Molecular Structure Formulas

$E_{SO} = {}^1/_2\, \mathcal{A} hc \{ J(J+1) - L(L+1) - S(S+1) \}$

$g_s(\alpha,r) = \left(\frac{2\alpha}{\pi}\right)^{3/4} e^{-\alpha r^2}$ $\quad g_x(\alpha,r) = \left(\frac{128\alpha^5}{\pi^3}\right)^{1/4} x\, e^{-\alpha r^2}$ $\quad \phi_\mu = \sum_{i=1}^{n} d_{mi}\, g_i(\alpha,r)$

$\Psi_a = 1/\sqrt{2} \begin{vmatrix} \Psi_{1s}(1)\alpha(1) & \Psi_{1s}(1)\beta(1) \\ \Psi_{1s}(2)\alpha(2) & \Psi_{1s}(2)\beta(2) \end{vmatrix}$ $\quad \frac{-\hbar^2}{2m}\nabla^2\Psi + \frac{e^2}{4\pi\varepsilon_o}\left(-\frac{1}{r_{1A}} - \frac{1}{r_{1B}} + \frac{1}{R}\right)\Psi = E\Psi$

$c_A(H_{AA} - E\,S_{AA}) + c_B(H_{AB} - E\,S_{AB}) = 0$ $\quad E_+ = \frac{H_{AA} + H_{AB}}{1 + S}$

$c_A(H_{AB} - E\,S_{AB}) + c_B(H_{BB} - E\,S_{BB}) = 0$ $\quad E_- = \frac{H_{AA} - H_{AB}}{1 - S}$

$\Psi_+ = \frac{1}{\sqrt{2+2\,S}}(\Psi_A + \Psi_B)$ $\quad \Psi_- = \frac{1}{\sqrt{2-2\,S}}(\Psi_A - \Psi_B)$

$E_+ = H_{AA} - \frac{(H_{AB} - H_{AA}\,S)^2}{H_{BB} - H_{AA}}$ $\quad E_- = H_{BB} + \frac{(H_{AB} - H_{BB}\,S)^2}{H_{BB} - H_{AA}}$

$d_a = \sum_{j\ on\ a} \sum_{i=1}^{m} n_i c_{ij}^{\,2}$ $\quad P_{ab} = \sum_{j\ on\ a} \sum_{k\ on\ b} \sum_{i=1}^{m} n_i\, 2c_{ij}\, c_{ik}\, S_{jk}$

$\hat{\vec{\mu}} = -\sum_{i=1}^{n} e\, \hat{\vec{r}}_i$ $\quad \langle\mu_x\rangle = -\sum_{i=1}^{n} e \int \Psi_{MO}^{*}\, x_i\, \Psi_{MO}\, d\tau$ $\quad 1\ D = 3.336\text{x}10^{-30}\ C\ m$

$(\chi_A - \chi_B)^2 = D_o(A\text{–}B) - [D_o(A\text{–}A)\, D_o(B\text{–}B)]^{1/2}$

$x_A = \frac{I_{1A} + (-EA_A)}{2}$ $\quad \chi_A = 0.336(x_A - 0.615)$

$D_o = D_e - \tfrac{1}{2} h\nu_o$ $\quad V = \tfrac{1}{2}\, k (r - r_o)^2$ $\quad k = \left(\frac{\partial^2 V}{\partial r^2}\right)$

symmetry	rotate 180°	reflect-σ_v
symmetric	a	1
antisymmetric	b	2

$\Psi_1 = \frac{1}{\sqrt{2}}(s + p)$ $\quad \Psi_2 = \frac{1}{\sqrt{2}}(s - p)$ $\quad \vec{u} \cdot \vec{v} = |u|\,|v| \cos\theta$

$\Psi_1 = \frac{1}{\sqrt{3}}s + \frac{\sqrt{2}}{\sqrt{3}}p_x$

$\Psi_2 = \frac{1}{\sqrt{3}}s - \frac{1}{\sqrt{6}}p_x + \frac{1}{\sqrt{2}}p_y$

$\Psi_3 = \frac{1}{\sqrt{3}}s - \frac{1}{\sqrt{6}}p_x - \frac{1}{\sqrt{2}}p_y$

$\Psi_1 = \tfrac{1}{2}(s + p_x + p_y + p_z)$

$\Psi_2 = \tfrac{1}{2}(s - p_x + p_y - p_z)$

$\Psi_3 = \tfrac{1}{2}(s + p_x - p_y - p_z)$

$\Psi_4 = \tfrac{1}{2}(s - p_x - p_y + p_z)$

$x = \frac{E - \alpha}{\beta}$ $\quad E = \alpha + x\beta$ $\quad P_{AB} = \sum_{i=1}^{m} n_i\, c_{iA}\, c_{iB}$ $\quad \rho_j = \sum_{i=1}^{m} n_i\, c_{ij}^{\,2}$