $(\sigma_a \pi_a; \pi_a \sigma_b) R$	0.00069 80 0.03110 56 0.02432 81 0.04306 32 0.01881 61	0.00080 74 0.03049 11 0.02494 95 0.04168 18 0.02205 18	0.00062 48 0.02924 46 0.02503 12 0.03968 97 0.02443 39	0.00010 32 0.01526 94 0.01714 61 0.02020 63 0.02264 36	
		$+$ $+$ $+$ $+$ $+$	$(\pi_a^+ \pi_a^+; \pi_a^+ \pi_b^+) R$ $(\pi_a^+ \pi_a^-; \pi_a^- \pi_b^+) R$	0.44048 94 0.04169 29	0.41648 43 0.03841 39	0.38923 14 0.03496 06	0.19103 60 0.01412 50
		$+$ $+$ $-$ $-$ $+$					