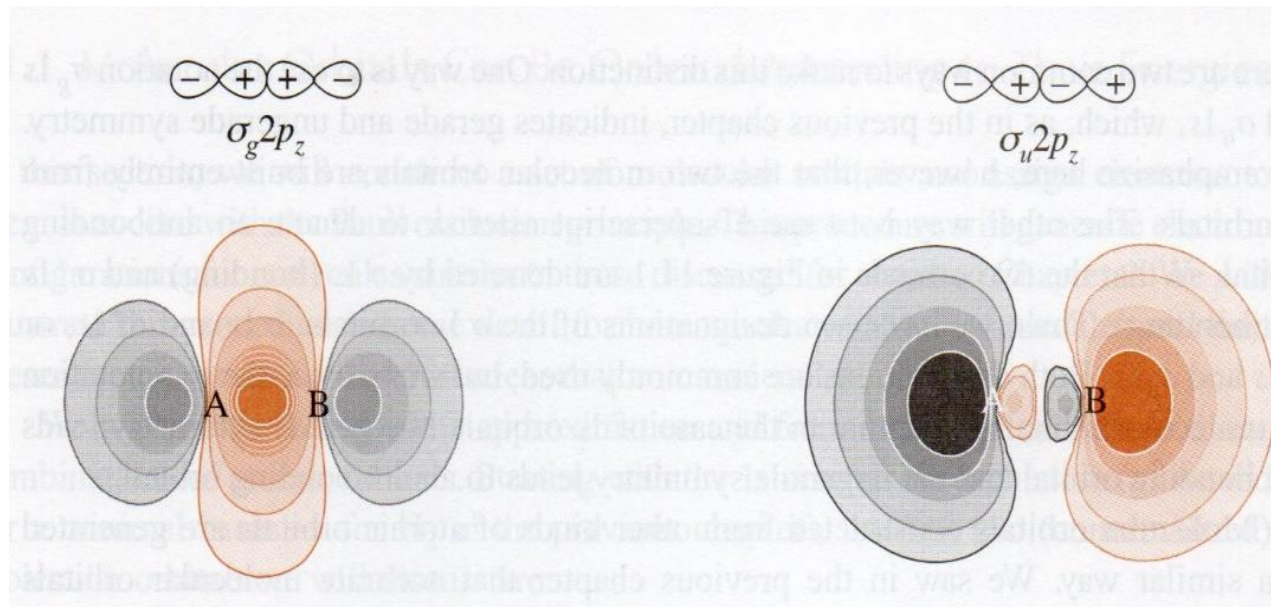
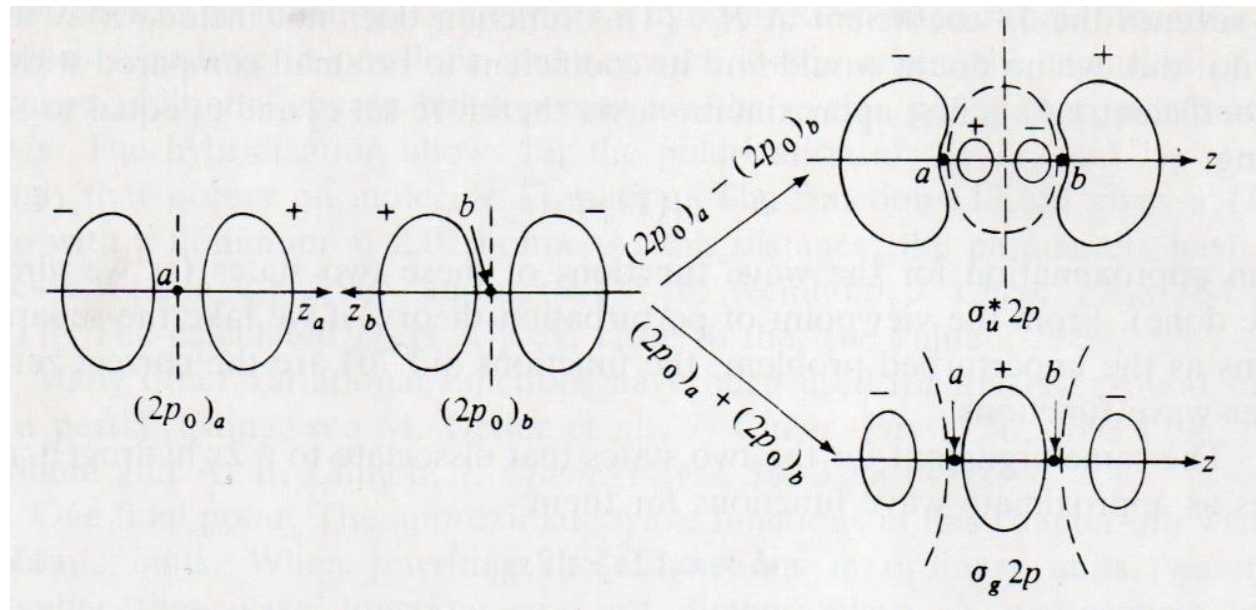


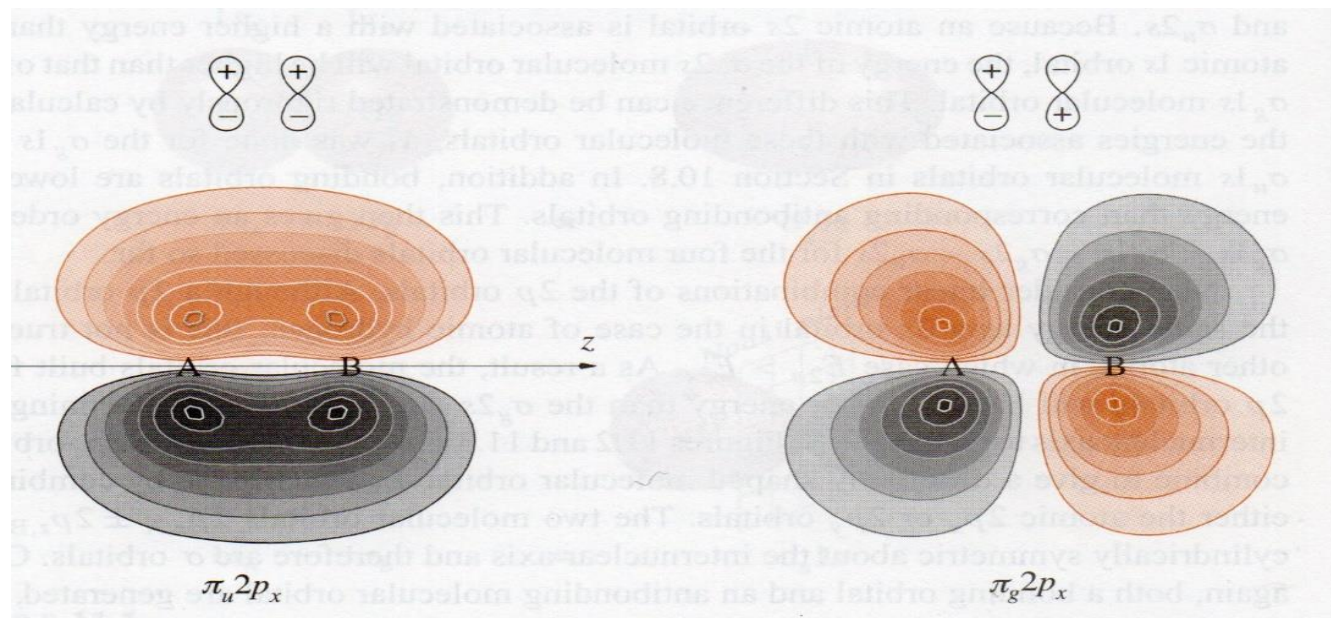
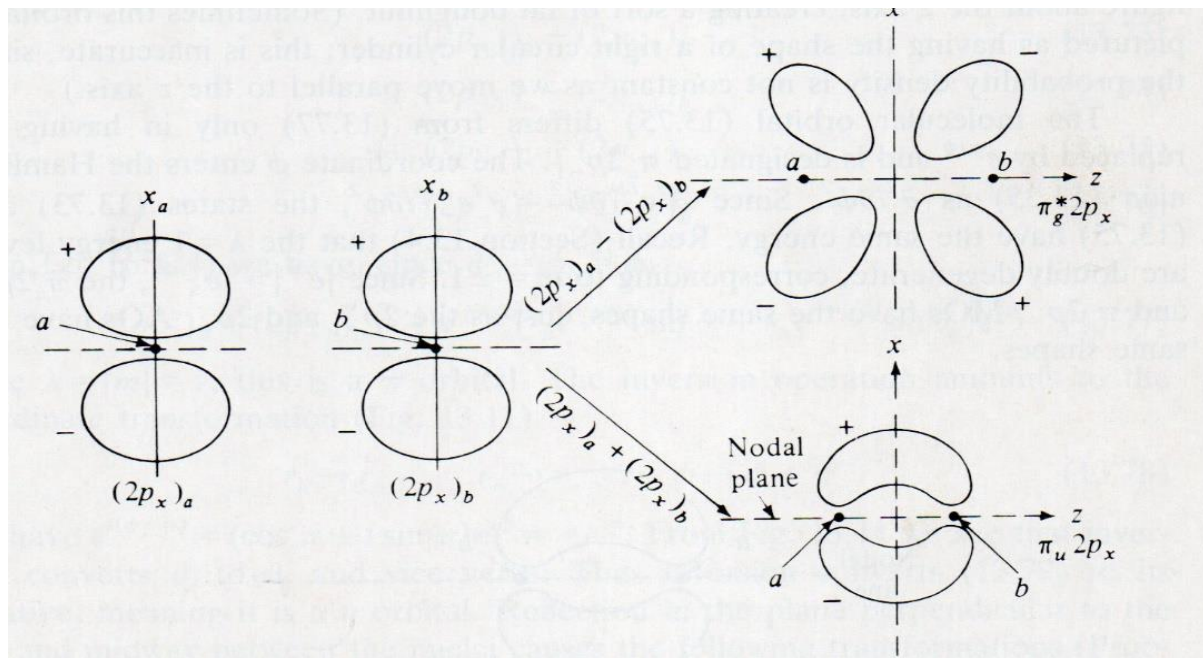
Figure 13.5 Atomic probability densities for H_2^+ . Note the cusps at the nuclei.

$$S(R) = e^{-R} \left(1 + R + \frac{R^2}{3} \right)$$

$$\psi_b = \psi_+ = \frac{1}{\sqrt{2(1+S)}} (1s_A + 1s_B)$$

$$\psi_a = \psi_- = \frac{1}{\sqrt{2(1-S)}} (1s_A - 1s_B)$$





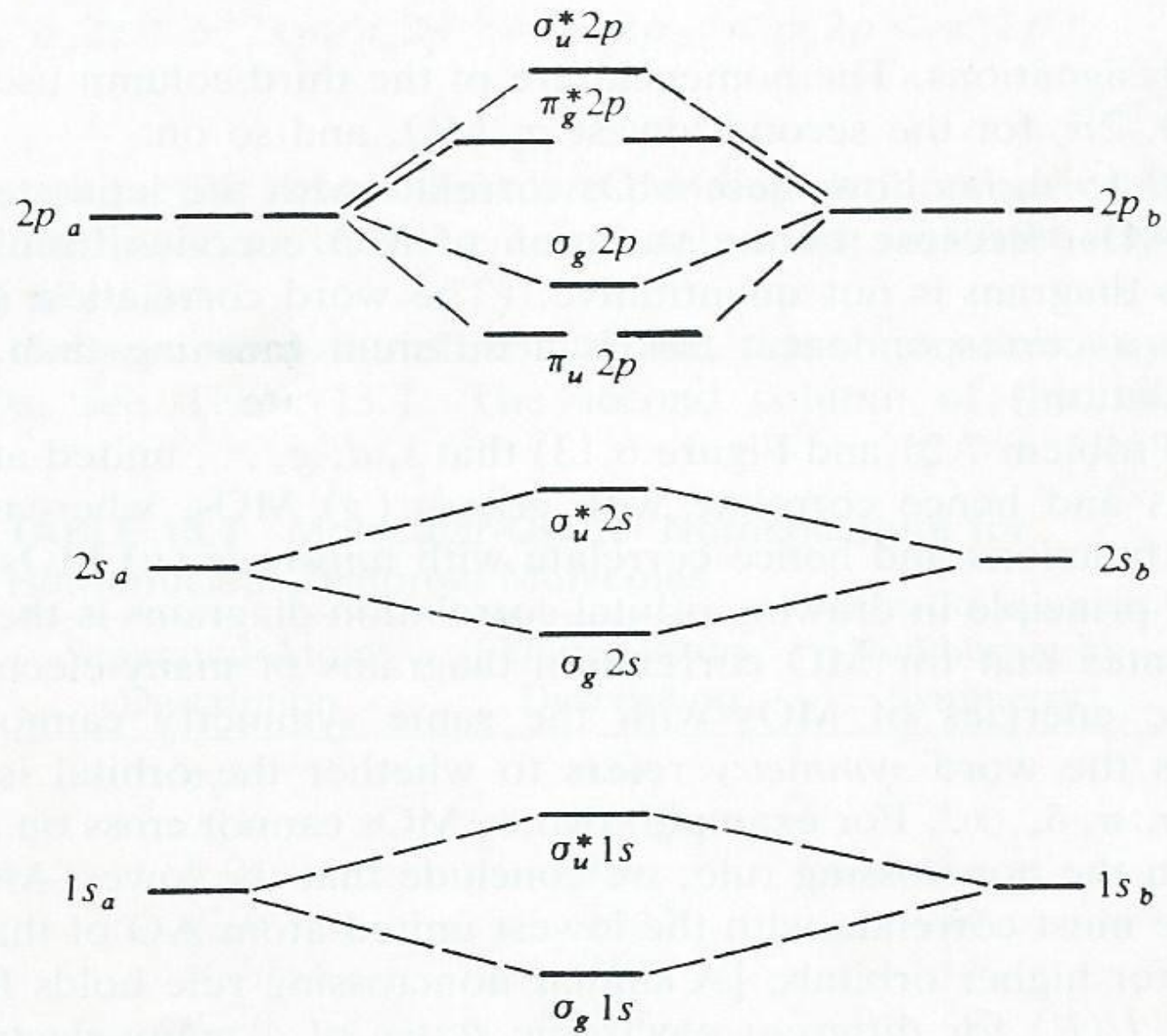


Figure 13.16 Homonuclear diatomic MOs formed from $1s$, $2s$, and $2p$ AOs.

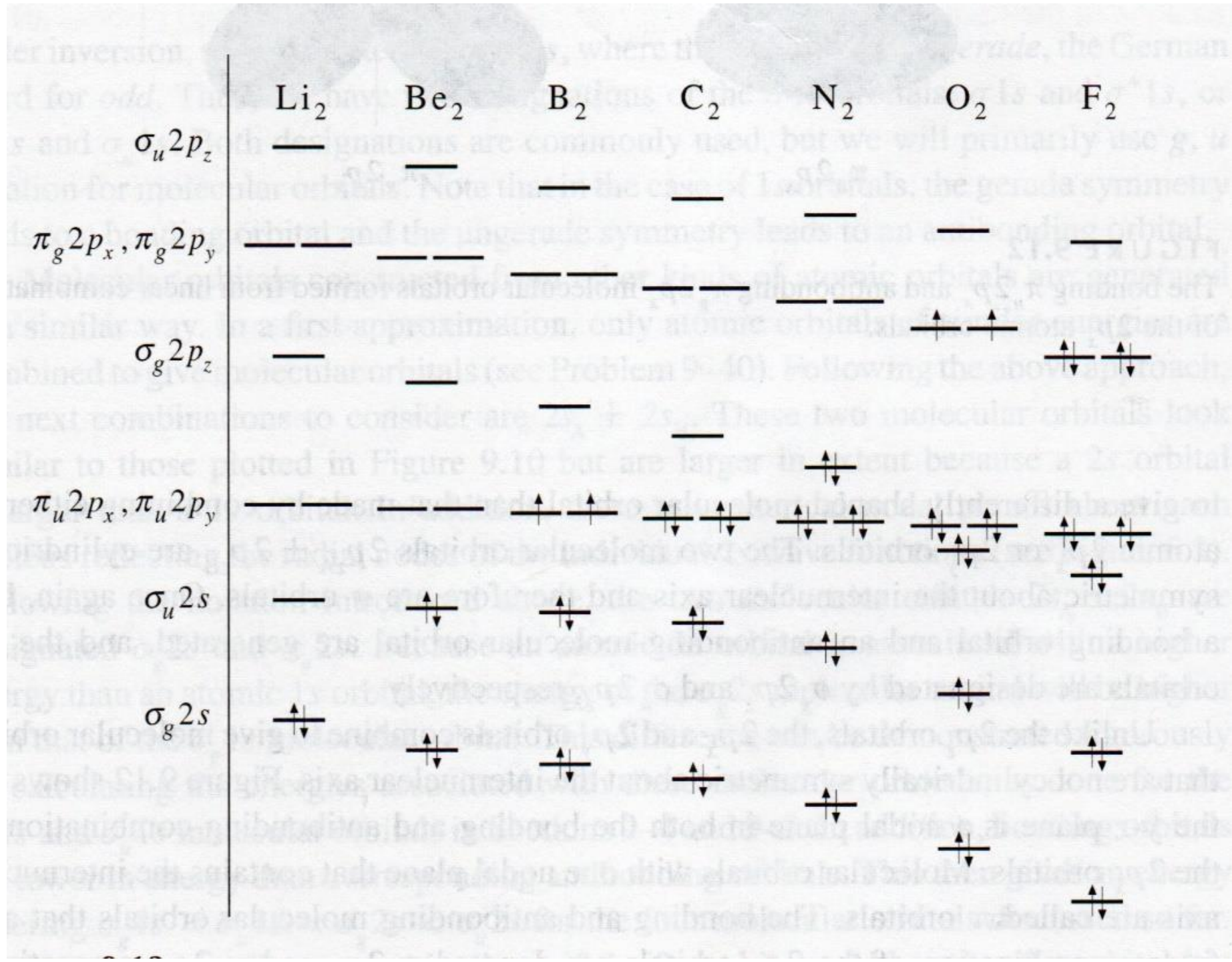


Table 6.4 Minimal-basis SCF-LCAO-MO's for N_2^*

		-15.72176	-1.45241	-0.54451
		<hr/>		
	ξ	$1\sigma_g$	$2\sigma_g$	$3\sigma_g$
<hr/>				
$1s\sigma_g$	6.70	0.70447	-0.16890	-0.06210
$2s\sigma_g$	1.95	0.00842	0.48828	0.40579
$2p\sigma_g$	1.95	0.00182	0.23970	-0.60324
		<hr/>		
		-15.71965	-0.73066	
		<hr/>		
	ξ	$1\sigma_u$	$2\sigma_u$	
<hr/>				
$1s\sigma_u$	6.70	0.70437	-0.16148	
$2s\sigma_u$	1.95	0.01972	0.74124	
$2p\sigma_u$	1.95	0.00857	-0.76578	
		<hr/>		
		-0.57951		
		<hr/>		
	ξ	$1\pi_u$		
<hr/>				
$2p\pi_u$	1.95	-0.62450		

* B. J. Ransil, *Rev. Mod. Phys.* 32, 245 (1960), with $R_e = 1.0456 \text{ \AA}$. The orbital energies ϵ_i in a.u. are given above the orbital designations.

Species	Ground-state electron configuration	Bond order	Bond length/pm	Bond energy/ kJ·mol ⁻¹
Li ₂	$KK(\sigma_g 2s)^2$	1	267	99.8
Be ₂	$KK(\sigma_g 2s)^2(\sigma_u 2s)^2$	0	245	≈ 9
B ₂	$KK(\sigma_g 2s)^2(\sigma_u 2s)^2(\pi_u 2p_x)^1(\pi_u 2p_y)^1$	1	159	289
C ₂	$KK(\sigma_g 2s)^2(\sigma_u 2s)^2(\pi_u 2p_x)^2(\pi_u 2p_y)^2$	2	124	599
N ₂	$KK(\sigma_g 2s)^2(\sigma_u 2s)^2(\pi_u 2p_x)^2(\pi_u 2p_y)^2(\sigma_g 2p_z)^2$	3	110	942
O ₂	$KK(\sigma_g 2s)^2(\sigma_u 2s)^2(\sigma_g 2p_z)^2(\pi_u 2p_x)^2(\pi_u 2p_y)^2$ $(\pi_g 2p_x)^1(\pi_g 2p_y)^1$	2	121	494
F ₂	$KK(\sigma_g 2s)^2(\sigma_u 2s)^2(\sigma_g 2p_z)^2(\pi_u 2p_x)^2(\pi_u 2p_y)^2$ $(\pi_g 2p_x)^2(\pi_g 2p_y)^2$	1	141	154
Ne ₂	$KK(\sigma_g 2s)^2(\sigma_u 2s)^2(\sigma_g 2p_z)^2(\pi_u 2p_x)^2(\pi_u 2p_y)^2$ $(\pi_g 2p_x)^2(\pi_g 2p_y)^2(\sigma_u 2p_z)^2$	0		

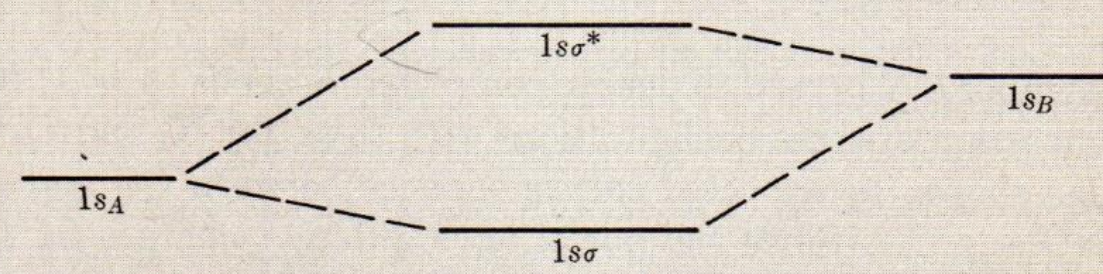
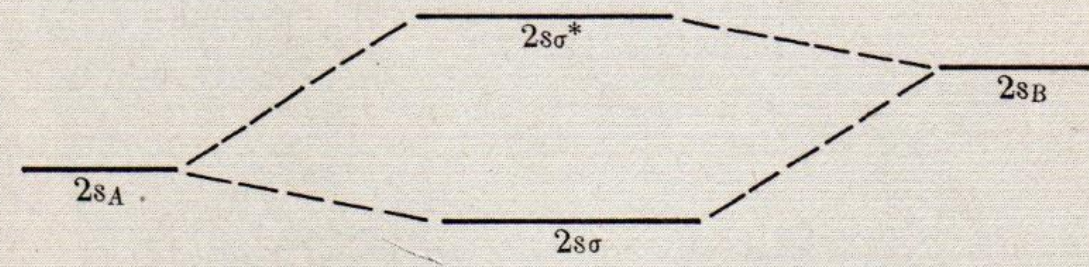
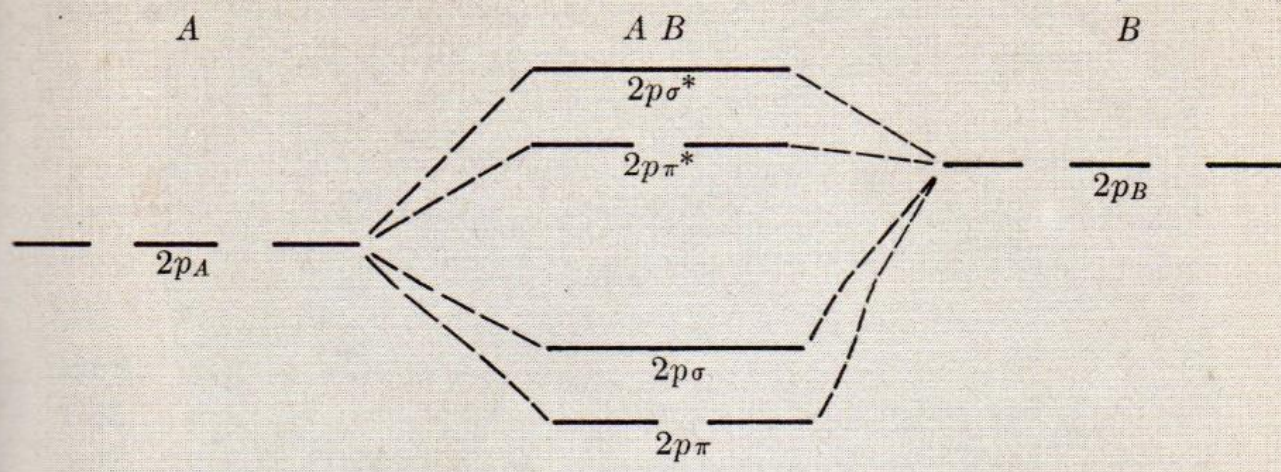


Table 6.6 SCF-LCAO-MO's for LiH^a

			-2.44695 ^b	-0.30350
			1 σ	2 σ
			ζ	
Li	1s	2.70	0.99658	0.13097
	2s	0.65	0.01605	-0.32335
	2p _z	0.65	-0.00514	-0.23106
H	1s	1.00	0.00600	-0.68526

^a B. J. Ransil, *Rev. Mod. Phys.* **32**, 245 (1960) with $R_e = 1.59536 \text{ \AA}$. For an extended basis set calculation, see P. F. Cade and W. Huo, *J. Chem. Phys.* **45**, 1063 (1966).

^b The orbital energies in a.u. are given above the orbital designations.

Table 16-4 Normalized SCF molecular orbitals and orbital energies of the ground state of the hydrogen fluoride molecule^a

<i>MO symbol</i>	$1s_F$	$2s_F$	$2p_{xF}$	$1s_H$	$2p_{zF}$ or $2p_{yF}$	<i>MO energy, a.u.</i>
1σ	0.99627	0.01632	0.00243	-0.00460		-26.139
2σ	0.24346	-0.93218	0.09066	-1.16060		-1.476
3σ	-0.08394	0.47149	-0.68695	-0.57613		-0.566
4σ	-0.08000	0.55994	0.80646	-1.05015		0.477
1π					1.00000	-0.465

^a From B. J. Ransil, *Rev. Mod. Phys.*, **32**, 245 (1960). By permission of the author and the American Institute of Physics.

Table 16-3 Normalized SCF molecular orbitals and orbital energies of the ground state of the carbon monoxide molecule^a

MO symbol	1s		2s		2p _z		MO energy, a.u.
	C	O	C	O	C	O	
1σ	-0.00021	-0.99603	0.00694	-0.02018	0.00626	-0.00576	-20.706
2σ	0.99643	-0.00024	-0.01707	-0.00542	0.00587	-0.00069	-11.353
3σ	-0.11522	-0.21481	0.24006	0.75883	0.16874	0.22322	-1.499
4σ	0.14683	0.12625	-0.53827	0.65294	-0.06682	-0.63503	-0.732
5σ	-0.14025	0.00215	0.75786	0.03656	-0.56582	-0.43792	-0.481
6σ	-0.09155	0.11970	0.96935	-1.12888	1.25088	-0.94147	0.932
			2p _x or 2p _y				
			C	O			
1π			-0.46864	-0.77124			-0.583
2π			-0.92245	0.68973			0.260

^a From B. J. Ransil, *Rev. Mod. Phys.*, **32**, 245 (1960). By permission of the author and the American Institute of Physics.

Table 6.11 *Energies of occupied orbitals in N₂, CO, BF⁺*

N ₂		CO		BF ⁺	
Orbital	Energy	Orbital	Energy	Orbital	Energy
1σ _g	-15.68195	1σ	-20.66123	1σ	-26.37504
1σ _u	-15.67833	2σ	-11.35927	2σ	-7.70897
2σ _g	-1.47360	3σ	-1.51920	3σ	-1.69759
2σ _u	-0.77796	4σ	-0.80235	4σ	-0.85373
3σ _g	-0.63495	5σ	-0.55304	5σ	-0.40424
1π _u	-0.61544	1π	-0.63771	1π	-0.74447

^a From the SCF-LCAO-MO calculations referred to in Tables 6.5 and 6.9. All values in a.u. are for the equilibrium internuclear distance.

TABLE 13.3 Electronic Terms of Diatomic Molecules

Configuration	Terms
$\sigma\sigma$	${}^1\Sigma^+, {}^3\Sigma^+$
$\sigma\pi; \sigma\pi^3$	${}^1\Pi, {}^3\Pi$
$\pi\pi; \pi\pi^3$	${}^1\Sigma^+, {}^3\Sigma^+, {}^1\Sigma^-, {}^3\Sigma^-, {}^1\Delta, {}^3\Delta$
$\pi\delta; \pi^3\delta; \pi\delta^3$	${}^1\Pi, {}^3\Pi, {}^1\Phi, {}^3\Phi$
σ	${}^2\Sigma^+$
$\sigma^2; \pi^4; \delta^4$	${}^1\Sigma^+$
$\pi; \pi^3$	${}^2\Pi$
π^2	${}^1\Sigma^+, {}^3\Sigma^-, {}^1\Delta$
$\delta; \delta^3$	${}^2\Delta$
δ^2	${}^1\Sigma^+, {}^3\Sigma^-, {}^1\Gamma$

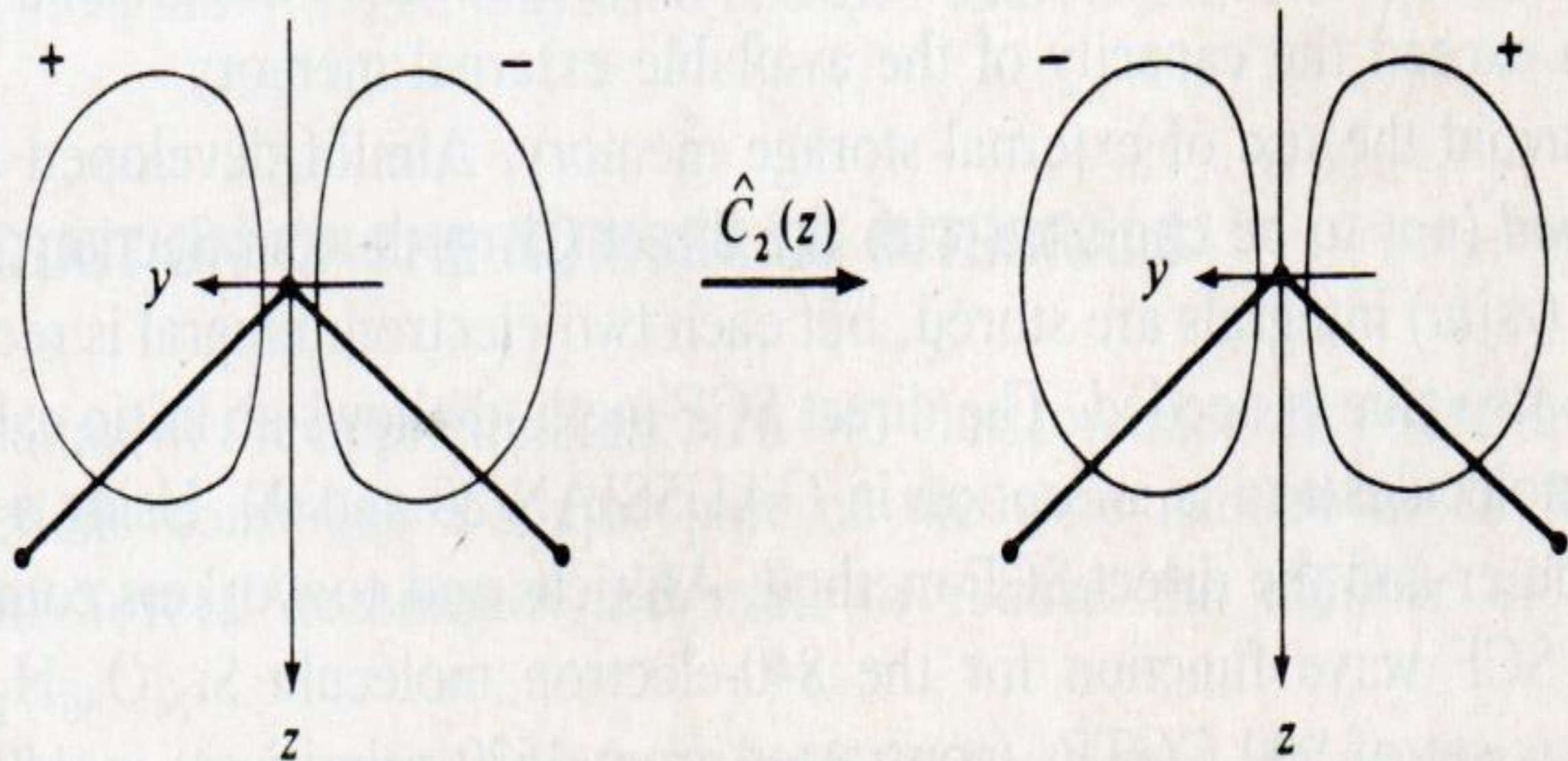


Figure 15.2 The effect of $\hat{C}_2(z)$ on the $2p_y$ oxygen AO in H_2O .

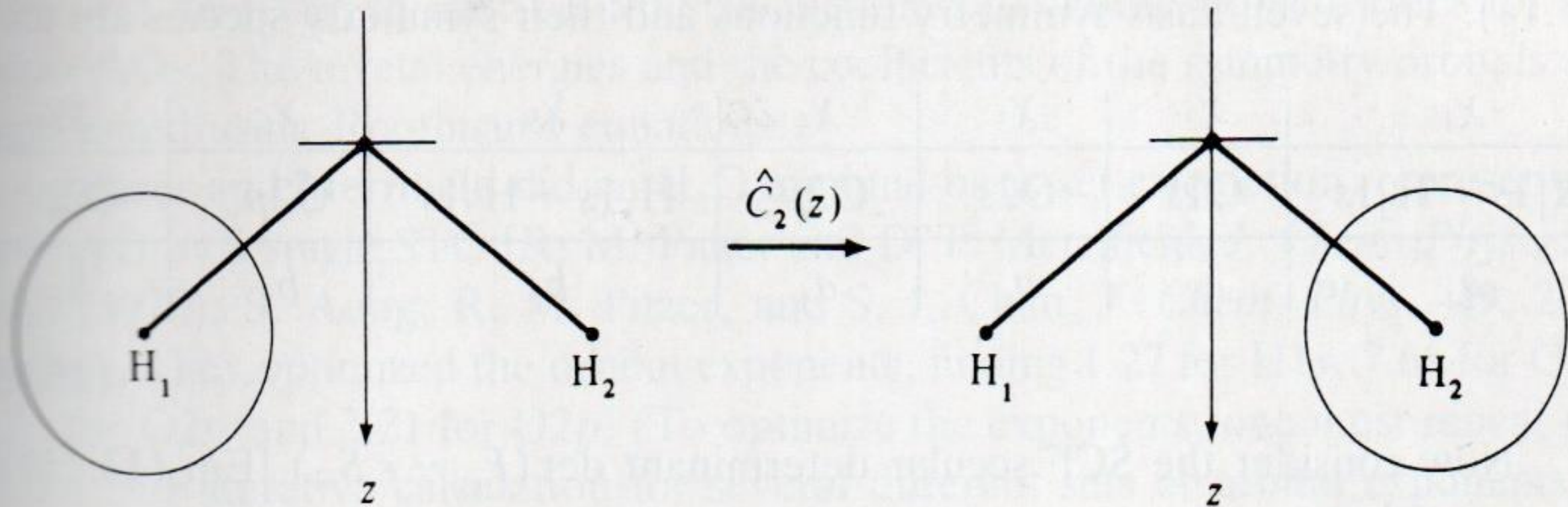


Figure 15.3 The effect of a $\hat{C}_2(z)$ rotation on the H₁1s AO in H₂O.

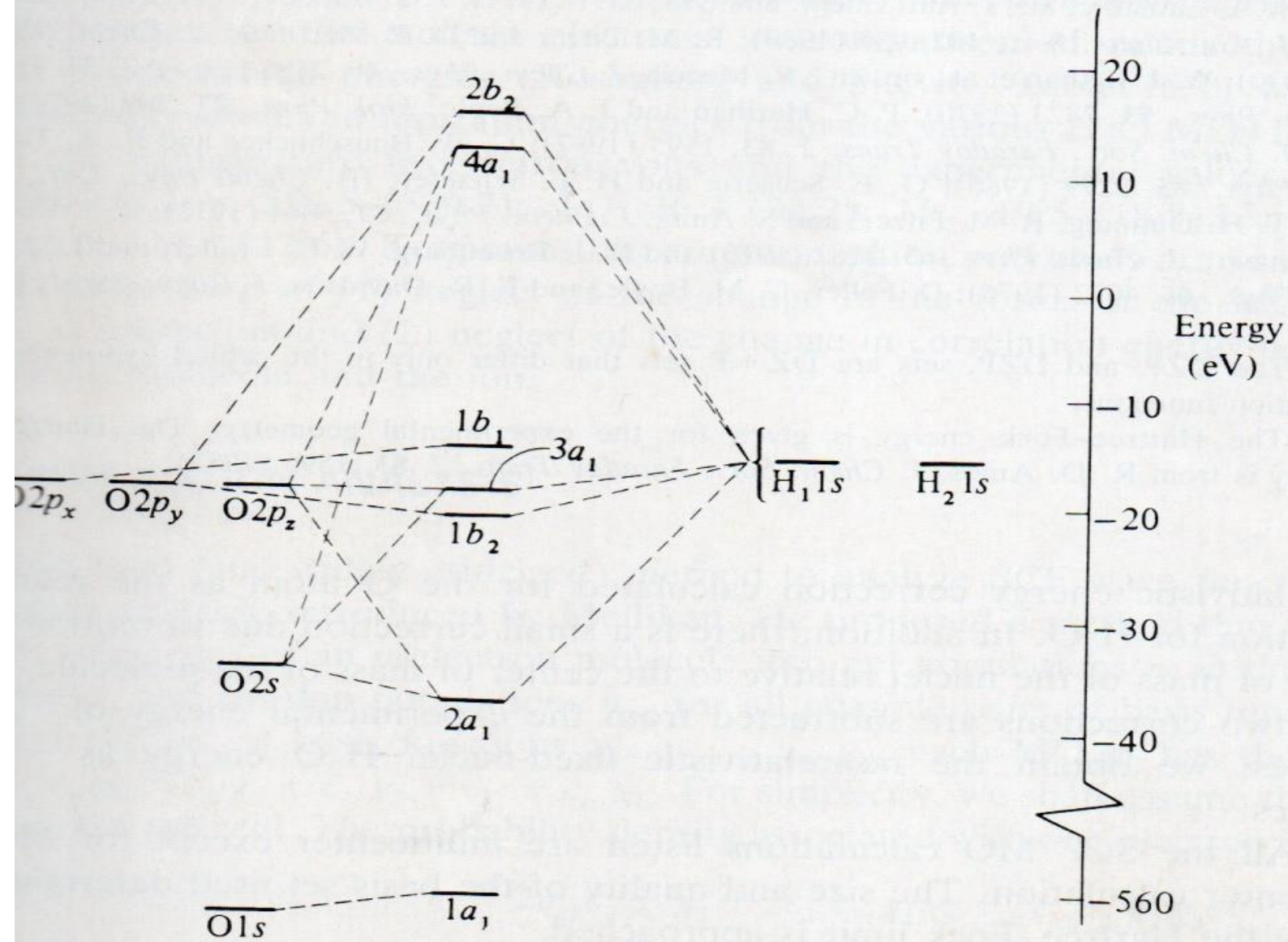


Figure 15.5 Formation of the H_2O MOs from the minimal-basis AOs. The five lowest MOs are filled in the ground state. (Note the break in the scale.)

completely are

$$1a_1 = 1.000(O1s) + 0.015(O2s_{\perp}) + 0.003(O2p_z) - 0.004(H_11s + H_21s)$$

$$2a_1 = -0.027(O1s) + 0.820(O2s_{\perp}) + 0.132(O2p_z) + 0.152(H_11s + H_21s)$$

$$1b_2 = 0.624(O2p_y) + 0.424(H_11s - H_21s) \quad (15.20)$$

$$3a_1 = -0.026(O1s) - 0.502(O2s_{\perp}) + 0.787(O2p_z) + 0.264(H_11s + H_21s)$$

$$1b_1 = O2p_x$$

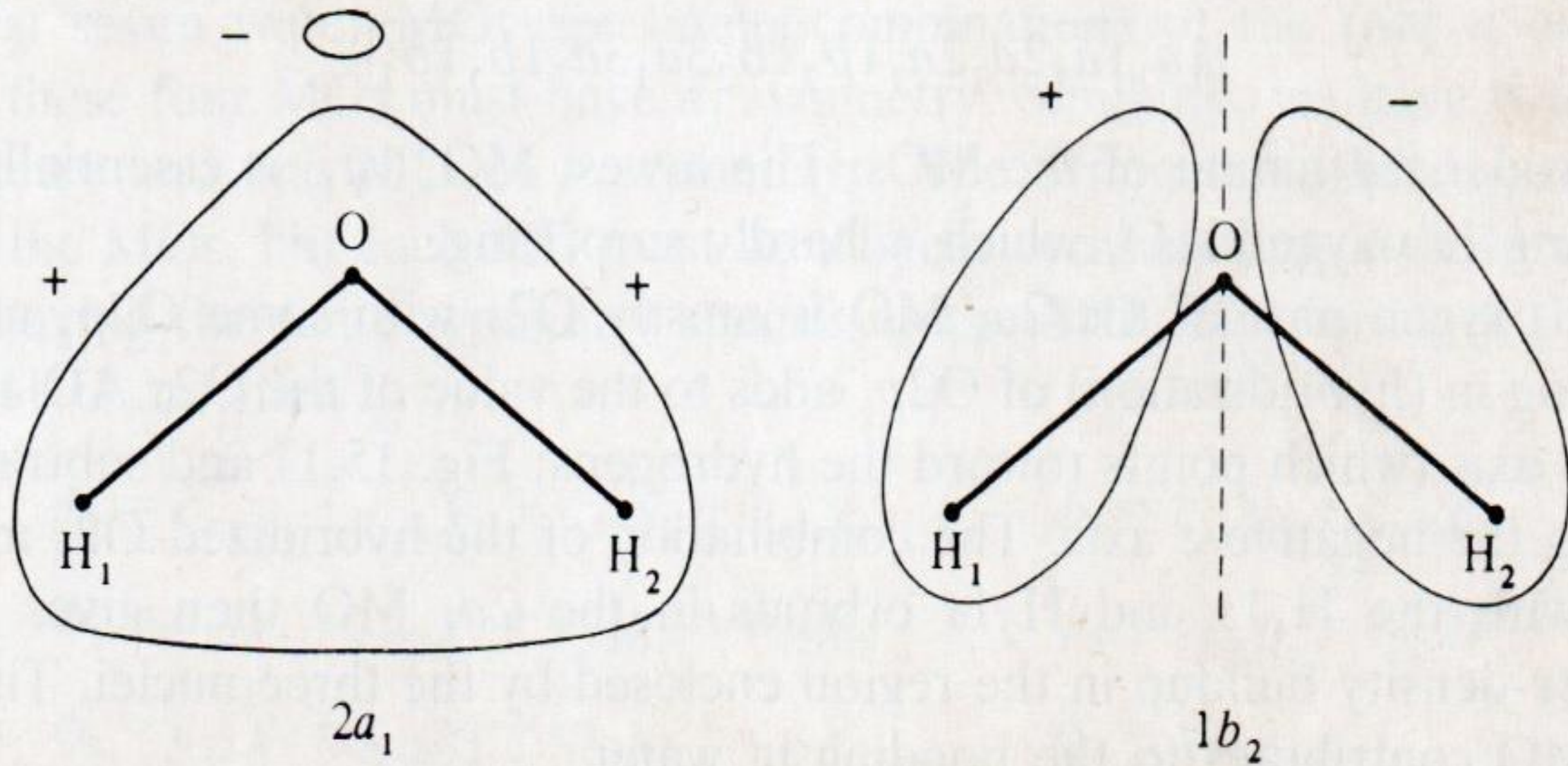


Figure 15.4 Sketches of the two main bonding MOs of H_2O .

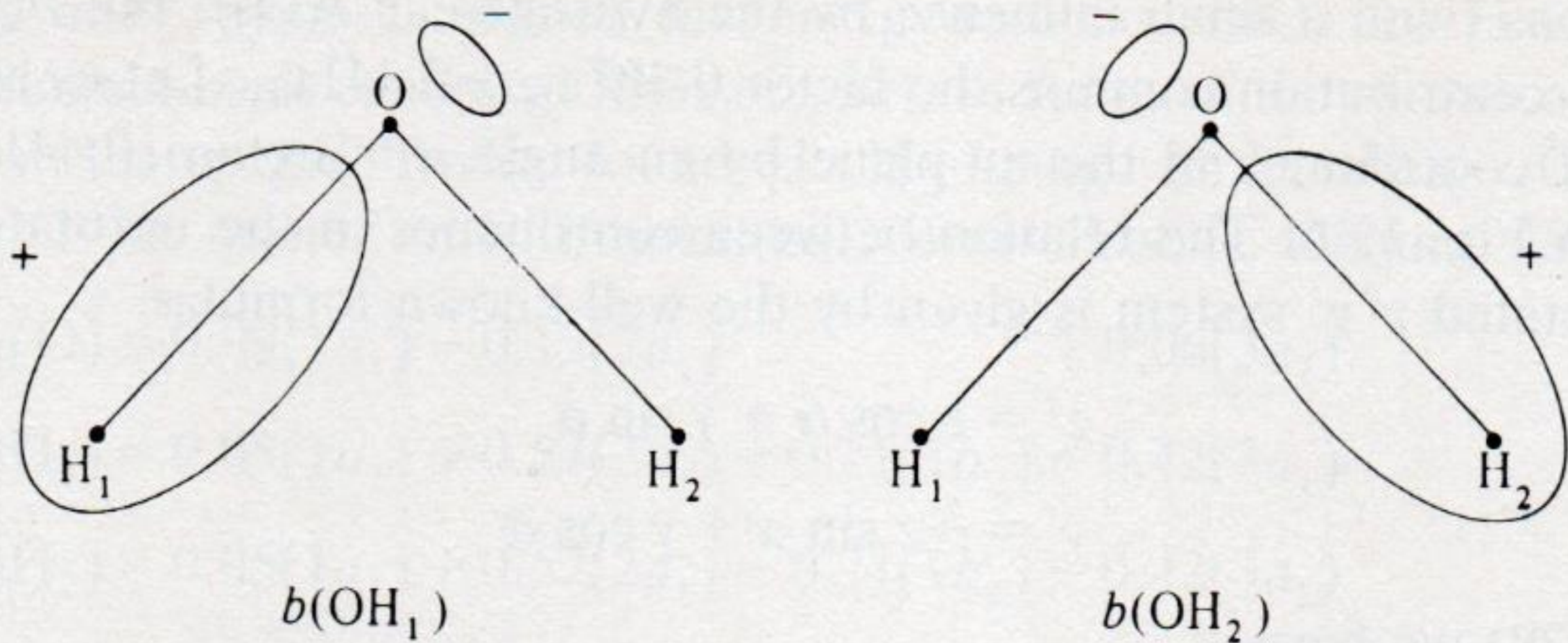


Figure 15.7 Rough sketches of the localized bonding MOs in H_2O .