

Tables Useful for the Calculation of the Molecular Integrals X

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Introductory Remarks

In the series of papers⁽¹⁾ we have given the molecular integrals involving $1s$, $2s$, $2s^o$ and $2p$ atomic orbitals for 4 sets of parameters α and β . The values of α and β considered are given in the following table.

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

In order to develop the molecular orbital theory, it is necessary to transform the integrals into those which involve molecular orbitals. We have considered the orthonormalized molecular orbitals (OMO) of the following form:

$$\begin{cases} \sigma_{1g} = \alpha_{11}(\sigma 1s)_g \\ \sigma_{2g} = \alpha_{21}(\sigma 1s)_g + \alpha_{22}(\sigma 2s)_g \\ \sigma_{3g} = \alpha_{31}(\sigma 1s)_g + \alpha_{32}(\sigma 2s)_g + \alpha_{33}(\sigma 2p)_g \\ \sigma_{1u} = \beta_{11}(\sigma 1s)_u \\ \sigma_{2u} = \beta_{21}(\sigma 1s)_u + \beta_{22}(\sigma 2s)_u \\ \sigma_{3u} = \beta_{31}(\sigma 1s)_u + \beta_{32}(\sigma 2s)_u + \beta_{33}(\sigma 2p)_u \\ \pi_g^\pm = \gamma_g(\pi^\pm 2p)_g \\ \pi_u^\pm = \gamma_u(\pi^\pm 2p)_u \end{cases} \quad (1)$$

where

$$\begin{aligned} (\sigma 1s)_{g,u} &= (1s)_a \pm (1s)_b \\ (\sigma 2s)_{g,u} &= (2s)_a \pm (2s)_b \\ (\sigma 2p)_{g,u} &= (2p\sigma)_a \pm (2p\sigma)_b \\ (\pi^\pm 2p)_{g,u} &= (2p\pi^\pm)_a \mp (2p\pi^\pm)_b \end{aligned} \quad (2)$$

The coefficients appeared in (1) are determined by the orthonormality condition and are given in Table XXIX.

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From the numerical tables of molecular integrals already published⁽¹⁾⁽²⁾⁽³⁾ we have obtained the values of molecular integrals involving OMO's and are given in Table XXX. The notations employed are as follows.

- (i) $R^{-1}(\varphi_i | z | \varphi_j) = 1/R \cdot \int \varphi_i^*(1) z_1 \varphi_j(1) d\tau_1,$
- (ii) $R^{-1}(\varphi_i | x \pm iy | \varphi_j) = 1/R \cdot \int \varphi_i^*(1) (x_1 \pm iy_1) \varphi_j(1) d\tau_1,$
- (iii) $R(\varphi_i | \zeta | \varphi_j) = R \int \varphi_i^*(1) \frac{\partial}{\partial z_1} \varphi_j(1) d\tau_1,$
- (iv) $R(\varphi_i | \xi \pm i\eta | \varphi_j) = R \int \varphi_i^*(1) \left(\frac{\partial}{\partial x_1} \pm i \frac{\partial}{\partial y_1} \right) \varphi_j(1) d\tau_1,$
- (v) $R^{-2}(\varphi_i | z^2 | \varphi_j) = 1/R^2 \cdot \int \varphi_i^*(1) z_1^2 \varphi_j(1) d\tau_1,$
- (vi) $R^{-2}(\varphi_i | x^2 + y^2 | \varphi_j) = 1/R^2 \cdot \int \varphi_i^*(1) (x_1^2 + y_1^2) \varphi_j(1) d\tau_1,$
- (vii) $2R^3(\varphi_i | q_a | \varphi_j) = R^3 \int \varphi_i^*(1) \frac{3 \cos^2 \theta_{a1} - 1}{r_{a1}^2} \varphi_j(1) d\tau_1,$
- (viii) $R^3(\varphi_i | \varphi_j)_0 = R^3 \int \varphi_i^*(1) \delta(r_{a1}) \varphi_j(1) d\tau_1,$
- (ix) $R^2(\varphi_i | -\frac{1}{2}A | \varphi_j) = R^2 \int \varphi_i^*(1) (-\frac{1}{2}A_1) \varphi_j(1) d\tau_1,$
- (x) $R(\varphi_i | \frac{1}{r_a} + \frac{1}{r_b} | \varphi_j) = R \int \varphi_i^*(1) \left(\frac{1}{r_a} + \frac{1}{r_b} \right) \varphi_j(1) d\tau_1,$
- (xi) $R(\varphi_i^*(1) \varphi_j(1) | \varphi_k^*(2) \varphi_l(2)) = R \int \varphi_i^*(1) \varphi_k^*(2) \frac{1}{r_{12}} \varphi_j(1) \varphi_l(2) d\tau_1 d\tau_2.$

In the above φ_i 's mean the OMO's, R is the internuclear distance. $R^3(\varphi_i | \varphi_j)_0$ are obtained only for the set IV.

As the basic integrals involving AO's for the calculation of (iii) $R(\varphi_i | \zeta | \varphi_j)$ and (iv) $R(\varphi_i | \xi \pm i\eta | \varphi_j)$ were not given in the previous reports, we have given these values in table XXXI. These values are obtained by the following formulae.

$$\begin{aligned}
 R \times \xi^0_h \pi &= R \times \eta^0_h \pi' = R \times \zeta^0_{h\sigma} = -R \times \xi^0_{\pi h} = -R \times \eta^0_{\pi' h} = -R \times \zeta^0_{\sigma h} = 8 \frac{\sqrt{\alpha^5 \beta^5}}{(\alpha + \beta)^4}, \\
 R \times \xi^0_s \pi &= R \times \eta^0_s \pi' = R \times \zeta^0_{s\sigma} = -R \times \xi^0_{\pi s} = -R \times \eta^0_{\pi' s} = -R \times \zeta^0_{\sigma s} = \frac{\beta}{2\sqrt{3}}, \\
 R \times \xi_h \pi &= R \times \eta_h \pi' = -R \times \xi_{\pi h} = -R \times \eta_{\pi' h} \\
 &= \frac{\sqrt{\alpha^5 \beta^5}}{16} [\{A_3(r) - A_1(r)\} \{B_0(\delta) - B_2(\delta)\} - \{A_2(r) - A_0(r)\} \{B_1(\delta) - B_3(\delta)\}], \\
 R \times \xi_s \pi &= R \times \eta_s \pi' = -R \times \xi_{\pi s} = -R \times \eta_{\pi' s} \\
 &= \frac{\beta^5}{120\sqrt{3}} [\beta \{5A_4(\beta) - 6A_2(\beta) + A_0(\beta)\} - 10 \{A_3(\beta) - A_1(\beta)\}], \\
 R \times \xi_\sigma \pi &= R \times \eta_\sigma \pi' = -R \times \xi_{\pi\sigma} = -R \times \eta_{\pi'\sigma} = \frac{\beta^6}{30} \{A_3(\beta) - A_1(\beta)\},
 \end{aligned}$$

$$R \times \zeta_{hh} = \frac{\alpha^4}{3} A_1(\alpha),$$

$$R \times \zeta_{hs} = R \times \zeta_{sh}$$

$$= \frac{\sqrt{\alpha^5 \beta^5}}{8\sqrt{3}} [A_2(r)B_0(\delta) - (2A_1(r) - A_3(r))B_1(\delta) + (A_0(r) - 2A_2(r))B_2(\delta) + A_1(r)B_3(\delta)]$$

$$= \frac{\sqrt{\alpha^3 \beta^5}}{8\sqrt{3}} [\beta \{A_2(r)B_0(\delta) - A_3(r)B_1(\delta) - A_0(r)B_2(\delta) + A_1(r)B_3(\delta)\} - 2A_1(r)B_0(\delta) + 2\{A_2(r) - A_0(r)\}B_1(\delta) + 2A_1(r)B_2(\delta)] ,$$

$$\begin{aligned} R \times \zeta_{h\sigma} &= R \times \zeta_{\sigma h} \\ &= \frac{\sqrt{\alpha^5 \beta^5}}{8} [A_1(r)B_0(\delta) - A_0(r)B_1(\delta) - A_3(r)B_2(\delta) + A_2(r)B_3(\delta)] \\ &= \frac{\sqrt{\alpha^3 \beta^5}}{8} [\beta \{A_1(r)B_0(\delta) - (2A_2(r) - A_0(r))B_1(\delta) + (A_3(r) - 2A_1(r))B_2(\delta) + A_2(r)B_3(\delta)\} - 2A_2(r)B_0(\delta) + 2A_0(r)B_2(\delta)] , \end{aligned}$$

$$\begin{aligned} R \times \zeta_{s\sigma} &= R \times \zeta_{\sigma s} \\ &= \frac{\beta^5}{120\sqrt{3}} [\beta \{-5A_4(\beta) + 18A_2(\beta) - 5A_0(\beta)\} - 10\{3A_1(\beta) - A_3(\beta)\}] \\ &= \frac{\beta^5}{120\sqrt{3}} [\beta \{5A_4(\beta) - 2A_2(\beta) + 5A_0(\beta)\} - 10\{3A_3(\beta) - A_1(\beta)\}] , \end{aligned}$$

$$R \times \zeta_{\sigma\sigma} = \frac{-\beta^5}{60} [\beta \{A_3(\beta) - 5A_1(\beta)\} + 5\{3A_2(\beta) - A_0(\beta)\}] ,$$

$$\begin{aligned} R \times \zeta_{\pi\pi} &= R \times \zeta_{\pi'\pi'} \\ &= \frac{\beta^6}{30} [A_3(\beta) - A_1(\beta)] , \end{aligned}$$

where

$$\xi^0_{\alpha\beta} = \int \alpha_a^*(1) \frac{\partial}{\partial x_1} \beta_a(1) d\tau_1 ,$$

$$\eta^0_{\alpha\beta} = \int \alpha_a^*(1) \frac{\partial}{\partial y_1} \beta_a(1) d\tau_1 ,$$

$$\varsigma^0_{\alpha\beta} = \int \alpha_a^*(1) \frac{\partial}{\partial z_1} \beta_a(1) d\tau_1 ,$$

$$\xi_{\alpha\beta} = \int \alpha_a^*(1) \frac{\partial}{\partial x_1} \beta_b(1) d\tau_1 ,$$

$$\eta_{\alpha\beta} = \int \alpha_a^*(1) \frac{\partial}{\partial y_1} \beta_b(1) d\tau_1 ,$$

$$\varsigma_{\alpha\beta} = \int \alpha_a^*(1) \frac{\partial}{\partial z_1} \beta_b(1) d\tau_1 ,$$

$$\gamma = \frac{1}{2}(\alpha + \beta) , \quad \delta = \frac{1}{2}(\alpha - \beta) .$$

In terms of OMO's (1), we have set up the configurations with which the lower electronic states of the Li_2 and O_2 molecules can be constructed within a reasonable approximation. These configurations are shown explicitly in table XXXII, where the letters in the first column are added so as to serve to distinguish each configuration.

Spins associated with two orbitals with the same superbar — or = are coupled to triplet, while spins associated with two orbitals with the same subbar — or

= are coupled to singlet.

The matrix elements of various interesting physical quantities with respect to the configurations shown in Table XXXII have been calculated. The matrix elements in the case of the Li_2 molecule are calculated with the use of the parameter sets I, II, and III and are given in Table XXXIII, and those in the case of the O_2 molecule are calculated with the use of the parameter set IV and are given in Table XXXIV.

The matrix elements considered are

$$(i) \quad R^{-1}(i|z|j) = 1/R \cdot \int \psi_i^*(1, 2, \dots, n) \sum_{k=1}^n z_k \psi_j(1, 2, \dots, n) d\tau_1 \dots d\tau_n,$$

$$(ii) \quad R(i|\varsigma|j) = R \cdot \int \psi_i^*(1, 2, \dots, n) \sum_{k=1}^n \frac{\partial}{\partial z_k} \psi_j(1, 2, \dots, n) d\tau_1 \dots d\tau_n,$$

$$(iii) \quad R^{-1}(i|x \pm iy|j) = 1/R \cdot \int \psi_i^*(1, 2, \dots, n) \sum_{k=1}^n (x_k \pm iy_k) \psi_j(1, 2, \dots, n) d\tau_1 \dots d\tau_n,$$

(for Li_2 only)

$$(iv) \quad R(i|\xi \pm i\eta|j) = R \cdot \int \psi_i^*(1, 2, \dots, n) \sum_{k=1}^n \left(\frac{\partial}{\partial x_k} \pm i \frac{\partial}{\partial y_k} \right) \psi_j(1, 2, \dots, n) d\tau_1 \dots d\tau_n,$$

(for Li_2 only)

$$(v) \quad R^{-2}(z^2)_{ij} = 1/R^2 \cdot \int \psi_i^*(1, 2, \dots, n) \sum_{k=1}^n z_k^2 \psi_j(1, 2, \dots, n) d\tau_1 \dots d\tau_n,$$

$$(vi) \quad R^{-2}(x^2 + y^2)_{ij} = 1/R^2 \cdot \int \psi_i^*(1, 2, \dots, n) \sum_{k=1}^n (x_k^2 + y_k^2) \psi_j(1, 2, \dots, n) d\tau_1 \dots d\tau_n,$$

$$(vii) \quad 2R^3(i|q_a|j) = R^3 \cdot \int \psi_i^*(1, 2, \dots, n) \sum_{k=1}^n \frac{3 \cos^2 \theta_{ak} - 1}{r_{ak}^3} \psi_j(1, 2, \dots, n) d\tau_1 \dots d\tau_n,$$

$$(viii) \quad 2R^3 q_{ij} = R^3 \cdot \int \psi_i^*(1, 2, \dots, n) \sum_{k=1}^n \frac{3 \cos^2 \theta_{ak} - 1}{r_{ak}^3} (2S_{kz}) \psi_j(1, 2, \dots, n) d\tau_1 \dots d\tau_n,$$

(for O_2 only)

$$(ix) \quad 1/2 \cdot R^3 \rho_{ij} = R^3 \cdot \int \psi_i^*(1, 2, \dots, n) \sum_{k=1}^n S_{kz} \psi_j(1, 2, \dots, n) d\tau_1 \dots d\tau_n,$$

(for O_2 only)

$$(x) \quad H_{ij} = \int \psi_i^*(1, 2, \dots, n) \left\{ -\frac{1}{2} \sum_{k=1}^n A_k - \sum_{k=1}^n \left(\frac{1}{r_{ak}} + \frac{1}{r_{bk}} \right) + \frac{1}{2} \sum_{k \neq l} \frac{1}{r_{kl}} \right\} \psi_j(1, 2, \dots, n) d\tau_1 \dots d\tau_n.$$

$(R=4.5, 5.0, 5.5 \text{ for } \text{Li}_2 \text{ and } 2.30 \text{ for } \text{O}_2)$

In the above, $\psi_i(1, 2, \dots, n)$ is the wave function of a molecule corresponding to the configuration i and $\frac{1}{2}S_{kz}$ is the z component of the spin angular momentum of the k -th electron in the units of \hbar .

Moreover for the Li_2 molecule, we have calculated H_{ij} by assuming that $\sigma_{1g^2} \sigma_{1u^2}$ electrons are shrunk into two nuclei. These values of H_{ij} are also given in Table XXXIII (1) for the case of the parameter set II and $R=5.00$.

For the ground state ${}^1\Sigma_g^+$ of the Li_2 molecule, we have obtained the matrix elements H_{ij} in the valence-bond (*VB*) scheme and are given in Table XXXV, where symbols such as $s-s$, $s-\sigma$, ... and $ss-$, $s\sigma-$, ... correspond to covalent and ionic structures respectively, while S_{ij} are the overlap integrals and are not necessarily equal to δ_{ij} in the *VB* case but independent of the value of R .

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Errata

Part	Page	Line	Column	
V⁽⁴⁾	177	49	5-6	$Ei(28.0) = 5 \ 36451 \ 18592$
VI⁽⁵⁾	58	5	5	$0.00048 \ 71994 \ 198$
VII⁽⁶⁾	203	8	4	$0.0^{10} \ 00521 \ 23671 \ 5720$
"	208	1	5	$17.75, \ 11.50$
IX⁽²⁾	207	3	7	$S_{hs^o} = 0.02214 \ 22$
"	209	13	1-3	$DR \ hhs^o\sigma \ (h_a s_a^o; h_b \sigma_b) R$
"	210	26	"	$CR \ hh\sigma\sigma \ (h_a \sigma_b; h_b \sigma_a) R$
"	211	13	"	$\pi s^o \pi s^o \ (\pi_a \pi_b; s_b^o s_a^o) R$
"	"	18	"	$\pi \pi \sigma s^o \ (\pi_a \sigma_b; \pi_b s_a) R$
"	"	26	"	$LR \ hh\bar{h} \ (h_a h_a; h_a h_b) R$
"	213	22	"	$\pi \pi' \pi \bar{\pi}' \ (\pi_a \pi_a; \pi_a' \pi_b') R$

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Table XXIX

	I	II	III	IV
α_{11}	0.70708 32	0.70706 15	0.70708 32	0.70710 59
α_{21}	-0.11365 46	-0.13810 93	-0.13813 95	-0.16451 50
α_{22}	0.55971 03	0.57121 90	0.57966 24	0.64420 46
α_{31}	-0.03735 83	-0.03024 54	-0.01969 30	0.01656 28
α_{32}	-0.21526 31	-0.21145 83	-0.20806 00	-0.15659 10
α_{33}	0.70763 78	0.68684 09	0.67083 84	0.63726 88
β_{11}	0.70713 04	0.70715 21	0.70713 04	0.70710 76
β_{21}	-0.08020 21	-0.11373 86	-0.12386 42	-0.18141 32
β_{22}	1.18160 28	1.11965 41	1.06407 36	0.85443 12
β_{31}	0.03898 60	-0.01013 22	-0.03304 84	-0.05226 28
β_{32}	2.77957 82	2.10767 48	1.63550 15	0.40917 14
β_{33}	1.98685 46	1.72124 92	1.52334 76	0.94154 01
γ_g	0.96945 70	0.92636 11	0.89099 07	0.76305 78
γ_u	0.58360 93	0.59394 58	0.60408 47	0.66189 67

Table XXX

(i)		$R^{-1}(\varphi_i z \varphi_j)$			
φ_i	φ_j	I	II	III	IV
σ_{1g}	σ_{1u}	-0.5	-0.5	-0.49999 97	-0.5
σ_{1g}	σ_{2u}	-0.00429 57	-0.00525 96	-0.00437 24	-0.00137 59
σ_{1g}	σ_{3u}	0.02991 43	0.03555 81	0.03351 23	0.02806 51
σ_{2g}	σ_{1u}	0.00203 13	0.00267 64	0.00237 87	0.00103 72
σ_{2g}	σ_{2u}	-0.65177 99	-0.62326 25	-0.59925 54	-0.52052 93
σ_{2g}	σ_{3u}	0.07312 27	0.08385 48	0.09402 40	0.13392 43
σ_{3g}	σ_{1u}	0.02179 27	0.02753 89	0.02583 30	0.02262 92
σ_{3g}	σ_{2u}	0.63267 33	0.59051 05	0.55285 24	0.36868 53
σ_{3g}	σ_{3u}	-0.55126 29	-0.54959 26	-0.54542 83	-0.51724 60
π_g^\pm	π_u^\pm	-0.56578 41	-0.55020 83	-0.53823 38	-0.50506 54

(ii)		$R^{-1}(\varphi_i x \pm iy \varphi_j)$			
φ_i	φ_j	I	II	III	IV
σ_{1g}	π_u^\mp	0.02415 88	0.03168 96	0.03078 76	0.03171 05
σ_{2g}	π_u^\mp	0.70443 80	0.65210 53	0.60549 26	0.40065 10
σ_{3g}	π_u^\mp	-0.00036 15	-0.00427 08	-0.00820 34	-0.01416 67

(ii)		$R^{-1}(\varphi_i x \pm iy \varphi_j)$			
φ_i	φ_j	I	II	III	IV
σ_{1u}	π_g^\mp	0.03123 43	0.03961 74	0.03800 69	0.03511 08
σ_{2u}	π_g^\mp	0.63018 79	0.58689 50	0.54939 81	0.38107 79
σ_{3u}	π_g^\mp	0.21766 11	0.17511 50	0.14235 29	0.04067 08

(iii)		$R(\varphi_i \varsigma \varphi_j)$			
φ_i	φ_j	I	II	III	IV
σ_{1g}	σ_{1u}	-0.34258 91	-0.36479 31	-0.25840 59	-0.03168 11
σ_{1g}	σ_{2u}	-0.17786 50	-0.17965 42	-0.17452 38	-0.09939 55
σ_{1g}	σ_{3u}	1.94434 51	2.14862 13	2.23945 39	2.94092 56
σ_{2g}	σ_{1u}	-0.04759 81	-0.05034 98	-0.06925 54	-0.07369 74
σ_{2g}	σ_{2u}	-0.69732 98	-0.71533 39	-0.73210 51	-0.67616 93
σ_{2g}	σ_{3u}	-0.26132 46	-0.31665 12	-0.27505 46	0.09791 95
σ_{3g}	σ_{1u}	-1.29277 71	-1.45664 21	-1.54033 98	-2.27681 35
σ_{3g}	σ_{2u}	-1.11193 18	-1.14353 59	-1.22153 33	-1.53788 19
σ_{3g}	σ_{3u}	-1.57100 95	-1.64076 12	-1.66708 06	-1.43600 53
$\pi_{g\pm}$	$\pi_{u\pm}$	0.70985 21	0.70042 94	0.68358 48	0.45108 37

(iv)		$\frac{1}{\sqrt{2}}R(\varphi_i \xi^{\pm i\eta} \varphi_j)$			
φ_i	φ_j	I	II	III	IV
σ_{1g}	$\pi_{u\mp}$	0.99829 13	1.20267 38	1.31291 53	2.27766 01
σ_{2g}	$\pi_{u\mp}$	0.73770 30	0.74125 07	0.79154 22	1.02300 40
σ_{3g}	$\pi_{u\mp}$	0.11996 77	0.10651 52	0.10193 74	0.05259 46

(iv)		$\frac{1}{\sqrt{2}}R(\varphi_i \xi^{\pm i\eta} \varphi_j)$			
φ_i	φ_j	I	II	III	IV
σ_{1u}	$\pi_{g\mp}$	1.34424 33	1.56554 28	1.67633 42	2.54643 20
σ_{2u}	$\pi_{g\mp}$	0.66599 80	0.65631 71	0.70039 28	0.92462 58
σ_{3u}	$\pi_{g\mp}$	-0.41719 66	-0.34279 41	-0.27433 27	-0.07422 82

(v)		$R^{-2}(\varphi_i z^2 \varphi_j)$			
φ_i	φ_j	I	II	III	IV
σ_{1g}	σ_{1g}	0.25508 95	0.25567 21	0.25508 92	0.25317 36
σ_{1g}	σ_{2g}	0.00077 52	0.00101 02	0.00092 67	0.00123 66
σ_{1g}	σ_{3g}	-0.02105 23	-0.02679 84	-0.02535 43	-0.02274 47
σ_{2g}	σ_{2g}	0.44807 20	0.41176 42	0.38235 44	0.29720 97
σ_{2g}	σ_{3g}	-0.49458 90	-0.44899 97	-0.41207 48	-0.27509 43
σ_{3g}	σ_{3g}	0.82664 19	0.74773 79	0.68457 94	0.44290 81
$\pi_{g\pm}$	$\pi_{g\pm}$	0.57709 72	0.52333 97	0.48075 38	0.33563 19

(v)		$R^{-2}(\varphi_i z^2 \varphi_j)$			
φ_i	φ_j	I	II	III	IV
σ_{1u}	σ_{1u}	0.25511 45	0.25572 00	0.25511 45	0.25317 44
σ_{1u}	σ_{2u}	0.00650 07	0.00824 27	0.00719 79	0.00368 84
σ_{1u}	σ_{3u}	-0.02984 91	-0.03523 91	-0.03295 90	-0.02760 37
σ_{2u}	σ_{2u}	0.91532 63	0.81021 19	0.72373 77	0.42840 61
σ_{2u}	σ_{3u}	-0.44682 50	-0.42269 40	-0.39693 58	-0.26481 48
σ_{3u}	σ_{3u}	0.59093 48	0.55289 77	0.52218 29	0.39949 86
$\pi_{u\pm}$	$\pi_{u\pm}$	0.35852 68	0.33802 48	0.32266 41	0.28093 83

(vi)		$R^{-2}(\varphi_i x^2 + y^2 \varphi_j)$			
φ_i	φ_j	I	II	III	IV
σ_{1g}	σ_{1g}	0.01020 57	0.01139 53	0.01020 57	0.00634 80
σ_{1g}	σ_{2g}	0.00535 43	0.00695 45	0.00622 93	0.00436 27
σ_{1g}	σ_{3g}	0.00098 51	0.00075 27	0.00032 72	-0.00049 82
σ_{2g}	σ_{2g}	0.57792 60	0.49794 02	0.43010 66	0.19453 97
σ_{2g}	σ_{3g}	-0.03988 34	-0.03166 05	-0.02579 26	-0.00481 95
σ_{3g}	σ_{3g}	0.29291 71	0.25481 43	0.22412 22	0.11025 69
π_g^\pm	π_g^\pm	0.55436 55	0.47939 61	0.41924 79	0.20151 53

(vi)		$R^{-2}(\varphi_i x^2 + y^2 \varphi_j)$			
φ_i	φ_j	I	II	III	IV
σ_{1u}	σ_{1u}	0.01020 25	0.01138 87	0.01020 25	0.00634 78
σ_{1u}	σ_{2u}	0.00496 47	0.00680 17	0.00635 79	0.00487 04
σ_{1u}	σ_{3u}	0.00312 98	0.00446 26	0.00395 09	0.00150 17
σ_{2u}	σ_{2u}	0.51686 91	0.44602 89	0.38718 46	0.18042 36
σ_{2u}	σ_{3u}	0.13008 93	0.08513 22	0.05648 51	0.00307 57
σ_{3u}	σ_{3u}	0.26095 96	0.21274 85	0.18001 70	0.08667 89
π_u^\pm	π_u^\pm	0.70736 45	0.60449 06	0.52222 49	0.22985 52

(vii)		$2R^3(\varphi_i q_a \varphi_j)$			
φ_i	φ_j	I	II	III	IV
σ_{1g}	σ_{1g}	1.00205 87	1.00363 92	1.00205 77	1.00010 47
σ_{1g}	σ_{2g}	0.12982 64	0.16381 62	0.18512 46	0.23863 86
σ_{1g}	σ_{3g}	0.33966 92	0.39737 79	0.41272 15	0.43082 98
σ_{2g}	σ_{2g}	0.44932 56	0.55519 73	0.68316 03	1.37104 31
σ_{2g}	σ_{3g}	0.69156 63	0.83333 09	0.98574 50	1.65351 44
σ_{3g}	σ_{3g}	5.42057 85	6.38639 67	7.44476 18	18.90908 55
π_g^\pm	π_g^\pm	-2.33760 11	-2.89691 07	-3.52617 90	-10.34673 45

(vii)		$2R^3(\varphi_i q_a \varphi_j)$			
φ_i	φ_j	I	II	III	IV
σ_{1u}	σ_{1u}	0.99794 11	0.99636 00	0.99794 11	0.99989 53
σ_{1u}	σ_{2u}	-0.27466 47	-0.32213 40	-0.34031 41	-0.31652 24
σ_{1u}	σ_{3u}	-1.43144 10	-1.40596 79	-1.30981 90	-0.68623 79
σ_{2u}	σ_{2u}	0.24326 50	0.22973 90	0.19540 33	0.11020 21
σ_{2u}	σ_{3u}	-1.92388 19	-1.98599 45	-2.05668 91	-1.71145 17
σ_{3u}	σ_{3u}	9.60814 12	10.96078 07	12.49625 10	28.46910 53
π_u^\pm	π_u^\pm	-1.21005 78	-1.54867 91	-1.96475 37	-7.92423 34

(vii)		$2R^3(\varphi_i q_a \varphi_j)$			
φ_i	φ_j	I	II	III	IV
σ_{1g}	σ_{1u}	-1	-1	-0.99999 94	-1
σ_{1g}	σ_{2u}	-0.24553 48	-0.28552 53	-0.30945 97	-0.30639 08
σ_{1g}	σ_{3u}	-1.58896 19	-1.59023 07	-1.48897 46	-0.85000 24
σ_{2g}	σ_{1u}	0.11635 72	0.14576 70	0.16863 10	0.23100 68
σ_{2g}	σ_{2u}	-0.54706 66	-0.61937 54	-0.69247 58	-0.95219 28
σ_{2g}	σ_{3u}	-0.92079 51	-0.87130 48	-0.86111 21	-0.57628 13
σ_{3g}	σ_{1u}	0.20507 07	0.22628 90	0.25258 77	0.29288 52
σ_{3g}	σ_{2u}	-1.06573 10	-1.14028 75	-1.18542 32	-1.10638 86
σ_{3g}	σ_{3u}	5.49284 91	6.58865 42	7.81316 45	20.98085 40
π_g^\pm	π_u^\pm	-2.36499 34	-2.90029 02	-3.50949 55	-10.43402 70

(viii)		$R^3(\varphi_i \varphi_j)_0$	(viii)		$R^3(\varphi_i \varphi_j)_0$
φ_i	φ_j	IV	φ_i	φ_j	IV
σ_{1g}	σ_{1g}	890.04945 3	σ_{2g}	σ_{1u}	-205.00440 1
σ_{1g}	σ_{2g}	-205.00391 7	σ_{2g}	σ_{2u}	53.22905 0
σ_{1g}	σ_{3g}	23.89838 4	σ_{2g}	σ_{3u}	16.66520 8
σ_{2g}	σ_{2g}	47.21828 2	σ_{3g}	σ_{1u}	23.89844 1
σ_{2g}	σ_{3g}	-5.50448 3	σ_{3g}	σ_{2u}	-6.20519 0
σ_{3g}	σ_{3g}	0.64168 7	σ_{3g}	σ_{3u}	-1.94275 1
σ_{1u}	σ_{1u}	890.05365 9			
σ_{1u}	σ_{2u}	-231.10094 3			
σ_{1u}	σ_{3u}	-72.35420 1			
σ_{2u}	σ_{2u}	60.00497 3			
σ_{2u}	σ_{3u}	18.78664 7			
σ_{3u}	σ_{3u}	5.88181 4			
σ_{1g}	σ_{1u}	890.05155 6			
σ_{1g}	σ_{2u}	-231.10039 7			
σ_{1g}	σ_{3u}	-72.35403 0			

(ix)		$R^2(\varphi_i -\frac{1}{2}A \varphi_j)$			
φ_i	φ_j	I	II	III	IV
σ_{1g}	σ_{1g}	97.98935	87.76317	97.98925	157.53061
σ_{1g}	σ_{2g}	-17.71831	-19.18655	-21.51338	-41.29515
σ_{1g}	σ_{3g}	-4.22141	-2.82015	-1.75828	4.73003
σ_{2g}	σ_{2g}	4.45974	5.66345	6.40203	14.57782
σ_{2g}	σ_{3g}	1.13473	0.98046	0.71651	-1.55387
σ_{3g}	σ_{3g}	5.74251	6.28968	6.89064	12.78124
π_g^\pm	π_g^\pm	6.52142	7.38486	8.28344	15.71555
σ_{1u}	σ_{1u}	98.01065	87.79935	98.01065	157.53189
σ_{1u}	σ_{2u}	-15.41359	-18.22025	-21.53674	-46.37732
σ_{1u}	σ_{3u}	-5.26413	-9.41794	-11.56863	-14.36702
σ_{2u}	σ_{2u}	4.83928	6.59081	7.93423	20.00011
σ_{2u}	σ_{3u}	1.44400	2.78434	3.57376	6.09647
σ_{3u}	σ_{3u}	13.31319	14.87311	16.11765	22.76984
π_u^\pm	π_u^\pm	3.76744	4.41649	5.13283	12.32582

(x)		$R'(\varphi_i \frac{1}{r_a} + \frac{1}{r_b} \varphi_j)$			
φ_i	φ_j	I	II	III	IV
σ_{1g}	σ_{1g}	14.99934 7	14.24884 1	14.99933 2	18.74996 8
	σ_{2g}	-1.26343 2	-1.44516 2	-1.53409 0	-2.32534 4
	σ_{3g}	-0.27945 3	-0.18487 8	-0.09938 9	0.28926 7
σ_{2g}	σ_{2g}	2.57792 0	2.75582 1	2.89955 3	3.86455 8
	σ_{3g}	0.45754 2	0.43392 8	0.40460 5	0.19528 7
	σ_{3g}	2.63241 1	2.74595 1	2.85788 4	3.64067 6
$\pi_g \pm$	$\pi_g \pm$	2.44242 2	2.59295 0	2.73833 1	3.66289 6
σ_{1u}	σ_{1u}	15.00065 3	14.25116 2	15.00065 3	18.75003 2
	σ_{2u}	-1.10555 8	-1.38083 0	-1.54309 7	-2.61432 6
	σ_{3u}	-0.34777 4	-0.67743 2	-0.79445 4	-0.78168 3
σ_{2u}	σ_{2u}	2.28829 5	2.52079 5	2.71975 2	4.00585 8
	σ_{3u}	0.19217 2	0.32508 9	0.40236 2	0.54668 9
	σ_{3u}	3.04844 9	3.25204 6	3.41132 0	4.16249 9
$\pi_u \pm$	$\pi_u \pm$	2.30955 9	2.44773 4	2.58292 4	3.50136 9

(xi)				$R(\varphi_i^*(1)\varphi_j(1) \varphi_k^*(2)\varphi_l(2))$			
φ_i	φ_j	φ_k	φ_l	I	II	III	IV
σ_{1g}	σ_{1g}	σ_{1g}	σ_{1g}	4.87467 81	4.64006 20	4.87466 84	6.04685 88
	σ_{1g}	σ_{1g}	σ_{2g}	-0.27653 69	-0.31381 80	-0.33304 67	-0.49855 14
	σ_{1g}	σ_{1g}	σ_{3g}	-0.05205 60	-0.03064 99	-0.01318 22	0.06712 48
	σ_{1g}	σ_{1g}	σ_{2g}	1.23915 81	1.30808 99	1.37526 72	1.79417 82
	σ_{1g}	σ_{2g}	σ_{3g}	0.21626 81	0.20616 17	0.19579 40	0.11362 74
σ_{1g}	σ_{1g}	σ_{3g}	σ_{3g}	1.31070 77	1.36765 84	1.42446 01	1.81058 36
	σ_{1g}	σ_{2g}	σ_{2g}	0.02859 29	0.03934 05	0.04190 44	0.07488 98
	σ_{1g}	σ_{2g}	σ_{3g}	0.00738 30	0.00676 39	0.00441 07	-0.00770 52
	σ_{1g}	σ_{2g}	σ_{2g}	-0.00415 95	-0.00698 44	-0.00755 98	-0.01778 12
	σ_{2g}	σ_{2g}	σ_{3g}	0.00043 73	0.00100 70	0.00148 78	0.00373 22
σ_{1g}	σ_{2g}	σ_{3g}	σ_{3g}	-0.00206 97	-0.00351 67	-0.00377 65	-0.00939 88
	σ_{1g}	σ_{3g}	σ_{3g}	0.01201 90	0.01608 89	0.01617 60	0.02866 70
	σ_{1g}	σ_{3g}	σ_{2g}	0.00873 18	0.01268 02	0.01374 56	0.01922 16
	σ_{1g}	σ_{3g}	σ_{2g}	0.02025 48	0.02756 09	0.02898 66	0.04379 22
	σ_{1g}	σ_{3g}	σ_{3g}	0.01150 76	0.01397 88	0.01303 98	0.00970 26
σ_{2g}	σ_{2g}	σ_{2g}	σ_{2g}	0.97978 74	1.04057 91	1.10242 85	1.44927 40
	σ_{2g}	σ_{2g}	σ_{3g}	0.14312 47	0.15086 45	0.15870 86	0.16851 38
	σ_{2g}	σ_{3g}	σ_{3g}	0.99619 39	1.05533 42	1.11453 67	1.46628 38
	σ_{2g}	σ_{3g}	σ_{2g}	0.16394 60	0.17578 43	0.18940 15	0.26741 00
	σ_{2g}	σ_{3g}	σ_{3g}	0.13219 97	0.13356 72	0.13519 13	0.13036 58
σ_{3g}	σ_{3g}	σ_{3g}	σ_{3g}	1.09232 56	1.15248 23	1.21029 59	1.57474 78
σ_{1u}	σ_{1u}	σ_{1u}	σ_{1u}	4.87532 19	4.64118 99	4.87532 19	6.04689 12
	σ_{1u}	σ_{1u}	σ_{2u}	-0.24784 50	-0.30343 58	-0.33737 66	-0.55864 98
	σ_{1u}	σ_{1u}	σ_{3u}	-0.08632 60	-0.14441 85	-0.16659 14	-0.15638 70
	σ_{1u}	σ_{1u}	σ_{2u}	1.10758 18	1.19788 95	1.28534 42	1.82732 36
	σ_{1u}	σ_{2u}	σ_{3u}	0.08647 60	0.13211 44	0.16237 64	0.21857 00
σ_{1u}	σ_{1u}	σ_{3u}	σ_{3u}	1.51300 15	1.59935 25	1.67377 80	2.04943 02
	σ_{1u}	σ_{2u}	σ_{2u}	0.02242 17	0.03620 10	0.04256 20	0.09438 38
	σ_{1u}	σ_{2u}	σ_{3u}	0.00585 93	0.01574 22	0.02008 52	0.02770 92
	σ_{1u}	σ_{2u}	σ_{2u}	-0.00273 40	-0.00638 97	-0.00829 22	-0.02615 14
	σ_{1u}	σ_{2u}	σ_{3u}	-0.00333 98	-0.00640 81	-0.00745 41	-0.00988 20

(xi)				$R(\varphi_i^*(1)\varphi_j(1) \varphi_k^*(2)\varphi_l(2))$			
φ_i	φ_j	φ_k	φ_l	I	II	III	IV
σ_{1u}	σ_{2u}	σ_{3u}	σ_{3u}	-0.00934 15	-0.01577 48	-0.01699 72	-0.02234 20
σ_{1u}	σ_{3u}	σ_{1u}	σ_{3u}	0.03040 90	0.04580 96	0.04855 75	0.05695 08
σ_{1u}	σ_{3u}	σ_{2u}	σ_{2u}	-0.00803 05	-0.01129 36	-0.01155 60	-0.00800 10
σ_{1u}	σ_{3u}	σ_{2u}	σ_{3u}	0.02202 58	0.02769 70	0.02991 19	0.05335 94
σ_{1u}	σ_{3u}	σ_{3u}	σ_{3u}	0.00867 31	0.01392 31	0.01696 69	0.02370 36
σ_{2u}	σ_{2u}	σ_{2u}	σ_{2u}	0.88318 53	0.94451 28	1.00682 11	1.39988 78
σ_{2u}	σ_{2u}	σ_{2u}	σ_{3u}	-0.01456 31	-0.00115 45	0.01031 64	0.06332 00
σ_{2u}	σ_{2u}	σ_{3u}	σ_{3u}	0.95995 26	1.02475 77	1.08948 78	1.48295 74
σ_{2u}	σ_{3u}	σ_{2u}	σ_{3u}	0.10123 97	0.11266 93	0.12682 89	0.21864 90
σ_{2u}	σ_{3u}	σ_{3u}	σ_{3u}	0.03834 13	0.06830 48	0.09139 87	0.14926 08
σ_{3u}	σ_{3u}	σ_{3u}	σ_{3u}	1.19722 90	1.28251 38	1.35632 40	1.72671 46
σ_{1g}	σ_{1g}	σ_{1u}	σ_{1u}	4.87500 00	4.64062 58	4.87499 51	6.04687 50
σ_{1g}	σ_{1g}	σ_{1u}	σ_{2u}	-0.24782 62	-0.30338 83	-0.33734 60	-0.55864 74
σ_{1g}	σ_{1g}	σ_{1u}	σ_{3u}	-0.08634 21	-0.14441 82	-0.16658 09	-0.15638 56
σ_{1g}	σ_{1g}	σ_{2u}	σ_{2u}	1.10756 97	1.19786 00	1.28532 56	1.82732 26
σ_{1g}	σ_{1g}	σ_{2u}	σ_{3u}	0.08648 29	0.13212 39	0.16238 57	0.21857 14
σ_{1g}	σ_{1g}	σ_{3u}	σ_{3u}	1.51294 01	1.59924 05	1.67374 06	2.04943 06
σ_{1g}	σ_{2g}	σ_{1u}	σ_{1u}	-0.27657 33	-0.31389 58	-0.33309 00	-0.49855 32
σ_{1g}	σ_{2g}	σ_{1u}	σ_{2u}	0.02503 88	0.03735 14	0.04191 68	0.08399 98
σ_{1g}	σ_{2g}	σ_{1u}	σ_{3u}	0.01112 76	0.02192 35	0.02477 76	0.02711 68
σ_{1g}	σ_{2g}	σ_{2u}	σ_{2u}	-0.00441 20	-0.00822 01	-0.00952 80	-0.02357 50
σ_{1g}	σ_{2g}	σ_{2u}	σ_{3u}	0.00043 84	-0.00129 05	-0.00216 57	-0.00508 22
σ_{1g}	σ_{2g}	σ_{3u}	σ_{3u}	-0.00715 70	-0.01167 92	-0.01218 82	-0.01784 70
σ_{1g}	σ_{3g}	σ_{1u}	σ_{1u}	-0.05207 94	-0.03069 37	-0.01320 25	0.06712 46
σ_{1g}	σ_{3g}	σ_{1u}	σ_{2u}	0.00416 46	0.00307 88	0.00124 05	-0.01073 80
σ_{1g}	σ_{3g}	σ_{1u}	σ_{3u}	0.01932 36	0.02621 50	0.02573 18	0.03344 18
σ_{1g}	σ_{3g}	σ_{2u}	σ_{2u}	-0.00533 52	-0.00641 49	-0.00560 03	0.00238 56
σ_{1g}	σ_{3g}	σ_{2u}	σ_{3u}	0.01461 27	0.02017 06	0.02257 15	0.04452 34
σ_{1g}	σ_{3g}	σ_{3u}	σ_{3u}	0.00818 82	0.01485 86	0.01803 70	0.02607 78
σ_{2g}	σ_{2g}	σ_{1u}	σ_{1u}	1.23914 78	1.30806 94	1.37525 65	1.79417 78
σ_{2g}	σ_{2g}	σ_{1u}	σ_{2u}	-0.00640 43	-0.01047 28	-0.01123 80	-0.02166 08
σ_{2g}	σ_{2g}	σ_{1u}	σ_{3u}	0.01157 50	0.01367 72	0.01396 84	0.01517 14
σ_{2g}	σ_{2g}	σ_{2u}	σ_{2u}	0.88027 76	0.94079 72	1.00316 56	1.39111 44
σ_{2g}	σ_{2g}	σ_{2u}	σ_{3u}	0.07198 14	0.09110 36	0.10763 07	0.15735 72
σ_{2g}	σ_{2g}	σ_{3u}	σ_{3u}	1.04508 29	1.11269 77	1.17763 88	1.52682 44
σ_{2g}	σ_{3g}	σ_{1u}	σ_{1u}	0.21623 57	0.20609 36	0.19575 41	0.11362 50
σ_{2g}	σ_{3g}	σ_{1u}	σ_{2u}	-0.00517 88	-0.00658 28	-0.00578 76	-0.00043 74
σ_{2g}	σ_{3g}	σ_{1u}	σ_{3u}	0.02828 47	0.03597 56	0.03793 79	0.05579 62
σ_{2g}	σ_{3g}	σ_{2u}	σ_{2u}	0.01639 88	0.01885 62	0.02203 72	0.04134 50
σ_{2g}	σ_{3g}	σ_{2u}	σ_{3u}	0.10735 06	0.12090 15	0.13594 88	0.22468 26
σ_{2g}	σ_{3g}	σ_{3u}	σ_{3u}	0.13948 81	0.15273 43	0.16212 30	0.15926 60
σ_{3g}	σ_{3g}	σ_{1u}	σ_{1u}	1.31068 12	1.36760 73	1.42443 46	1.81058 28
σ_{3g}	σ_{3g}	σ_{1u}	σ_{2u}	-0.00546 53	-0.00778 13	-0.00760 37	-0.01175 90
σ_{3g}	σ_{3g}	σ_{1u}	σ_{3u}	0.01364 55	0.01416 04	0.01272 20	0.00652 30
σ_{3g}	σ_{3g}	σ_{2u}	σ_{2u}	0.91805 25	0.97959 47	1.04087 07	1.41966 42
σ_{3g}	σ_{3g}	σ_{2u}	σ_{3u}	0.02162 95	0.03725 95	0.05020 33	0.09160 38
σ_{3g}	σ_{3g}	σ_{3u}	σ_{3u}	1.12021 96	1.19055 42	1.25433 44	1.62022 00
σ_{1g}	σ_{1u}	σ_{1g}	σ_{1u}	3.87500 00	3.64062 50	3.87499 54	5.04687 50
σ_{1g}	σ_{1u}	σ_{1g}	σ_{2u}	-0.24323 07	-0.29766 66	-0.33257 86	-0.55712 88
σ_{1g}	σ_{1u}	σ_{1g}	σ_{3u}	-0.11456 26	-0.17777 18	-0.19844 93	-0.18411 18
σ_{1g}	σ_{1u}	σ_{2g}	σ_{1u}	-0.27873 58	-0.31678 56	-0.33567 25	-0.49969 66
σ_{1g}	σ_{1u}	σ_{2g}	σ_{2u}	0.36809 14	0.41852 90	0.46875 06	0.84246 16
σ_{1g}	σ_{1u}	σ_{2g}	σ_{3u}	0.11205 70	0.14468 15	0.16079 91	0.14947 08

(xi)				$R(\varphi_i^*(1)\varphi_j(1) \varphi_k^*(2)\varphi_l(2))$			
φ_i	φ_j	φ_k	φ_l	I	II	III	IV
σ_{1g}	σ_{1u}	σ_{3g}	σ_{1u}	-0.07414 89	-0.05864 03	-0.03939 70	0.04433 90
σ_{1g}	σ_{1u}	σ_{3g}	σ_{2u}	-0.16822 25	-0.18614 09	-0.20267 28	-0.26352 16
σ_{1g}	σ_{1u}	σ_{3g}	σ_{3u}	0.44218 76	0.48210 62	0.52192 95	0.84086 22
σ_{1g}	σ_{2u}	σ_{1g}	σ_{2u}	0.02239 77	0.03614 23	0.04252 37	0.09438 06
σ_{1g}	σ_{2u}	σ_{1g}	σ_{3u}	0.00623 94	0.01620 69	0.02045 32	0.02780 34
σ_{1g}	σ_{2u}	σ_{2g}	σ_{1u}	0.02504 80	0.03737 46	0.04193 35	0.08400 16
σ_{1g}	σ_{2u}	σ_{2g}	σ_{2u}	-0.00195 26	-0.00493 86	-0.00662 19	-0.02237 74
σ_{1g}	σ_{2u}	σ_{2g}	σ_{3u}	-0.00355 46	-0.00671 02	-0.00761 20	-0.00943 96
σ_{1g}	σ_{2u}	σ_{3g}	σ_{1u}	0.00435 50	0.00339 54	0.0148 82	-0.01066 78
σ_{1g}	σ_{2u}	σ_{3g}	σ_{2u}	-0.00304 92	-0.00378 01	-0.00326 17	0.00121 92
σ_{1g}	σ_{2u}	σ_{3g}	σ_{3u}	-0.00327 52	-0.00577 75	-0.00641 43	-0.01259 88
σ_{1g}	σ_{3u}	σ_{1g}	σ_{3u}	0.02954 25	0.04410 45	0.04688 20	0.05545 14
σ_{1g}	σ_{3u}	σ_{2g}	σ_{1u}	0.01094 48	0.02167 92	0.02457 31	0.02704 58
σ_{1g}	σ_{3u}	σ_{2g}	σ_{2u}	-0.01427 14	-0.01931 44	-0.01977 31	-0.02076 92
σ_{1g}	σ_{3u}	σ_{2g}	σ_{3u}	0.01587 13	0.01899 00	0.02082 90	0.04201 92
σ_{1g}	σ_{3u}	σ_{3g}	σ_{1u}	0.01800 44	0.02432 27	0.02403 88	0.03217 60
σ_{1g}	σ_{3u}	σ_{3g}	σ_{2u}	0.02050 58	0.02701 30	0.02913 46	0.04725 84
σ_{1g}	σ_{3u}	σ_{3g}	σ_{3u}	-0.01016 66	-0.01340 53	-0.01290 22	-0.01488 50
σ_{2g}	σ_{1u}	σ_{2g}	σ_{1u}	0.02859 46	0.03934 38	0.04190 36	0.07488 88
σ_{2g}	σ_{1u}	σ_{2g}	σ_{2u}	-0.00531 76	-0.00912 49	-0.01003 85	-0.02148 52
σ_{2g}	σ_{1u}	σ_{2g}	σ_{3u}	-0.00123 07	-0.00369 34	-0.00423 29	-0.00563 88
σ_{2g}	σ_{1u}	σ_{3g}	σ_{1u}	0.00729 90	0.00661 60	0.00428 26	-0.00775 80
σ_{2g}	σ_{1u}	σ_{3g}	σ_{2u}	0.00071 10	0.00140 08	0.00179 47	0.00430 16
σ_{2g}	σ_{1u}	σ_{3g}	σ_{3u}	-0.00551 14	-0.00849 92	-0.00842 55	-0.01232 44
σ_{2g}	σ_{2u}	σ_{2g}	σ_{2u}	0.22026 35	0.24207 19	0.26676 09	0.47589 98
σ_{2g}	σ_{2u}	σ_{2g}	σ_{3u}	0.02019 80	0.02583 46	0.02919 32	0.02604 80
σ_{2g}	σ_{2u}	σ_{3g}	σ_{1u}	-0.01050 59	-0.01358 27	-0.01285 22	-0.00923 90
σ_{2g}	σ_{2u}	σ_{3g}	σ_{2u}	-0.15839 09	-0.16749 72	-0.17575 24	-0.20105 64
σ_{2g}	σ_{2u}	σ_{3g}	σ_{3u}	0.20383 16	0.22699 12	0.25245 27	0.46778 26
σ_{2g}	σ_{3u}	σ_{2g}	σ_{3u}	0.07568 30	0.08503 58	0.09560 51	0.16173 66
σ_{2g}	σ_{3u}	σ_{3g}	σ_{1u}	0.01005 77	0.01348 91	0.01572 16	0.03536 80
σ_{2g}	σ_{3u}	σ_{3g}	σ_{2u}	0.04682 49	0.05166 17	0.05984 14	0.13586 44
σ_{2g}	σ_{3u}	σ_{3g}	σ_{3u}	0.01639 32	0.02437 56	0.02881 83	0.01989 68
σ_{3g}	σ_{1u}	σ_{3g}	σ_{1u}	0.01105 42	0.01452 99	0.01480 63	0.02762 42
σ_{3g}	σ_{1u}	σ_{3g}	σ_{2u}	0.01399 19	0.01958 14	0.02116 21	0.03619 28
σ_{3g}	σ_{1u}	σ_{3g}	σ_{3u}	-0.00678 79	-0.00850 37	-0.00747 35	-0.00760 24
σ_{3g}	σ_{2u}	σ_{3g}	σ_{2u}	0.16729 30	0.17633 33	0.18482 82	0.21993 92
σ_{3g}	σ_{2u}	σ_{3g}	σ_{3u}	-0.15167 04	-0.16238 24	-0.17163 22	-0.20764 24
σ_{3g}	σ_{3u}	σ_{3g}	σ_{3u}	0.24255 03	0.27048 43	0.29902 87	0.53922 74
σ_{1g}	σ_{1g}	$\pi_g \pm$	$\pi_g \pm$	1.21811 47	1.29165 58	1.36393 08	1.82108 88
σ_{1g}	σ_{2g}	$\pi_g \pm$	$\pi_g \pm$	-0.00325 31	-0.00541 77	-0.00587 19	-0.10541 66
σ_{1g}	σ_{3g}	$\pi_g \pm$	$\pi_g \pm$	0.00088 86	0.00188 76	0.00255 66	0.00736 08
σ_{2g}	σ_{2g}	$\pi_g \pm$	$\pi_g \pm$	0.94514 45	1.00401 38	1.06274 13	1.41842 60
σ_{2g}	σ_{3g}	$\pi_g \pm$	$\pi_g \pm$	0.07826 17	0.08046 94	0.08230 69	0.08063 86
σ_{3g}	σ_{3g}	$\pi_g \pm$	$\pi_g \pm$	0.95120 26	1.00897 34	1.06432 40	1.40856 90
σ_{1g}	σ_{1g}	$\pi_u \pm$	$\pi_u \pm$	1.15326 45	1.22133 53	1.28854 01	1.74259 52
σ_{1g}	σ_{2g}	$\pi_u \pm$	$\pi_u \pm$	-0.00114 16	-0.00227 30	-0.00274 11	-0.00939 32
σ_{1g}	σ_{3g}	$\pi_u \pm$	$\pi_u \pm$	0.00755 00	0.01044 07	0.01067 35	0.01266 48
σ_{2g}	σ_{2g}	$\pi_u \pm$	$\pi_u \pm$	0.95575 55	1.01464 45	1.07251 03	1.41471 18
σ_{2g}	σ_{3g}	$\pi_u \pm$	$\pi_u \pm$	0.13538 76	0.13920 42	0.14196 85	0.12715 58
σ_{3g}	σ_{3g}	$\pi_u \pm$	$\pi_u \pm$	0.94460 48	1.00165 93	1.05634 73	1.39877 20
σ_{1u}	σ_{1u}	$\pi_g \pm$	$\pi_g \pm$	1.21811 96	1.29166 75	1.36393 97	1.82108 96
σ_{1u}	σ_{2u}	$\pi_g \pm$	$\pi_g \pm$	-0.00324 65	-0.00563 41	-0.00632 43	-0.01370 20
σ_{1u}	σ_{3u}	$\pi_g \pm$	$\pi_g \pm$	0.00121 13	0.00141 71	0.00162 27	0.00442 58
σ_{2u}	σ_{2u}	$\pi_g \pm$	$\pi_g \pm$	0.89883 30	0.96117 38	1.02356 84	1.41361 22

(xi)				$R(\varphi_i^*(1)\varphi_j(1) \varphi_k^*(2)\varphi_l(2))$			
φ_i	φ_j	φ_k	φ_l	I	II	III	IV
σ_{2u}	σ_{3u}	$\pi_{g\pm}$	$\pi_{g\pm}$	0.04475 17	0.06083 27	0.07365 66	0.11276 58
σ_{3u}	σ_{3u}	$\pi_{g\pm}$	$\pi_{g\pm}$	1.01476 57	1.07764 82	1.13740 08	1.48467 80
σ_{1u}	σ_{1u}	$\pi_{u\pm}$	$\pi_{u\pm}$	1.15325 75	1.22132 25	1.28853 52	1.74259 56
σ_{1u}	σ_{2u}	$\pi_{u\pm}$	$\pi_{u\pm}$	-0.00313 72	-0.00500 13	-0.00532 39	-0.01130 98
σ_{1u}	σ_{3u}	$\pi_{u\pm}$	$\pi_{u\pm}$	0.01056 01	0.01318 51	0.01304 41	0.01200 26
σ_{2u}	σ_{2u}	$\pi_{u\pm}$	$\pi_{u\pm}$	0.85698 43	0.91915 19	0.98170 33	1.38113 48
σ_{2u}	σ_{3u}	$\pi_{u\pm}$	$\pi_{u\pm}$	0.08209 72	0.09790 60	0.11078 94	0.14223 60
σ_{3u}	σ_{3u}	$\pi_{u\pm}$	$\pi_{u\pm}$	0.99868 80	1.06399 37	1.12378 01	1.46705 32
σ_{1g}	σ_{1u}	$\pi_{g\pm}$	$\pi_{u\pm}$	0.36847 99	0.41470 08	0.46335 26	0.83899 14
σ_{1g}	σ_{2u}	$\pi_{g\pm}$	$\pi_{u\pm}$	-0.00062 38	-0.00186 28	-0.00273 13	-0.01120 48
σ_{1g}	σ_{3u}	$\pi_{g\pm}$	$\pi_{u\pm}$	-0.00994 36	-0.01292 98	-0.01316 99	-0.01470 02
σ_{2g}	σ_{1u}	$\pi_{g\pm}$	$\pi_{u\pm}$	-0.00322 18	-0.00532 39	-0.00572 36	-0.01164 46
σ_{2g}	σ_{2u}	$\pi_{g\pm}$	$\pi_{u\pm}$	0.21478 07	0.23943 52	0.26652 34	0.49314 44
σ_{2g}	σ_{3u}	$\pi_{g\pm}$	$\pi_{u\pm}$	0.04520 91	0.05165 80	0.05525 17	0.04701 04
σ_{3g}	σ_{1u}	$\pi_{g\pm}$	$\pi_{u\pm}$	-0.00778 98	-0.01027 87	-0.00987 44	-0.00876 54
σ_{3g}	σ_{2u}	$\pi_{g\pm}$	$\pi_{u\pm}$	-0.13143 65	-0.14195 53	-0.15149 48	-0.18856 28
σ_{3g}	σ_{3u}	$\pi_{g\pm}$	$\pi_{u\pm}$	0.18843 56	0.21291 46	0.23841 27	0.45710 38
σ_{1g}	$\pi_{g\pm}$	σ_{1u}	$\pi_{u\mp}$	0.00831 18	0.01260 83	0.01404 83	0.03059 60
σ_{1g}	$\pi_{g\pm}$	σ_{2u}	$\pi_{u\mp}$	0.01203 80	0.01737 93	0.01969 16	0.04094 22
σ_{1g}	$\pi_{g\pm}$	σ_{3u}	$\pi_{u\mp}$	0.00707 77	0.01002 43	0.01065 28	0.01101 64
σ_{2g}	$\pi_{g\pm}$	σ_{1u}	$\pi_{u\mp}$	0.01075 77	0.01518 24	0.01697 68	0.03563 76
σ_{2g}	$\pi_{g\pm}$	σ_{2u}	$\pi_{u\mp}$	0.08943 71	0.09768 02	0.10710 50	0.17523 12
σ_{2g}	$\pi_{g\pm}$	σ_{3u}	$\pi_{u\mp}$	0.04250 39	0.04365 02	0.04436 75	0.03739 20
σ_{3g}	$\pi_{g\pm}$	σ_{1u}	$\pi_{u\mp}$	-0.00066 90	-0.00160 44	-0.00215 37	-0.00595 16
σ_{3g}	$\pi_{g\pm}$	σ_{2u}	$\pi_{u\mp}$	-0.02877 19	-0.03134 94	-0.03361 22	-0.04019 32
σ_{3g}	$\pi_{g\pm}$	σ_{3u}	$\pi_{u\mp}$	0.01393 79	0.01666 62	0.01958 63	0.04359 80
σ_{1g}	$\pi_{u\pm}$	σ_{1u}	$\pi_{g\mp}$	0.00868 41	0.01322 78	0.01462 83	0.03115 24
σ_{1g}	$\pi_{u\pm}$	σ_{2u}	$\pi_{g\mp}$	0.01392 52	0.02007 02	0.02232 98	0.04404 18
σ_{1g}	$\pi_{u\pm}$	σ_{3u}	$\pi_{g\mp}$	0.00744 96	0.01067 45	0.01120 30	0.01168 14
σ_{2g}	$\pi_{u\pm}$	σ_{1u}	$\pi_{g\mp}$	0.01899 43	0.02575 62	0.02736 82	0.04430 08
σ_{2g}	$\pi_{u\pm}$	σ_{2u}	$\pi_{g\mp}$	0.15723 10	0.16663 76	0.17661 20	0.23404 78
σ_{2g}	$\pi_{u\pm}$	σ_{3u}	$\pi_{g\mp}$	0.08395 33	0.08446 28	0.08370 87	0.06232 02
σ_{3g}	$\pi_{u\pm}$	σ_{1u}	$\pi_{g\mp}$	0.00415 91	0.00442 49	0.00361 87	-0.00151 16
σ_{3g}	$\pi_{u\pm}$	σ_{2u}	$\pi_{g\mp}$	0.00500 70	0.00281 17	0.00067 87	-0.01152 34
σ_{3g}	$\pi_{u\pm}$	σ_{3u}	$\pi_{g\mp}$	0.04223 00	0.04448 92	0.04638 65	0.06044 70
σ_{1g}	$\pi_{u\pm}$	σ_{1g}	$\pi_{u\mp}$	0.00634 75	0.01000 59	0.01130 23	0.02773 80
σ_{1g}	$\pi_{u\pm}$	σ_{2g}	$\pi_{u\mp}$	0.01475 62	0.02067 81	0.02221 46	0.03992 28
σ_{1g}	$\pi_{u\pm}$	σ_{3g}	$\pi_{u\mp}$	0.00368 74	0.00423 14	0.00355 38	-0.00104 86
σ_{2g}	$\pi_{u\pm}$	σ_{2g}	$\pi_{u\mp}$	0.19167 33	0.19914 25	0.20608 88	0.23866 54
σ_{2g}	$\pi_{u\pm}$	σ_{3g}	$\pi_{u\mp}$	0.04537 91	0.04361 87	0.04121 68	0.01768 10
σ_{3g}	$\pi_{u\pm}$	σ_{3g}	$\pi_{u\mp}$	0.05150 70	0.05376 67	0.05586 94	0.06873 20
σ_{1u}	$\pi_{g\pm}$	σ_{1u}	$\pi_{g\mp}$	0.01192 34	0.01754 25	0.01897 66	0.03499 16
σ_{1u}	$\pi_{g\pm}$	σ_{2u}	$\pi_{g\mp}$	0.01840 11	0.02566 67	0.02808 50	0.04901 82
σ_{1u}	$\pi_{g\pm}$	σ_{3u}	$\pi_{g\mp}$	0.00919 25	0.01279 77	0.01334 26	0.01267 14
σ_{2u}	$\pi_{g\pm}$	σ_{2u}	$\pi_{g\mp}$	0.15863 23	0.16916 14	0.18062 58	0.24582 08
σ_{2u}	$\pi_{g\pm}$	σ_{3u}	$\pi_{g\mp}$	0.05411 89	0.05496 29	0.05516 37	0.04372 76
σ_{3u}	$\pi_{g\pm}$	σ_{3u}	$\pi_{g\mp}$	0.06195 82	0.06474 50	0.06666 42	0.07442 38
σ_{1g}	$\pi_{g\pm}$	σ_{1g}	$\pi_{g\mp}$	0.01147 98	0.01683 40	0.01830 88	0.03438 54
σ_{1g}	$\pi_{g\pm}$	σ_{2g}	$\pi_{g\mp}$	0.01435 26	0.01962 43	0.02150 87	0.03970 24
σ_{1g}	$\pi_{g\pm}$	σ_{3g}	$\pi_{g\mp}$	-0.00127 71	-0.00259 99	-0.00321 85	-0.00689 52
σ_{2g}	$\pi_{g\pm}$	σ_{2g}	$\pi_{g\mp}$	0.09787 09	0.10415 14	0.11194 13	0.16986 18
σ_{2g}	$\pi_{g\pm}$	σ_{3g}	$\pi_{g\mp}$	-0.02679 80	-0.02873 95	-0.03040 37	-0.03490 68

(xi)				$R(\varphi_i^*(1)\varphi_j(1) \varphi_k^*(2)\varphi_l(2))$			
φ_i	φ_j	φ_k	φ_l	I	II	III	IV
σ_{3g}	$\pi_g \pm$	σ_{3g}	$\pi_g \mp$	0.03460 51	0.03738 53	0.04007 98	0.05547 66
σ_{1u}	$\pi_u \pm$	σ_{1u}	$\pi_u \mp$	0.00603 41	0.00946 30	0.01079 68	0.02722 72
σ_{1u}	$\pi_u \pm$	σ_{2u}	$\pi_u \mp$	0.00898 48	0.01338 56	0.01549 04	0.03672 88
σ_{1u}	$\pi_u \pm$	σ_{3u}	$\pi_u \mp$	0.00561 92	0.00817 91	0.00881 02	0.01013 80
σ_{2u}	$\pi_u \pm$	σ_{2u}	$\pi_u \mp$	0.08258 72	0.09236 74	0.10321 40	0.18115 94
σ_{2u}	$\pi_u \pm$	σ_{3u}	$\pi_u \mp$	0.03522 88	0.03682 49	0.03804 76	0.03419 02
σ_{3u}	$\pi_u \pm$	σ_{3u}	$\pi_u \mp$	0.04346 95	0.04663 83	0.04922 76	0.06292 64
$\pi_g +$	$\pi_g +$	$\pi_g +$	$\pi_g +$	0.95496 46	1.01728 51	1.07749 96	1.45467 92
$\pi_g +$	$\pi_g +$	$\pi_g -$	$\pi_g -$	0.95496 46	1.01728 51	1.07749 96	1.45467 92
$\pi_g +$	$\pi_g -$	$\pi_g -$	$\pi_g +$	0.08278 00	0.08811 54	0.09324 94	0.12547 96
$\pi_g +$	$\pi_g +$	$\pi_g +$	$\pi_u +$	0.22145 86	0.24945 87	0.27919 09	0.52940 58
$\pi_g +$	$\pi_u +$	$\pi_g -$	$\pi_u -$	0.22145 86	0.24945 87	0.27919 09	0.52940 58
$\pi_g +$	$\pi_u -$	$\pi_g -$	$\pi_u +$	0.05586 19	0.06120 71	0.06663 95	0.10601 48
$\pi_g +$	$\pi_g +$	$\pi_u +$	$\pi_u +$	0.92795 04	0.98894 87	1.04803 41	1.42425 14
$\pi_g +$	$\pi_g +$	$\pi_u -$	$\pi_u -$	0.92795 04	0.98894 87	1.04803 41	1.42425 14
$\pi_g +$	$\pi_g -$	$\pi_u -$	$\pi_u +$	0.07561 89	0.08038 66	0.08503 64	0.11672 54
$\pi_u +$	$\pi_u +$	$\pi_u +$	$\pi_u +$	0.94302 46	1.00120 20	1.05698 97	1.41023 88
$\pi_u +$	$\pi_u +$	$\pi_u -$	$\pi_u -$	0.94302 46	1.00120 20	1.05698 97	1.41023 88
$\pi_u +$	$\pi_u +$	$\pi_u -$	$\pi_u +$	0.08825 92	0.09137 93	0.09419 21	0.11441 86

Table XXXI

	$\alpha\beta$	I	II	III	IV
$\xi^0 R$	$h\pi$	1.09500 86	1.31341 60	1.43360 00	2.39647 44
	$s\pi$	0.86602 54	0.93819 42	1.01036 30	1.51554 45
ξR	$h\pi$	0.11457 13	0.11848 78	0.10327 44	0.03676 16
	$s\pi$	0.50877 90	0.50042 12	0.48613 11	0.30543 91
	$\sigma\pi$	0.62731 71	0.63651 30	0.63502 58	0.44655 97
ξR	hh	0.34258 91	0.36479 31	0.25840 61	0.03168 11
	hs	0.12969 67	0.15052 32	0.14605 98	0.08898 40
	$h\sigma$	0.21484 15	0.24851 51	0.24284 90	0.15089 31
	ss	0.55761 52	0.60195 69	0.63810 84	0.65412 06
	$s\sigma$	0.06036 36	0.14958 45	0.23645 49	0.59145 58
	$\sigma\sigma$	-0.80655 05	-0.68386 75	-0.54562 90	0.32136 02
	$\pi\pi$	0.62731 71	0.63651 30	0.63502 58	0.44655 97

Table XXXII Table of configurations

(i) ${}^1\Sigma_g^+$ (Li_2)

	σ_{1g}	σ_{1u}	σ_{2g}	σ_{2u}	σ_{3g}	σ_{3u}	π_{u+}	π_{u-}	π_{g+}	π_{g-}
1	2	2		2						
2	2	2			2					
3	2	2				2				
4	2	2					2			
5	2	2				1				
6	2	2				1				
7	2	2						1		
8	2	2						1		1

(ii) $^1\Sigma_u^+$ and $^3\Sigma_u^+$ (Li_2)

	σ_{1g}	σ_{1u}	σ_{2g}	σ_{2u}	σ_{3g}	σ_{3u}	π_{u^+}	π_{u^-}	π_{g^+}	π_{g^-}
1	2	2	1	1						
2	2	2	1		1	1				
3	2	2		1	1	1				
4	2	2			1	1	1			
5	2	2								1

(iii) $^1\Pi_u$ (Li_2)

	σ_{1g}	σ_{1u}	σ_{2g}	σ_{2u}	σ_{3g}	σ_{3u}	π_{u^+}	π_{u^-}	π_{g^+}	π_{g^-}
1	2	2	1		1		1			
2	2	2		1			1			
3	2	2				1			1	
4	2	2							1	

(iv) $^3\Sigma_g^-$ (O_2)*

	σ_{1g}	σ_{1u}	σ_{2g}	σ_{2u}	σ_{3g}	σ_{3u}	π_{u^+}	π_{u^-}	π_{g^+}	π_{g^-}
A	2	2	2	2	2		2	2	1	1
B	2	2	2	2		2	2	2	1	1
C	2	2	2	2	2		1	1	2	2
D	2	2	2	2		2	1	1	2	2
E ₁	2	2	2	2	2	2	1	1	1	1
E ₂	2	2	2	2	2	2	1	1	1	1
F ₁	2	2	2	2	1	1	1	2	2	1
F ₂	2	2	2	2	1	1	1	2	2	1
F ₃	2	2	2	2	1	1	1	2	2	2
H	2	2	2		2	2	2	2	1	1
J ₁	2	2	2	1	2	1	2	2	1	1
J ₃	2	2	2	1	2	1	2	2	1	1
L	2	2		2	2	2	2	2	1	1
M ₁	2	2	1	2	2	1	1	2	2	1
M ₂	2	2	1	2	2	1	1	2	2	1
M ₃	2	2	1	2	2	1	1	2	2	1
O ₁	2	2	1	2	1	2	2	2	1	1

* pins associated with two orbitals with the same superbar $\overline{\quad}$ or $\overline{\overline{\quad}}$ are coupled to triplet, while spins associated with two orbitals with the same subbar $\underline{\quad}$ or $\underline{\underline{\quad}}$ are coupled to singlet.

(v) $^1\Sigma_u^-$ (O_2)

	σ_{1g}	σ_{1u}	σ_{2g}	σ_{2u}	σ_{3g}	σ_{3u}	π_{u^+}	π_{u^-}	π_{g^+}	π_{g^-}
<i>A</i>	2	2	2	2	2		2	1	1	2
<i>B</i>	2	2	2	2		2	2	1	1	2
<i>I</i> ₁	2	2	2	1	2	1	2	1	1	2

(vi) $^3\Sigma_u^+$ and $^3\Sigma_u^-$ (O_2)

	σ_{1g}	σ_{1u}	σ_{2g}	σ_{2u}	σ_{3g}	σ_{3u}	π_{u^+}	π_{u^-}	π_{g^+}	π_{g^-}
<i>A</i>	2	2	2	2	2		2	1	1	2
<i>B</i>	2	2	2	2		2	2	1	1	2
<i>E</i> ₁	2	2	2	2	1	1	2	2	1	1
<i>F</i> ₁	2	2	2	2	1	1	1	1	2	2
<i>I</i> ₁	2	2	2	1	2	1	2	1	1	2

(vii) $^1\Sigma_g^+$ (O_2)

	σ_{1g}	σ_{1u}	σ_{2g}	σ_{2u}	σ_{3g}	σ_{3u}	π_{u^+}	π_{u^-}	π_{g^+}	π_{g^-}
<i>A</i>	2	2	2	2	2		2	2	1	1
<i>B</i>	2	2	2	2	2		1	1	2	2
<i>E</i>	2	2	2	2		2	2	2	1	1
<i>J</i> ₁	2	2	2	2	1	1	2	1	1	2
<i>N</i> ₁	2	2	2	1	2	1	2	2	1	1

(viii) 1A_g (O_2)

	σ_{1g}	σ_{1u}	σ_{2g}	σ_{2u}	σ_{3g}	σ_{3u}	π_{u^+}	π_{u^-}	π_{g^+}	π_{g^-}
<i>A</i>	2	2	2	2	2		2	2	2	
<i>C</i>	2	2	2	2	2		2		2	2
<i>D</i>	2	2	2	2		2	2	2	2	
<i>G</i> ₁	2	2	2	2	1	1	2	1	2	1
<i>J</i>	2	2	2	1	2	1	2	2	2	

Table XXXIII

(a) Li_2

$^1\Sigma_g^+$	$^1\Pi_u$	$R^{-1}(i z j)$		
i	j	I	II	III
1	1	-0.92176	-0.88143	-0.84748
1	2	0.10341	0.11859	0.13297
2	3	0.89474	0.83511	0.78185
2	4	-0.77960	-0.77724	-0.77135
3	1	-0.92176	-0.88143	-0.84748
3	3	0.89474	0.83511	0.78185
4	2	0.10341	0.11859	0.13297
4	4	-0.77960	-0.77724	-0.77135
5	1	0.63267	0.59051	0.55285
5	2	-0.55126	-0.54959	-0.54543
5	3	-0.65178	-0.62326	-0.59926
5	4	0.07312	0.08385	0.09402
6	1	0.07312	0.08385	0.09402
6	2	-0.65178	-0.62326	-0.59926
6	3	-0.55126	-0.54959	-0.54543
6	4	0.63267	0.59051	0.55285
7	5	-0.80014	-0.77811	-0.76118
8	5	-0.80014	-0.77811	-0.76118

(b) Li_2

$^1\Sigma_g^+$	$^1\Pi_u$	$R(i \varsigma j)$		
i	j	I	II	III
1	1	-0.98617	-1.01163	-1.03535
1	2	-0.36957	-0.44781	-0.38899
2	3	-1.57251	-1.61720	-1.72751
2	4	-2.22174	-2.32039	-2.35761
3	1	0.98617	1.01163	1.03535
3	3	1.57251	1.61720	1.72751
4	2	0.36957	0.44781	0.38899
4	4	2.22174	2.32039	2.35761
5	1	-1.11193	-1.14354	-1.22153
5	2	-1.57101	-1.64076	-1.66708
5	3	-0.69733	-0.71533	-0.73211
5	4	-0.26132	-0.31665	-0.27505
6	1	0.26132	0.31665	0.27505
6	2	0.69733	0.71533	0.73211
6	3	1.57101	1.64076	1.66708
6	4	1.11193	1.14354	1.22153
7	5	1.00388	0.99056	0.96673
8	5	-1.00388	-0.99056	-0.96673

(c) Li₂

$^1\Sigma_g^+$	$^1\Pi_u$	$R^{-1}(i x+iy j)$		
i	j	I	II	III
1	1	0.99623	0.92222	0.85630
2	2	-0.00051	-0.00604	-0.01160
3	3	0.89122	0.82999	0.77697
4	4	0.30782	0.24765	0.20132
5	1	-0.00036	-0.00427	-0.00820
5	2	0.70444	0.65211	0.60549
6	3	0.21766	0.17512	0.14235
6	4	0.63019	0.58690	0.54940
7	3	0.63019	0.58690	0.54940
7	4	0.21766	0.17512	0.14235
8	1	0.70444	0.65211	0.60549
8	2	-0.00036	-0.00427	-0.00820

(d) Li₂

$^1\Sigma_g^+$	$^1\Pi_u$	$\frac{1}{\sqrt{2}}R(i \xi+i\eta j)$		
i	j	I	II	III
1	1	1.04327	1.04829	1.11941
2	2	0.16966	0.15064	0.14416
3	3	0.94186	0.92817	0.99051
4	4	-0.59001	-0.48478	-0.38797
5	1	0.11997	0.10652	0.10194
5	2	0.73770	0.74125	0.79154
6	3	-0.41720	-0.34279	-0.27433
6	4	0.66600	0.65632	0.70039
7	3	-0.66600	-0.65632	-0.70039
7	4	0.41720	0.34279	0.27433
8	1	-0.73770	-0.74125	-0.79154
8	2	-0.11997	-0.10652	-0.10194

(e) Li₂

$^1\Sigma_g^+$		$R^{-2}(z^2)_{ij}$		
i	j	I	II	III
1	1	1.91655	1.84631	1.78512
2	2	2.67369	2.51826	2.38957
3	3	2.85106	2.64321	2.46788
4	4	2.20228	2.12858	2.06477
5	5	2.29512	2.18229	2.08734
6	6	2.52667	2.38589	2.26633
7	7	2.17460	2.06946	1.98192
8	8	1.73746	1.69883	1.66574
1	5	-0.69945	-0.63498	-0.58276
2	5	-0.69945	-0.63498	-0.58276
3	6	-0.63191	-0.59778	-0.56135
4	6	-0.63191	-0.59778	-0.56135

(f) Li_2

${}^1\Sigma_g^+$		$R^{-2}(x^2+y^2)_{ij}$		
<i>i</i>	<i>j</i>	I	II	III
1	1	1.19667	1.04145	0.90103
2	2	0.62665	0.55520	0.48906
3	3	1.07455	0.93763	0.81519
4	4	0.56274	0.47107	0.40085
5	5	0.91166	0.79832	0.69505
6	6	0.81865	0.70435	0.60802
7	7	1.14955	1.00436	0.87931
8	8	1.45555	1.25455	1.08527
1	5	-0.05640	-0.04477	-0.03648
2	5	-0.05640	-0.04477	-0.03648
3	6	0.18397	0.12040	0.07988
4	6	0.18397	0.12040	0.07988

(g) Li_2

${}^1\Sigma_g^+$		$2R^3(i q_a j)$		
<i>i</i>	<i>j</i>	I	II	III
1	1	4.89865	5.11039	5.36632
2	2	14.84116	16.77279	18.88952
3	3	4.48653	4.45948	4.39080
4	4	23.21628	25.92156	28.99250
5	5	9.86990	10.94159	12.12792
6	6	13.85141	15.19052	16.69165
7	7	-0.67520	-1.79382	-3.05236
8	8	1.57988	0.90264	0.07049
1	5	0.97802	1.17851	1.39405
2	5	0.97802	1.17851	1.39405
3	6	-2.72078	-2.80862	-2.90860
4	6	-2.72078	-2.80862	-2.90860

(h) Li₂

¹ Σ_g^+		H_{ij}			
<i>i</i>	<i>j</i>	R	I	II	III
11	4.5	-16.46570 5	-16.68437 9	-16.44531 4	
	5.0	-16.60099 9	-16.62684 0	-16.59991 1	
	5.5	-16.41717 0	-16.31349 9	-16.42902 3	
12	4.5	0.03643 2	0.03906 3	0.04208 9	
	5.0	0.03278 9	0.03515 7	0.03788 0	
	5.5	0.02980 8	0.03196 1	0.03443 7	
13	4.5	0.04894 7	0.05379 4	0.05928 0	
	5.0	0.04405 3	0.04841 4	0.05335 2	
	5.5	0.04004 8	0.04401 3	0.04850 2	
14	4.5	0.01681 8	0.01889 7	0.02124 5	
	5.0	0.01513 7	0.01700 7	0.01912 1	
	5.5	0.01376 1	0.01546 1	0.01738 3	
15	4.5	-0.03991 7	-0.03831 3	-0.03817 7	
	5.0	-0.04305 7	-0.04034 4	-0.03886 3	
	5.5	-0.04444 8	-0.04153 3	-0.03868 0	
16	4.5	0.00634 8	0.00811 9	0.00917 3	
	5.0	0.00571 3	0.00730 7	0.00825 6	
	5.5	0.00519 4	0.00664 3	0.00750 5	
17	4.5	0.03075 8	0.03273 2	0.03518 0	
	5.0	0.02768 2	0.02945 9	0.03166 2	
	5.5	0.02516 6	0.02678 0	0.02878 3	
18	4.5	0.06023 7	0.06258 4	0.06476 8	
	5.0	0.05421 3	0.05632 6	0.05829 1	
	5.5	0.04928 5	0.05120 6	0.05299 2	
22	4.5	-16.24430 9	-16.45726 7	-16.20660 5	
	5.0	-16.41314 5	-16.42800 6	-16.38941 7	
	5.5	-16.25487 6	-16.13688 1	-16.24089 5	
23	4.5	0.03717 6	0.03918 5	0.04107 3	
	5.0	0.03345 9	0.03526 7	0.03696 6	
	5.5	0.03041 7	0.03206 1	0.03360 5	
24	4.5	0.05390 0	0.06010 8	0.06645 1	
	5.0	0.04851 0	0.05409 7	0.05980 6	
	5.5	0.04410 0	0.04917 9	0.05436 9	
25	4.5	-0.04335 0	-0.04374 9	-0.04556 8	
	5.0	-0.04614 7	-0.04553 6	-0.04551 5	
	5.5	-0.04725 7	-0.04598 0	-0.04472 7	
26	4.5	-0.04766 5	-0.05103 2	-0.05394 9	
	5.0	-0.04289 9	-0.04592 9	-0.04855 4	
	5.5	-0.03899 9	-0.04175 3	-0.04414 0	
27	4.5	0.01087 5	0.01174 9	0.01259 6	
	5.0	0.00978 8	0.01057 4	0.01133 6	
	5.5	0.00889 8	0.00961 3	0.01030 6	
28	4.5	0.01618 7	0.01689 7	0.01755 8	
	5.0	0.01456 8	0.01520 8	0.01580 2	
	5.5	0.01324 4	0.01382 5	0.01436 6	

$^1\Sigma_g^+$		H_{ij}		
ij	R	I	II	III
33	4.5	-16.29193 7	-16.49386 8	-16.23593 6
	5.0	-16.44798 1	-16.46362 4	-16.42509 1
	5.5	-16.28057 3	-16.17125 3	-16.28022 6
34	4.5	0.02249 8	0.02503 8	0.02818 4
	5.0	0.02024 8	0.02253 4	0.02536 6
	5.5	0.01840 7	0.02048 5	0.02306 0
35	4.5	-0.04977 8	-0.05263 9	-0.05523 4
	5.0	-0.04480 0	-0.04737 5	-0.04971 0
	5.5	-0.04072 7	-0.04306 9	-0.04519 1
36	4.5	0.01999 7	0.04363 6	0.06486 0
	5.0	0.00892 2	0.02177 2	0.03591 1
	5.5	0.00135 9	0.00677 6	0.01593 9
37	4.5	0.04985 3	0.05316 2	0.05676 5
	5.0	0.04486 8	0.04784 6	0.05108 9
	5.5	0.04078 9	0.04349 6	0.04644 4
38	4.5	0.02595 5	0.02902 8	0.03243 7
	5.0	0.02335 9	0.02612 5	0.02919 3
	5.5	0.02123 6	0.02375 0	0.02653 9
44	4.5	-15.68478 2	-15.86992 4	-15.58618 9
	5.0	-15.97686 5	-15.97569 5	-15.91306 0
	5.5	-15.90831 1	-15.78243 9	-15.86884 9
45	4.5	0.00515 2	0.00766 1	0.00905 7
	5.0	0.00463 7	0.00689 5	0.00815 1
	5.5	0.00421 5	0.00626 8	0.00741 0
46	4.5	0.03662 4	0.06546 5	0.09034 2
	5.0	0.02388 5	0.04141 8	0.05884 5
	5.5	0.01496 3	0.02463 6	0.03678 8
47	4.5	0.01947 2	0.02034 7	0.02095 1
	5.0	0.01752 4	0.01831 3	0.01885 6
	5.5	0.01593 1	0.01664 8	0.01714 1
48	4.5	0.01366 1	0.01465 7	0.01547 1
	5.0	0.01229 5	0.01319 1	0.01392 4
	5.5	0.01117 7	0.01199 2	0.01265 8
55	4.5	-16.32743 3	-16.54091 5	-16.29316 5
	5.0	-16.48225 5	-16.50050 6	-16.46514 9
	5.5	-16.31346 2	-16.20072 0	-16.30812 7
56	4.5	0.05570 1	0.06192 3	0.06939 9
	5.0	0.05013 1	0.05573 1	0.06245 9
	5.5	0.04557 4	0.05066 4	0.05678 1
57	4.5	-0.01191 0	-0.01277 3	-0.01351 3
	5.0	-0.01071 9	-0.01149 6	-0.01216 2
	5.5	-0.00974 5	-0.01045 1	-0.01105 6
58	4.5	0.02016 9	0.01938 6	0.01831 9
	5.0	0.01815 2	0.01744 8	0.01648 7
	5.5	0.01650 2	0.01586 1	0.01498 8
66	4.5	-15.98369 6	-16.17658 2	-15.90334 2
	5.0	-16.20822 6	-16.21487 7	-16.16212 7
	5.5	-16.09062 7	-15.97249 8	-16.06822 0

$^1\Sigma_g^+$		H_{ij}		
ij	R	I	II	III
67	4.5	0.02405 3	0.02442 8	0.02451 7
	5.0	0.02164 7	0.02198 5	0.02206 6
	5.5	0.01968 0	0.01998 7	0.02006 0
68	4.5	0.01565 7	0.01636 7	0.01691 0
	5.0	0.01409 2	0.01473 0	0.01521 9
	5.5	0.01281 1	0.01339 1	0.01383 6
77	4.5	-16.09092 0	-16.29229 4	-16.02881 2
	5.0	-16.28201 8	-16.28926 5	-16.24178 3
	5.5	-16.14081 9	-16.01799 3	-16.11589 1
78	4.5	0.06162 7	0.06903 7	0.07685 1
	5.0	0.05546 4	0.06213 3	0.06916 6
	5.5	0.05042 2	0.05648 5	0.06287 8
88	4.5	-16.29760 4	-16.51310 3	-16.26441 2
	5.0	-16.44355 4	-16.46160 8	-16.42581 8
	5.5	-16.26946 2	-16.15504 3	-16.26236 5

(i) Li_2

$^1\Sigma_u^+$		H_{ij}		
ij	R	I	II	III
11	4.5	-16.34125	-16.54683	-16.29278
	5.0	-16.49068	-16.50717	-16.46944
	5.5	-16.31813	-16.20777	-16.31548
12	4.5	0.03786	0.05710	0.07397
	5.0	0.02766	0.03901	0.05069
	5.5	0.02037	0.02626	0.03427
13	4.5	-0.09158	-0.09365	-0.09642
	5.0	-0.08747	-0.08864	-0.08997
	5.5	-0.08327	-0.08382	-0.08416
14	4.5	0.03426	0.03835	0.04351
	5.0	0.03084	0.03451	0.03916
	5.5	0.02803	0.03138	0.03560
15	4.5	0.07752	0.08307	0.08916
	5.0	0.06977	0.07476	0.08025
	5.5	0.06343	0.06796	0.07295
22	4.5	-16.06807	-16.26911	-16.00600
	5.0	-16.28248	-16.29403	-16.24771
	5.5	-16.15688	-16.04139	-16.14096
23	4.5	0.06916	0.07731	0.08631
	5.0	0.06224	0.06958	0.07768
	5.5	0.05658	0.06325	0.07062
24	4.5	-0.02539	-0.02126	-0.01983
	5.0	-0.02789	-0.02349	-0.02103
	5.5	-0.02911	-0.02460	-0.02149
25	4.5	0.03974	0.04026	0.04025
	5.0	0.03577	0.03624	0.03623
	5.5	0.03252	0.03294	0.03293

$^1\Sigma_u^+$		H_{ij}		
ij	R	I	II	III
33	4.5	-16.24644	-16.45169	-16.19524
	5.0	-16.41105	-16.42433	-16.38383
	5.5	-16.24998	-16.13453	-16.23926
34	4.5	-0.01152	0.00331	0.01658
	5.0	-0.01679	-0.00940	-0.00096
	5.5	-0.02003	-0.01775	-0.01269
35	4.5	-0.00747	-0.00897	-0.01035
	5.0	-0.00672	-0.00807	-0.00932
	5.5	-0.00611	-0.00734	-0.00847
44	4.5	-15.91610	-16.10948	-15.83640
	5.0	-16.15141	-16.15314	-16.09724
	5.5	-16.04196	-15.91538	-16.00578
45	4.5	0.01765	0.01922	0.02067
	5.0	0.01589	0.01730	0.01860
	5.5	0.01444	0.01572	0.01691
55	4.5	-16.27155	-16.48685	-16.23784
	5.0	-16.43234	-16.45117	-16.41590
	5.5	-16.26837	-16.15537	-16.26377

(j) Li_2

$^3\Sigma_u^+$		H_{ij}		
ij	R	I	II	III
11	4.5	-16.43915	-16.65442	-16.41134
	5.0	-16.57878	-16.60400	-16.57615
	5.5	-16.39823	-16.29580	-16.41248
12	4.5	0.02888	0.04562	0.06100
	5.0	0.01958	0.02868	0.03902
	5.5	0.01302	0.01687	0.02366
13	4.5	-0.02119	-0.01920	-0.01831
	5.0	-0.02411	-0.02164	-0.01966
	5.5	-0.02567	-0.02292	-0.02025
14	4.5	0.01345	0.01539	0.01691
	5.0	0.01211	0.01385	0.01522
	5.5	0.01100	0.01259	0.01384
15	4.5	-0.02131	-0.02167	-0.02184
	5.0	-0.01918	-0.01950	-0.01966
	5.5	-0.01743	-0.01773	-0.01787
22	4.5	-16.10171	-16.30690	-16.04849
	5.0	-16.31275	-16.32804	-16.28595
	5.5	-16.18440	-16.07231	-16.17573
23	4.5	-0.02144	-0.02358	-0.02589
	5.0	-0.01930	-0.02122	-0.02330
	5.5	-0.01754	-0.01929	-0.02118
24	4.5	-0.03268	-0.03209	-0.03264
	5.0	-0.03445	-0.03324	-0.03256
	5.5	-0.03507	-0.03346	-0.03197

$^3\Sigma_u^+$		H_{ij}		
ij	R	I	II	III
25	4.5	-0.01303	-0.01283	-0.01236
	5.0	-0.01172	-0.01154	-0.01113
	5.5	-0.01066	-0.01049	-0.01012
33	4.5	-16.32079	-16.53006	-16.27739
	5.0	-16.47796	-16.49486	-16.45776
	5.5	-16.31081	-16.19866	-16.30647
34	4.5	0.05589	0.07548	0.09287
	5.0	0.04388	0.05555	0.06770
	5.5	0.03512	0.04130	0.04973
35	4.5	-0.01062	-0.01074	-0.01078
	5.0	-0.00955	-0.00966	-0.00970
	5.5	-0.00869	-0.00878	-0.00882
44	4.5	-16.02390	-16.22969	-15.96928
	5.0	-16.24843	-16.26134	-16.21683
	5.5	-16.13016	-16.01374	-16.11450
45	4.5	-0.00889	-0.00874	-0.00842
	5.0	-0.00800	-0.00787	-0.00758
	5.5	-0.00727	-0.00715	-0.00689
55	4.5	-16.19795	-16.40318	-16.14337
	5.0	-16.36610	-16.37587	-16.33088
	5.5	-16.20816	-16.08691	-16.18648

(k) Li₂

$^1\Pi_u$		H_{ij}		
ij	R	I	II	III
11	4.5	-16.35012	-16.56603	-16.32113
	5.0	-16.49390	-16.51478	-16.48251
	5.5	-16.31752	-16.20751	-16.31810
12	4.5	-0.01986	-0.01999	-0.02156
	5.0	-0.02292	-0.02235	-0.02259
	5.5	-0.02459	-0.02356	-0.02290
13	4.5	0.06760	0.07491	0.08303
	5.0	0.06084	0.06742	0.07473
	5.5	0.05531	0.06129	0.06793
14	4.5	0.01949	0.02118	0.02214
	5.0	0.01754	0.01906	0.01992
	5.5	0.01595	0.01733	0.01811
22	4.5	-16.28556	-16.50010	-16.25074
	5.0	-16.44149	-16.45823	-16.42132
	5.5	-16.27411	-16.15816	-16.26409
23	4.5	-0.03560	-0.03851	-0.04113
	5.0	-0.03204	-0.03466	-0.03702
	5.5	-0.02913	-0.03151	-0.03366
24	4.5	0.04497	0.05102	0.05733
	5.0	0.04047	0.04592	0.05160
	5.5	0.03680	0.04174	0.04691

$^1\Pi_u$		H_{ij}		
ij	R	I	II	III
33	4.5	-16.16987	-16.36966	-16.10659
	5.0	-16.34560	-16.35537	-16.31023
	5.5	-16.19306	-16.07546	-16.17696
34	4.5	0.03935	0.05684	0.07220
	5.0	0.02900	0.03879	0.04909
	5.5	0.02159	0.02605	0.03282
44	4.5	-15.89691	-16.09257	-15.82072
	5.0	-16.13759	-16.14279	-16.08932
	5.5	-16.03198	-15.90959	-16.00318

(1) Li_2 : inner shells neglected.

Set II		$R = 5.0$	H_{ij}		
ij		$^1\Sigma_g^+$	$^1\Sigma_u^+$	$^3\Sigma_u^+$	$^1\Pi_u$
11		-0.44114	-0.32858	-0.42541	-0.39476
22		-0.36471	-0.14056	-0.17458	-0.39941
33		-0.29215	-0.30694	-0.37748	-0.23766
44		0.14553	-0.06088	-0.16907	-0.05020
55		-0.37601	-0.26008	-0.38435	
66		-0.06853			
77		-0.22531			
88		-0.40726			
15		-0.02460			
25		-0.02949			
36		0.06523			
46		0.08448			
12			0.06974	0.05941	-0.01100
13			-0.07730	-0.01030	
24			-0.01215	-0.02190	
34			0.02133	0.08629	0.06952

Table XXXIV

(a) O_2 (Set IV)

$^3\Sigma_g^-$		$^3\Sigma_u^-$	$R^{-1}(i z j)$	$R(i \varsigma j)$
i	j			
A	A	0.71427	0.63793	
A	E ₁	-0.73150	-2.03082	
B	B	0.71427	0.63793	
B	E ₁	-0.73150	2.03082	
C	A	0.71427	-0.63793	
C	F ₁	-0.73150	-2.03082	
J ₁	E ₁	-0.36869	1.53788	
J ₁	I ₁	0.71427	0.63793	
F ₁	A	-0.73150	2.03082	
F ₁	E ₁	0.71427	-0.63793	
F ₁	F ₁	0.71427	0.63793	
F ₁	I ₁	-0.36869	-1.53788	
F ₁	B	-0.73150	-2.03082	

(b) O₂

(Set IV)

$^3\Sigma_g^-$	$\frac{1}{2}R^3\rho_{ij}$	$2R^3q_{ij}$	$R^{-2}(z^2)_{ij}$	$R^{-2}(x^2+y^2)_{ij}$
$i \ j$				
AA	0	-10.34673	5.14476	2.31828
AJ_1	0	0	-0.37450	0.00435
AJ_3	-9.39332	0.85573	0	0
BB	0	-10.34673	5.05794	2.27113
BO_1	0	0	-0.38904	-0.00682
CC	0	-7.92423	5.25415	2.26160
DD	0	-7.92423	5.16733	2.21445
E_1E_1	0	-7.92423	5.38188	2.03193
E_2E_2	0	-10.34673	5.38188	2.03193
F_1F_1	0	-9.13549	5.15604	2.26637
F_1F_3	1.85267	3.37998	0	0
F_2F_2	3.26175	23.68910	5.15604	2.26637
F_2F_3	0	0.85648	0	0
F_3F_3	1.63088	7.27681	5.15604	2.26637
HH	0	-10.34673	5.08695	2.13079
HJ_1	0	0	-0.37450	0.00435
HJ_3	9.39332	-0.85573	0	0
J_1J_1	0	-10.34673	5.11585	2.22454
J_1J_3	19.13543	-10.02639	0	0
J_3J_3	16.47170	1.97146	5.11585	2.22454
LL	0	-10.34673	5.34934	2.10256
M_1M_1	0	-9.13549	5.30174	2.18208
M_1M_3	14.61465	-9.58061	0	0
M_2M_2	26.55005	14.92007	5.30174	2.18208
M_2M_3	0	0.85648	0	0
M_3M_3	13.27502	2.89230	5.30174	2.18208
O_1O_1	0	-10.34673	5.20364	2.18684
F_1M_1	0	0	0.27509	0.00482
F_1M_3	-1.94613	0.58461	0	0
F_2M_2	2.75224	-0.82676	-0.27509	-0.00482
F_3M_1	1.94613	-0.58461	0	0
F_3M_3	1.37612	-0.41338	-0.27509	-0.00482
LO_1	0	0	-0.38904	-0.00682

(c) O₂

(R = 2.30. Set IV)

$^3\Sigma_g^-$	H_{ij}	$^3\Sigma_g^-$	H_{ij}	$^3\Sigma_g^-$	H_{ij}
		$i \ j$		$i \ j$	
AA	-149.00734	AM_3	0.02299	BM_2	0
AB	0.23445	AO_1	-0.01223	BM_3	0
AC	0.18408	BB	-147.34109	BO_1	-0.21372
AD	0	BC	0	CC	-148.40205
AE_1	0	BD	0.18408	CD	0.23445
AE_2	-0.03869	BE_1	0	CE_1	-0.04576
AF_1	-0.37853	BE_2	-0.04226	CE_2	0
AF_2	0.01896	BF_1	-0.37120	CF_1	-0.37120
AF_3	-0.02681	BF_2	-0.02628	CF_2	-0.02628
AH	0.09506	BF_3	0.03717	CF_3	-0.03717
AJ_1	0.32041	BH	0.09563	CH	0
AJ_3	0.03802	BJ_1	0.12767	CJ_1	0
AL	0.07032	BJ_3	0	CJ_3	0
AM_1	-0.02462	BL	0.11627	CL	0
AM_2	-0.01626	BM_1	0	CM_1	-0.01378

$^3\Sigma_g^-$	H_{ij}	$^3\Sigma_g^-$	H_{ij}	$^3\Sigma_g^-$	H_{ij}
$i \ j$		$i \ j$		$i \ j$	
CM_2	0.02709	F_1M_3	0.00530	J_1O_1	0.26246
CM_3	0.03832	F_1O_1	0.00975	J_3J_3	-147.85011
CO_1	0	F_2F_2	-148.30751	J_3L	0
DD	-146.74371	F_2F_3	-0.00054	J_3M_1	-0.07619
DE_1	-0.03411	F_2H	0	J_3M_2	-0.07619
DE_2	0	F_2J_1	0.01236	J_3M_3	0.30322
DF_1	-0.37853	F_2J_3	-0.01748	J_3O_1	0
DF_2	0.01896	F_2L	0	LL	-145.84116
DF_3	0.02681	F_2M_1	-0.00374	LM_1	-0.01378
E_1E_1	-147.60107	F_2M_2	-0.12140	LM_2	0.02710
E_1E_2	-0.18408	F_2M_3	0.01617	LM_3	-0.03832
E_1F_1	-0.03199	F_2O_1	0.01916	LO_1	-0.23718
E_1F_2	0.00518	F_3F_3	-147.88248	M_1M_1	-146.90737
E_1F_3	0.00733	F_3H	0	M_1M_2	0.01746
E_2E_2	-147.61068	F_3J_1	-0.01748	M_1M_3	-0.08337
E_2F_1	-0.03199	F_3J_3	0.11594	M_1O_1	0.26248
E_2F_2	0.00518	F_3L	0	M_2M_2	-147.41618
E_2F_3	-0.00733	F_3M_1	-0.00530	M_2M_3	-0.01762
E_2H	-0.11139	F_3M_2	0.01617	M_2O_1	-0.01858
E_2J_1	0.02973	F_3M_3	-0.11766	M_3M_3	-146.92934
E_2J_3	0	F_3O_1	-0.02710	M_3O_1	0.02628
E_2L	-0.14675	HH	-146.71136	O_1O_1	-146.49474
E_2M_1	-0.03066	HJ_1	0.37326		
E_2M_2	-0.00766	HJ_3	-0.03802		
E_2M_3	0.01084	HL	0.20691		
E_2O_1	0.01537	HM_1	0		
F_1F_1	-147.47045	HM_2	0		
F_1F_2	-0.00538	HM_3	0		
F_1F_3	-0.00404	HO_1	0.12362		
F_1H	0	J_1J_1	-147.79922		
F_1J_1	-0.10359	J_1J_3	-0.10539		
F_1J_3	0.01748	J_1L	-0.01602		
F_1L	0	J_1M_1	0.24935		
F_1M_1	0.13870	J_1M_2	0.05387		
F_1M_2	0.01143	J_1M_3	-0.07619		

(d) O_2 ($R=2.30$, Set IV)

$^1\Sigma_u^-$	H_{ij}
$i \ j$	
A A	-148.89094
A B	0.23445
A I ₁	0.29936
B B	-147.22865
B I ₁	0.12767
I ₁ I ₁	-147.71467

(f) O_2 ($R=2.30$, Set IV)

$^3\Sigma_u^-$	H_{ij}
$i \ j$	
A A	-148.52278
A B	0.23445
A E ₁	-0.37120
A F ₁	-0.37853
A I ₁	0.29936

(e) O_2 ($R=2.30$, Set IV)

$^3\Sigma_u^+$	H_{ij}
$i \ j$	
A A	-148.88163
A B	0.23445
A I ₁	0.29936
B B	-147.21934
B I ₁	0.12767
I ₁ I ₁	-147.66841

$^3\Sigma_u^+$	H_{ij}
$i \ j$	
E ₁ F ₁	0.18408
E ₁ I ₁	-0.11240
F ₁ F ₁	-147.35170
F ₁ I ₁	-0.10359
I ₁ I ₁	-147.30955

(g) O_2 ($R=2.30$, Set IV)

$^1\Sigma_g^+$		H_{ij}
i	j	
A	A	-148.89823
A	B	0.27627
A	E	0.23445
A	J_1	-0.37853
A	N_1	0.32041
B	B	-148.30255
B	E	0
B	J_1	-0.37120
B	N_1	0
E	E	-147.23198
E	J_1	-0.37120
E	N_1	0.12767
J_1	J_1	-147.27676
J_1	N_1	-0.10359
N_1	N_1	-147.69010

(h) ($R=2.30$, Set IV)

1A_g		H_{ij}
i	j	
A	A	-148.95279
A	C	0.23018
A	D	0.23445
A	G_1	0.37853
A	J	0.32041
C	C	-148.35230
C	D	0
C	G_1	0.37120
C	J	0
D	D	-147.28654
D	G_1	0.12767
D	J	0.37120
G_1	G_1	-147.37361
G_1	J	0.10359
J	J	-147.74466

Table XXXV
 Li_2 ; The matrix elements in Heitler-London Method for $^1\Sigma_g^+$

structure		I	II	III
$s-s ; s-s$	S	1	1	1
	H			
	R	4.5 5.0 5.5	-16.47828 9 -16.61248 6 -16.42773 4	-16.69851 8 -16.64008 6 -16.32592 8
$s-s ; s-\sigma$	S	0.31852 9	0.29177 4	0.26851 5
	H			
	R	4.5 5.0 5.5	-5.26724 2 -5.31346 6 -5.25658 3	-4.89020 4 -4.87572 3 -4.78544 0
$s-s ; \sigma-\sigma$	S	0.21048 1	0.20386 3	0.19472 4
	H	H	H	H
	R	4.5 5.0 5.5	-3.46355 9 -3.49469 9 -3.45778 1	-3.39534 5 -3.38601 3 -3.32379 9
$s-s ; \pi-\pi$	S	0	0	0
	H			
	R	4.5 5.0 5.5	0.04341 0 0.03906 9 0.03551 7	0.04230 3 0.03807 3 0.03461 1
$s-s ; ss-$	S	0.90409 2	0.87310 7	0.83812 2
	H			
	R	4.5 5.0 5.5	-14.89553 3 -15.01686 2 -14.84986 9	-14.57933 5 -14.52736 4 -14.25245 2

structure		I	II	III
<i>s-s ; sσ-</i>	<i>S</i>	0.51047 4	0.50699 8	0.50403 1
	<i>H</i>			
	<i>R</i>	4.5	-8.43579 5	-8.48555 1
		5.0	-8.50730 9	-8.45859 7
		5.5	-8.41456 5	-8.30074 2
	<i>S</i>	-0.00660 7	-0.00705 2	-0.00523 9
<i>s-s ; σσ-</i>	<i>H</i>			
	<i>R</i>	4.5	0.12156 5	0.13186 0
		5.0	0.11828 2	0.12720 0
		5.5	0.11413 0	0.12197 8
	<i>S</i>	0	0	0
	<i>H</i>			
<i>s-s ; ππ-</i>	<i>R</i>	4.5	0.05642 3	0.05620 8
		5.0	0.05078 1	0.05058 7
		5.5	0.04616 4	0.04598 8
	<i>S</i>	1	1	1
	<i>H</i>			
	<i>R</i>	4.5	-16.39642 6	-16.61152 1
		5.0	-16.54717 1	-16.56727 1
		5.5	-16.37457 5	-16.26380 9
<i>s-σ ; s-σ'</i>	<i>S</i>	0.08781 5	0.11884 3	0.14186 1
	<i>H</i>			
	<i>R</i>	4.5	-1.45179 3	-1.98171 1
		5.0	-1.47002 0	-1.98103 3
		5.5	-1.45792 3	-1.94783 6
	<i>S</i>	0	0	0
	<i>H</i>			
<i>s-σ ; π-π'</i>	<i>R</i>	4.5	0.03997 7	0.03861 1
		5.0	0.03597 9	0.03475 0
		5.5	0.03270 8	0.03159 1
	<i>S</i>	0.51047 4	0.50699 8	0.50403 1
	<i>H</i>			
	<i>R</i>	4.5	-8.40347 5	-8.45331 2
		5.0	-8.47822 1	-8.42958 3
		5.5	-8.38812 1	-8.27436 6
<i>s-σ ; ss-</i>	<i>S</i>	0.58095 7	0.58345 2	0.58482 9
	<i>H</i>			
	<i>R</i>	4.5	-9.54745 9	-9.71218 3
		5.0	-9.63579 9	-9.68632 1
		5.5	-9.53566 5	-9.50890 3

structure		I	II	III
$s-\sigma ; \sigma\sigma-$	S	0.60102 2	0.57753 0	0.55593 3
	H			
	R	4.5 5.0 5.5	-9.83913 5 -9.93401 2 -9.83332 6	-9.57844 9 -9.55677 4 -9.38430 1
$s-\sigma ; \pi\pi-$	S	0	0	0
	H			
	R	4.5 5.0 5.5	0.05527 3 0.04974 6 0.04522 3	0.05551 6 0.04996 4 0.04542 2
$\sigma-\sigma ; \sigma-\sigma$	S	1	1	1
	H			
	R	4.5 5.0 5.5	-16.29682 9 -16.46192 2 -16.30034 1	-16.51059 1 -16.47908 8 -16.18561 8
$\sigma-\sigma ; \pi-\pi$	S	0	0	0
	H			
	R	4.5 5.0 5.5	0.01950 8 0.01755 7 0.01596 1	0.02012 8 0.01811 5 0.01646 8
$\sigma-\sigma ; ss-$	S	-0.01557 0	-0.00705 2	-0.00523 9
	H			
	R	4.5 5.0 5.5	0.08032 3 0.08116 4 0.08038 6	0.09599 2 0.09491 8 0.09263 1
$\sigma-\sigma ; s\sigma-$	S	0.60102 2	0.57753 0	0.55593 3
	H			
	R	4.5 5.0 5.5	-9.80946 0 -9.90730 4 -9.80904 6	-9.54895 8 -9.53023 5 -9.36017 1
$\sigma-\sigma ; \sigma\sigma-$	S	0.31467 6	0.42364 3	0.49961 7
	H			
	R	4.5 5.0 5.5	-5.15779 9 -5.21176 2 -5.16174 1	-7.02499 6 -7.01133 0 -6.88629 2
$\sigma-\sigma ; \pi\pi-$	S	0	0	0
	H			
	R	4.5 5.0 5.5	0.01066 8 0.00960 2 0.00872 9	0.01260 5 0.01134 4 0.01031 3

structure		I	II	III	
	S	1	1	1	
	H				
$\pi-\pi ; \pi-\pi$	R	4.5 5.0 5.5	-16.31309 2 -16.46033 5 -16.28683 1	-16.52973 9 -16.48039 3 -16.17495 6	-16.28164 9 -16.44621 7 -16.28454 4
		S	0	0	0
		H			
$\pi-\pi ; ss-$	R	4.5 5.0 5.5	0.04665 7 0.04199 1 0.03817 4	0.04564 5 0.04108 1 0.03734 6	0.04397 0 0.03957 3 0.03597 5
		S	0	0	0
		H			
$\pi-\pi ; s\sigma-$	R	4.5 5.0 5.5	0.03519 5 0.03167 5 0.02879 6	0.03481 9 0.03133 7 0.02848 8	0.03407 3 0.03066 5 0.02787 8
		S	0	0	0
		H			
$\pi-\pi ; \sigma\sigma-$	R	4.5 5.0 5.5	0.02408 5 0.02167 6 0.01970 6	0.02338 0 0.02104 2 0.01912 9	0.02240 2 0.02016 2 0.01832 9
		S	0.76782 6	0.71087 6	0.65111 9
		H			
$\pi-\pi ; \pi\pi-$	R	4.5 5.0 5.5	-12.53771 2 -12.64453 6 -12.50704 5	-11.77068 6 -11.72707 2 -11.50403 9	-10.63117 5 -10.72727 4 -10.61429 5
		S	1	1	1
		H			
$ss- ; ss-$	R	4.5 5.0 5.5	-16.43646 3 -16.57484 3 -16.39351 3	-16.64606 5 -16.59287 9 -16.28301 2	-16.39603 9 -16.55666 7 -16.39053 0
		S	0.31852 9	0.29177 4	0.26851 5
		H			
$ss- ; s\sigma-$	R	4.5 5.0 5.5	-5.31540 0 -5.35680 9 -5.29598 6	-4.94188 1 -4.92223 3 -4.82772 1	-4.49353 8 -4.53031 8 -4.48005 8
		S	0.21048 1	0.20386 3	0.19472 4
		H			
$ss- ; \sigma\sigma-$	R	4.5 5.0 5.5	-3.41159 0 -3.44792 7 -3.41526 1	-3.34527 4 -3.34094 9 -3.28283 2	-3.14477 2 -3.18160 5 -3.15367 3

structure		I	II	III
$ss^- ; \pi\pi^-$	S	0	0	0
	H			
	R	4.5 5.0 5.5	0.07454 5 0.06709 1 0.06099 2	0.07991 6 0.07192 4 0.06538 5
$s\sigma^- ; s\sigma^-$	S	1	1	1
	H			
	R	4.5 5.0 5.5	-16.34036 5 -16.49671 5 -16.32870 7	-16.54506 3 -16.50745 8 -16.20943 4
$s\sigma^- ; \sigma\sigma^-$	S	0.08781 5	0.11884 3	0.14186 1
	H			
	R	4.5 5.0 5.5	-1.50906 2 -1.52156 2 -1.50478 0	-2.04362 6 -2.03675 7 -1.99849 4
$s\sigma^- ; \pi\pi^-$	S	0	0	0
	H			
	R	4.5 5.0 5.5	0.02502 7 0.02252 4 0.02047 7	0.02314 4 0.02083 0 0.01893 6
$\sigma\sigma^- ; \sigma\sigma^-$	S	1	1	1
	H			
	R	4.5 5.0 5.5	-16.24372 1 -16.41412 4 -16.25688 9	-16.44725 0 -16.42208 1 -16.13379 4
$\sigma\sigma^- ; \pi\pi^-$	S	0	0	0
	H			
	R	4.5 5.0 5.5	0.04153 6 0.03738 3 0.03398 4	0.04167 7 0.03750 9 0.03410 0
$\pi\pi^- ; \pi\pi^-$	S	1	1	1
	H			
	R	4.5 5.0 5.5	-16.23412 8 -16.38926 7 -16.22222 4	-16.43262 9 -16.39299 4 -16.09550 3