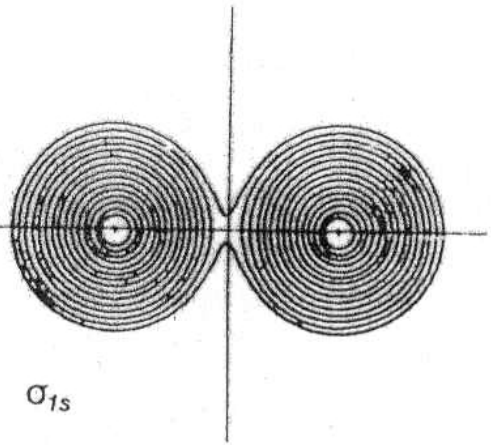
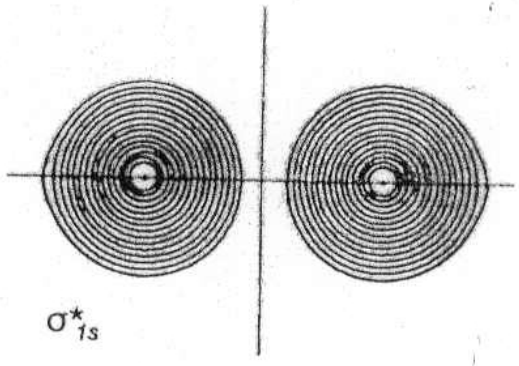
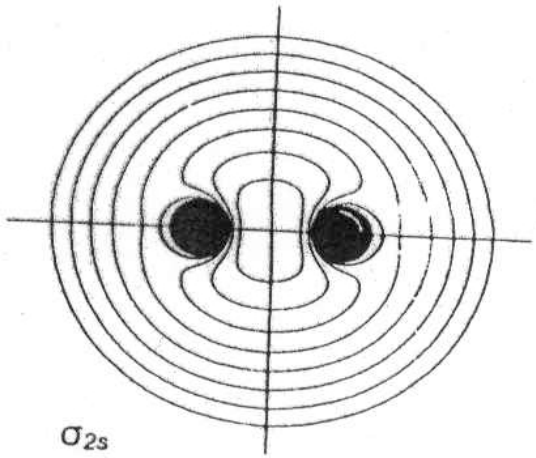
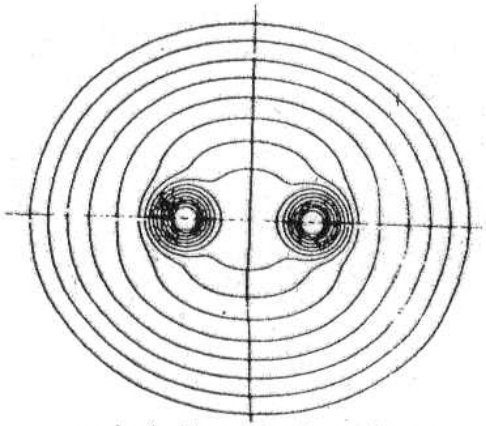
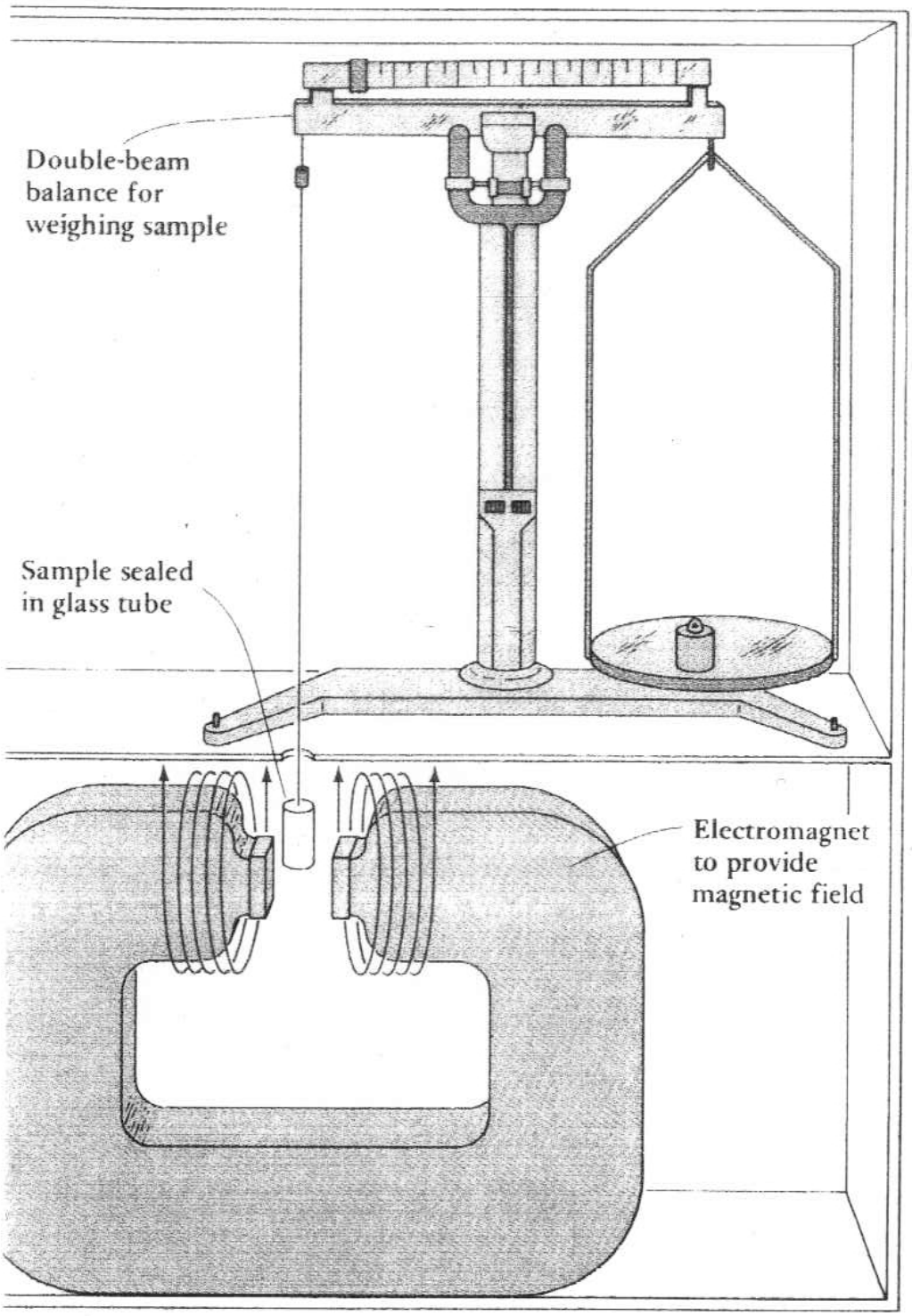




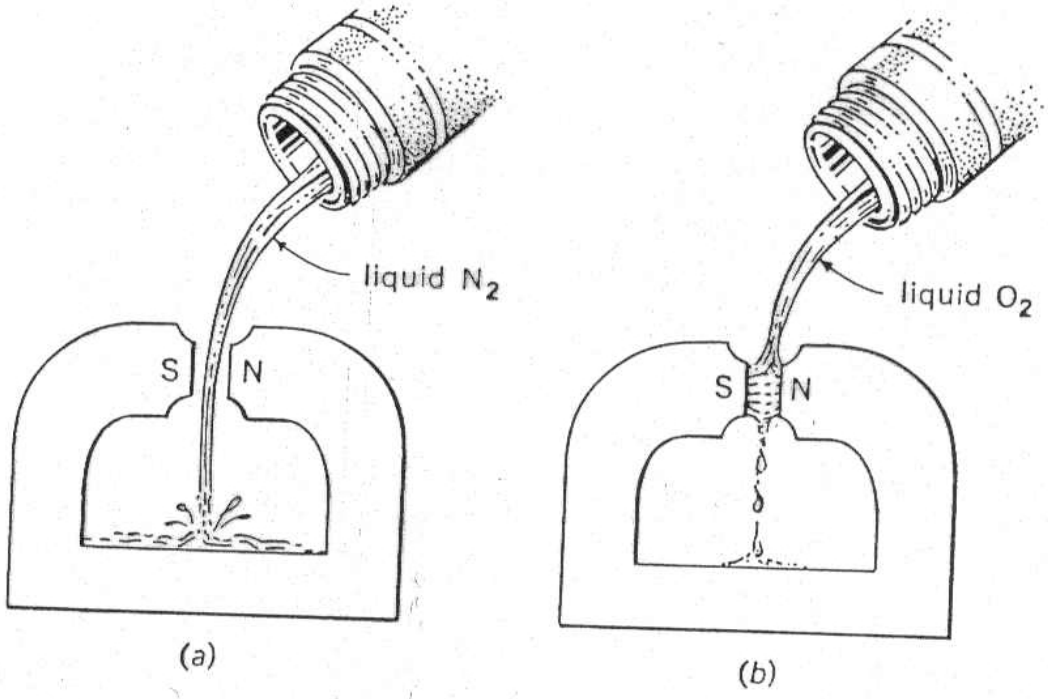




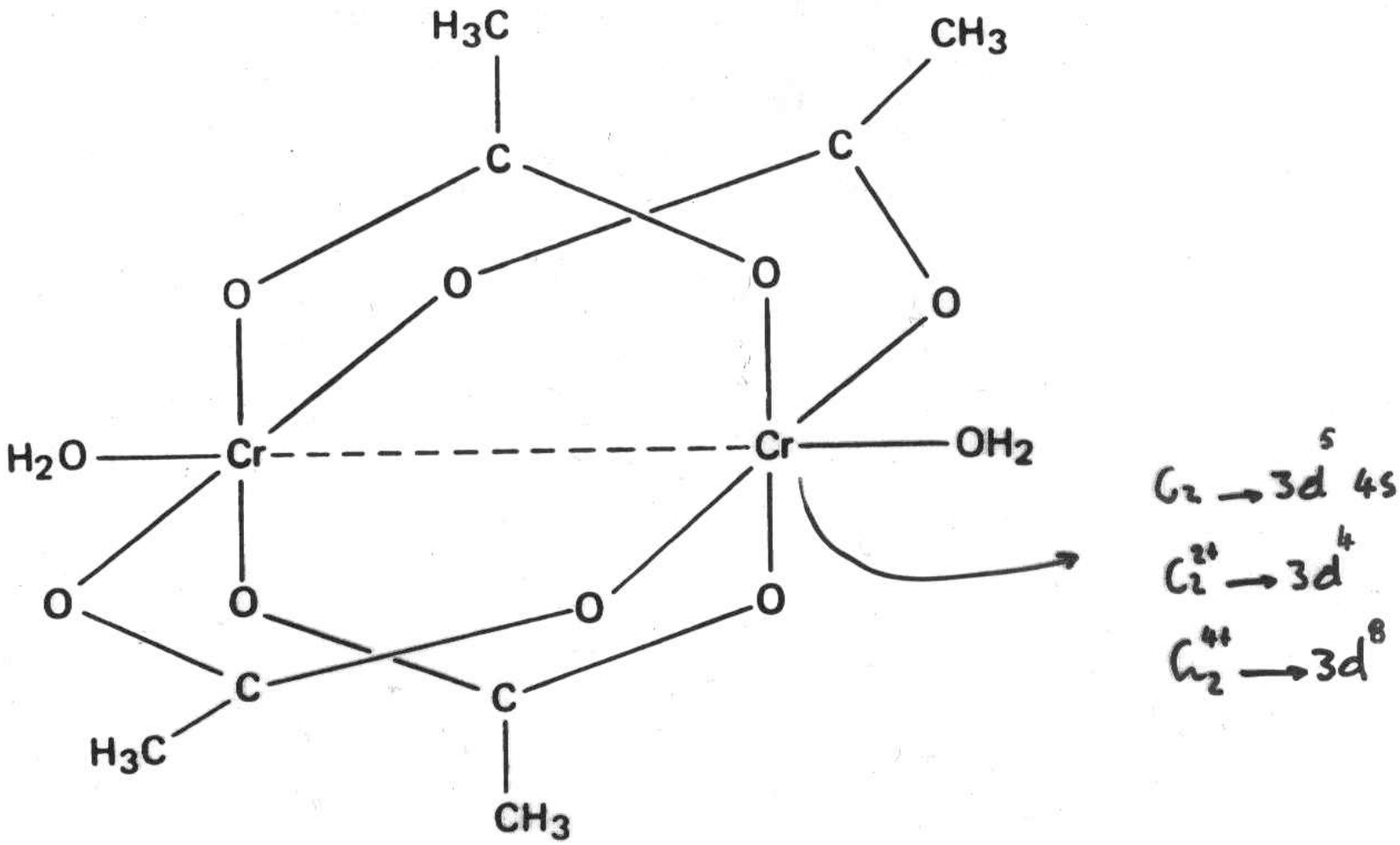
Περιγράμματα ηλεκτρονιακής πυκνότητας για τα συμπληρωμένα τροχιακά: σ_{1s} , σ^*_{1s} και σ_{2s} του μορίου Li_2 και της συνολικής ηλεκτρονιακής πυκνότητας του μορίου.



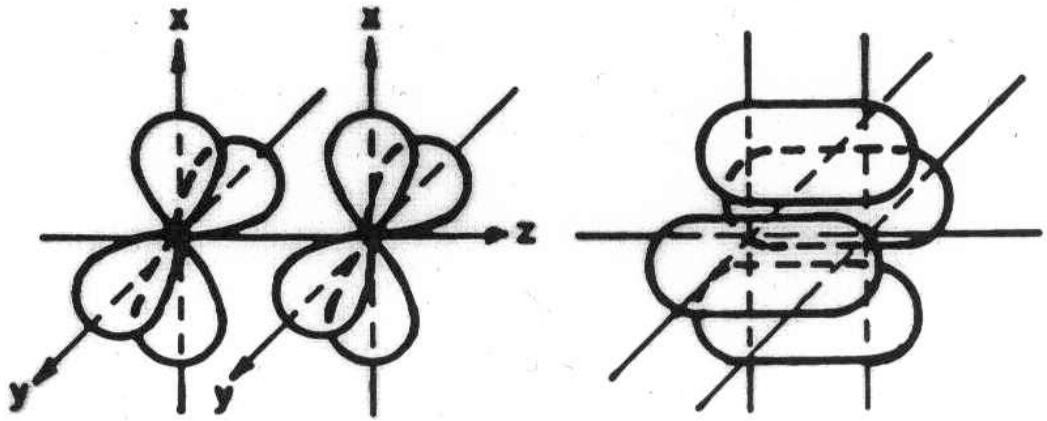
Magnetic balance used to measure the magnetic properties of a sample. The sample is first weighed with the electromagnet turned off. The magnet is then turned on and the sample reweighed. If paramagnetic, the sample is drawn into the magnetic field and the apparent weight increases.



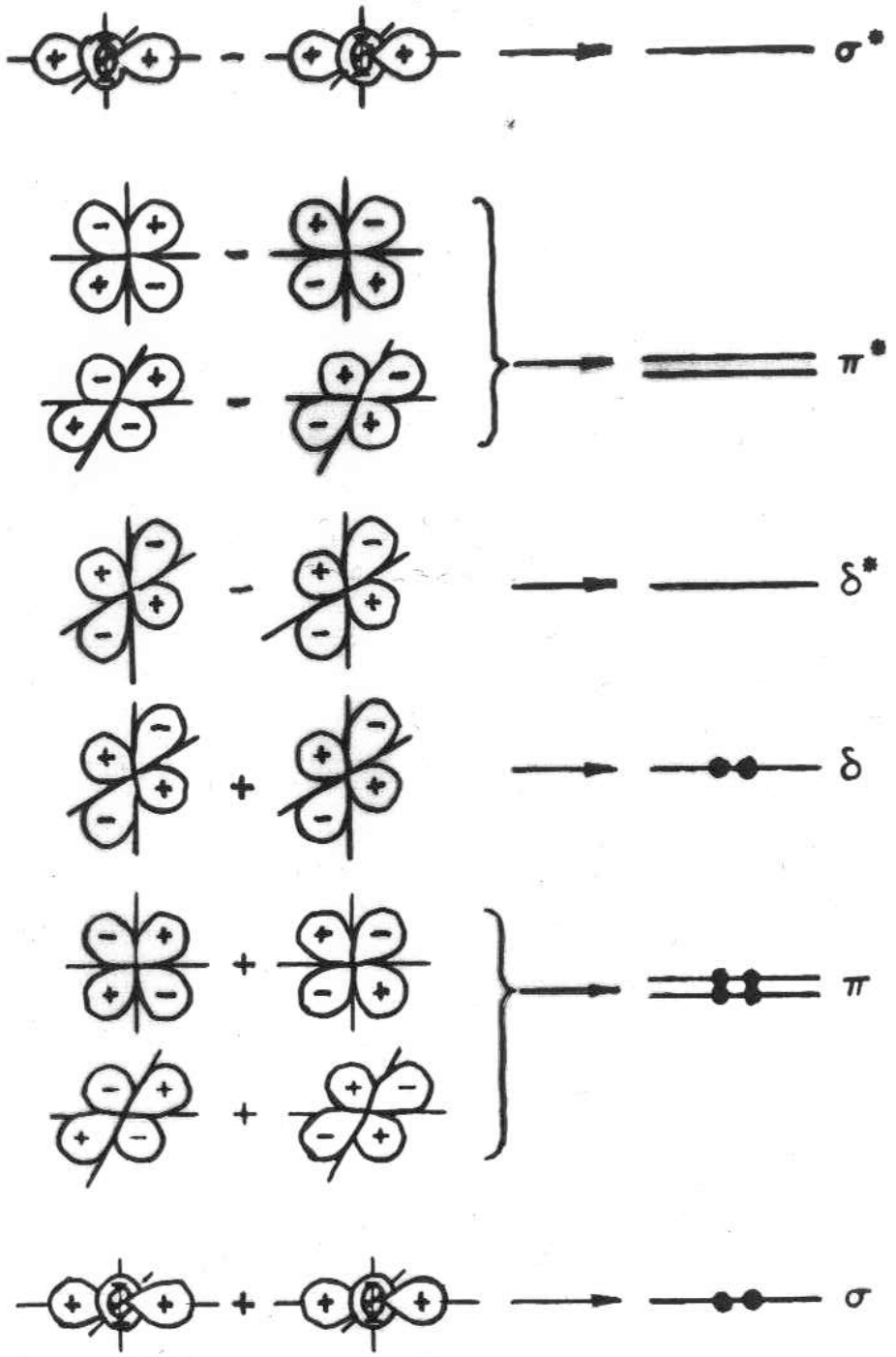
The oxygen molecule is magnetic, the nitrogen molecule is not. (a) Liquid nitrogen (b.p. = 77 degK) can be poured directly between the poles of a strong magnet. (b) Liquid oxygen (b.p. = 90 degK) is attracted by the magnet and fills up the gap between the two poles. Oxygen has two unpaired electrons (in antibonding orbitals) and is magnetic. Nitrogen has all its electrons paired and is not magnetic.



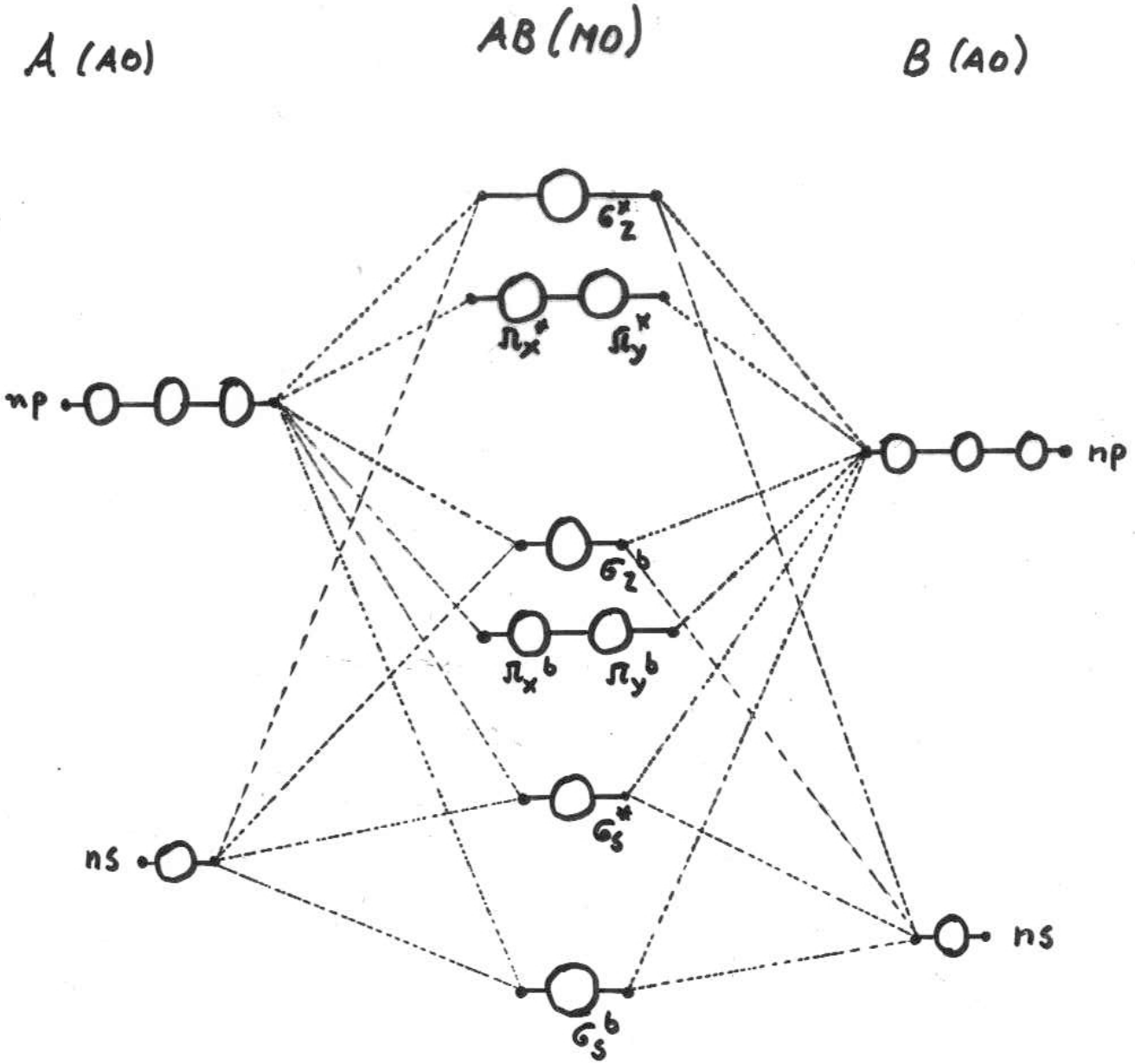
The structure of chromium(II) acetate hydrate.



Σχηματισμός δέλτα μοριακού τροχιακού.

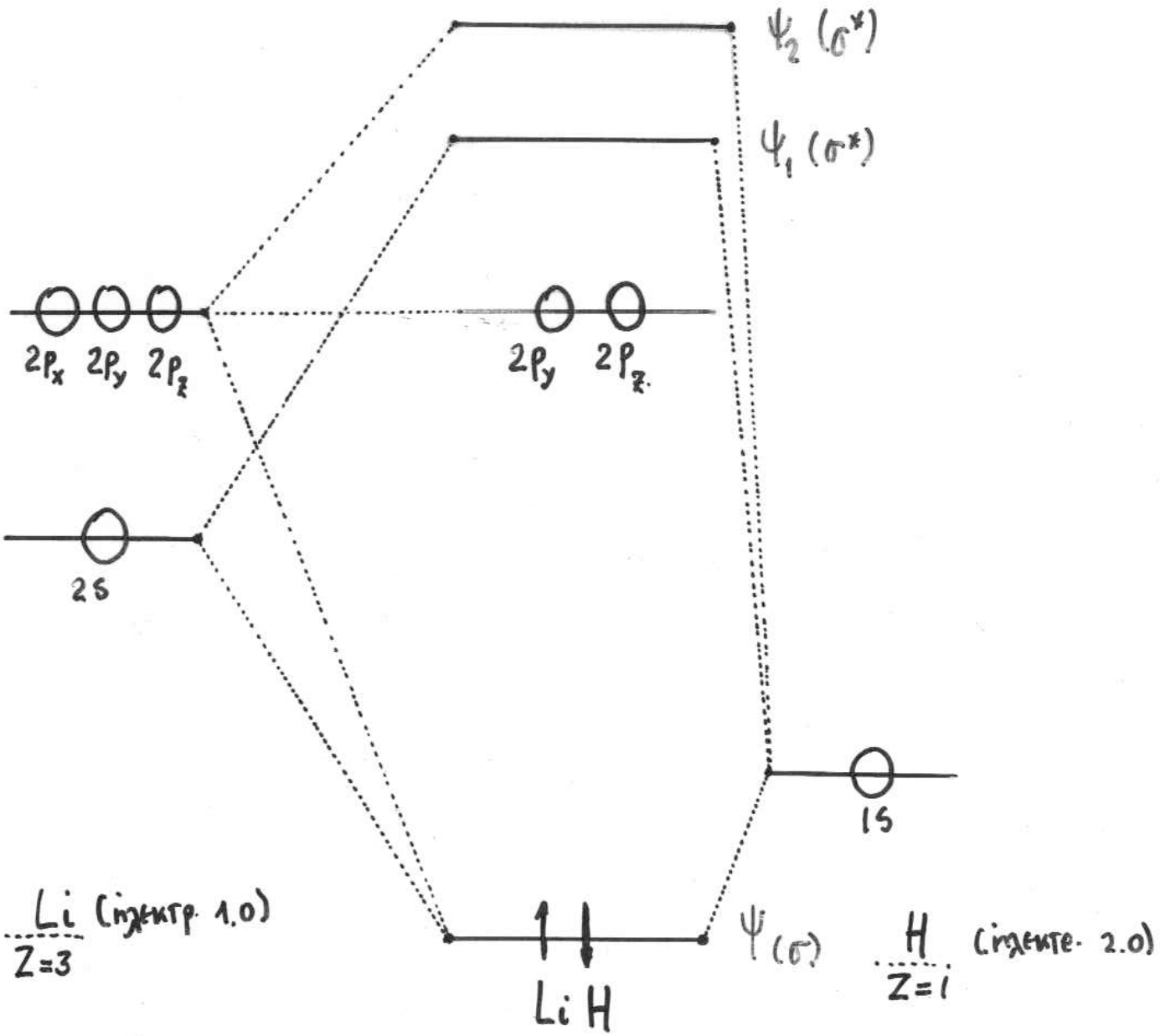


The d-orbital overlap scheme for the formation of a quadruple bond between two MX_4 units each having four electrons available.



Ενεργειακό διάγραμμα ΜΟ για ετεροπυρηνικό διατομικό μόριο ΑΒ όπου το Β είναι πιο ηλεκτραρνητικό του Α ($\chi_B > \chi_A$)

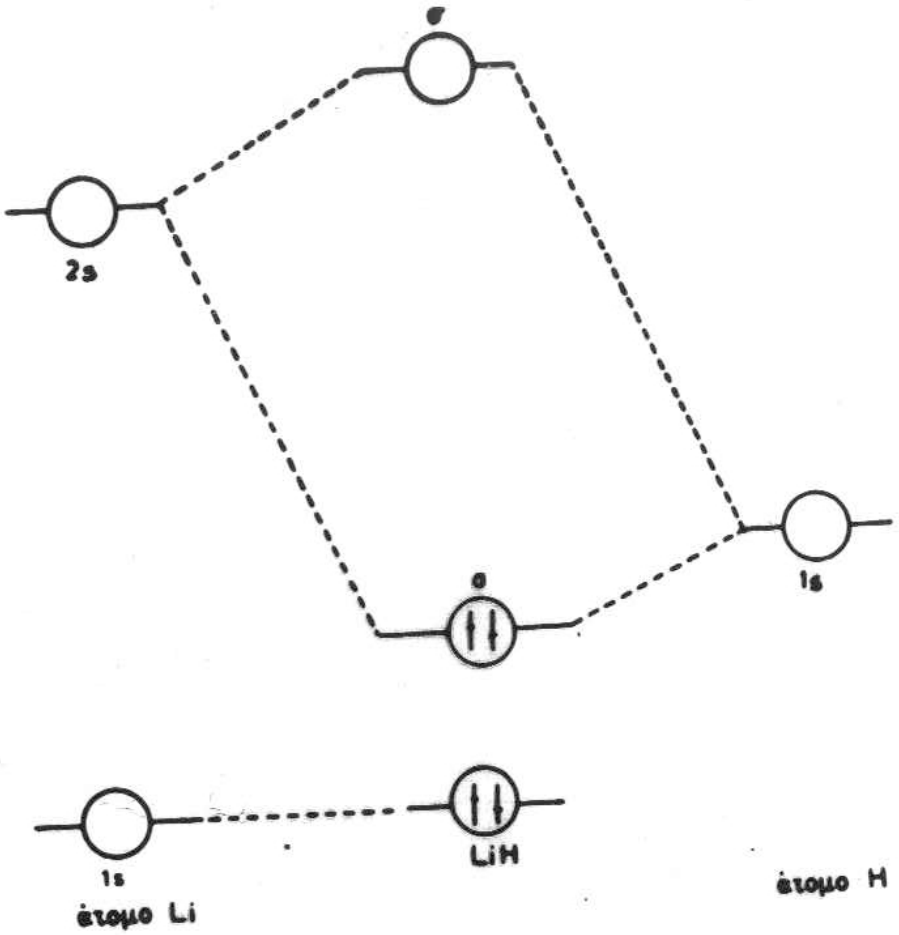
ΕΝΕΡΓΕΙΑΚΕΣ ΣΤΑΘΜΕΣ ΜΟΡΙΑΚΩΝ ΤΡΟΧΙΑΚΩΝ ΓΙΑ ΕΤΕΡΟΠΥΡΗΝΙΚΑ ΜΟΡΙΑ



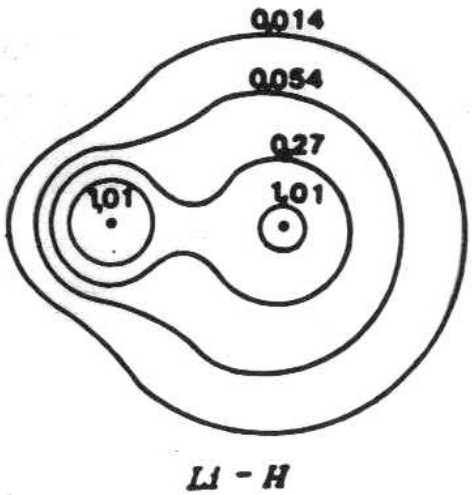
$\psi_{(\sigma)} = C_1(2s) + C_2(2p_x) + C_3(1s)$ $\quad C_3 > C_1 > C_2$

$\psi_1(\sigma^*) = C_4(2s) - C_5(1s)$ $\quad C_4 > C_5$

$\psi_2(\sigma^*) = C_6(2p_x) - C_7(1s)$ $\quad C_6 > C_7$



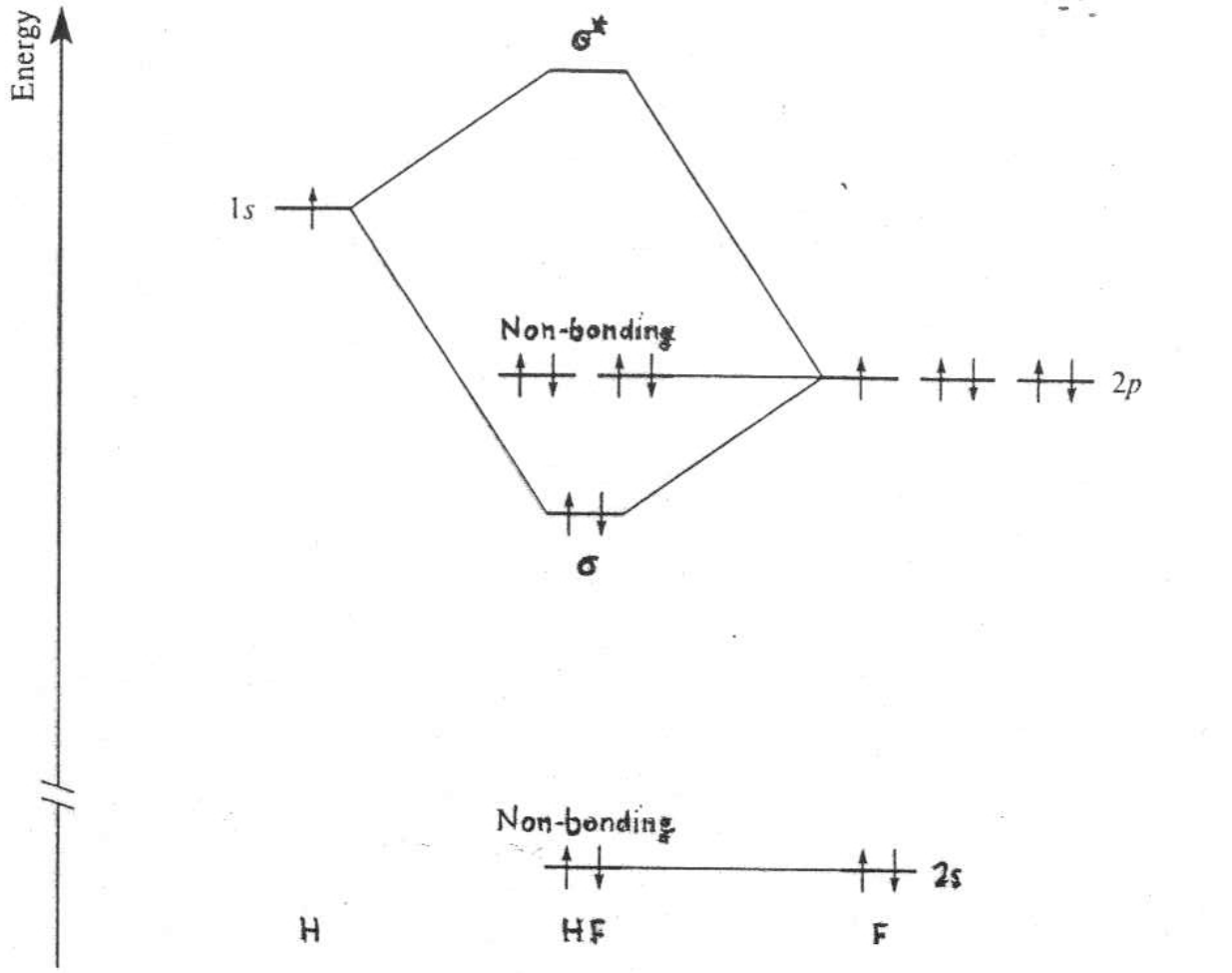
Ενεργειακό διάγραμμα LiH.

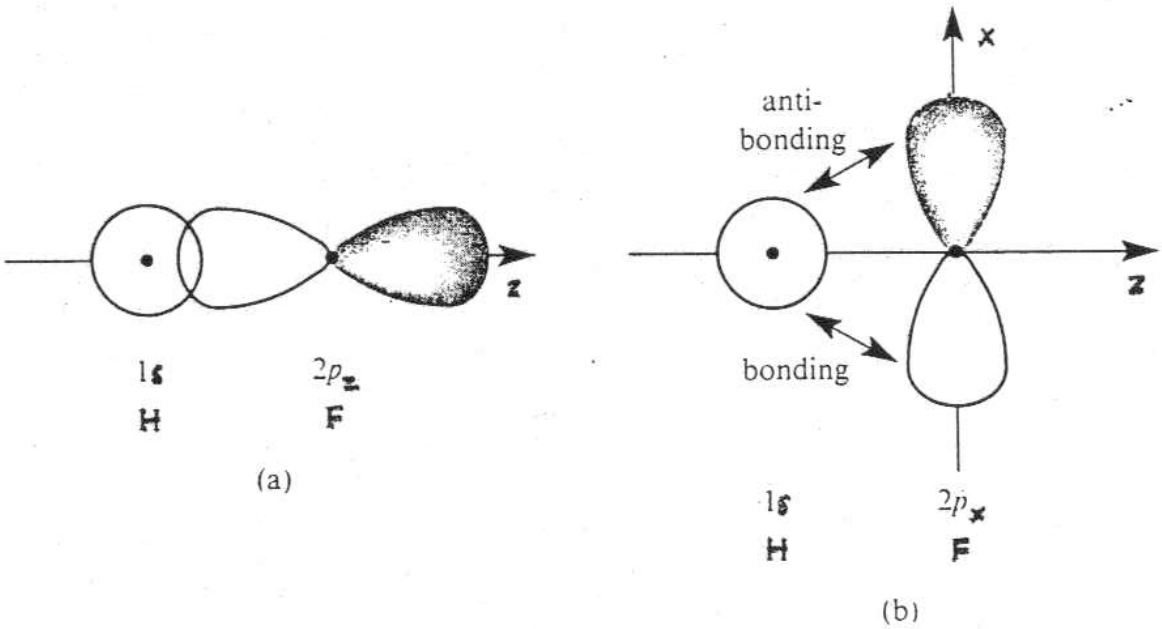


Ισόπυκνες του συνολικού ηλεκτρονικού νέφους του LiH. Η πυκνότητα του νέφους δίδεται σε ηλεκτρόνια ανά κυβικό Ångstrom.

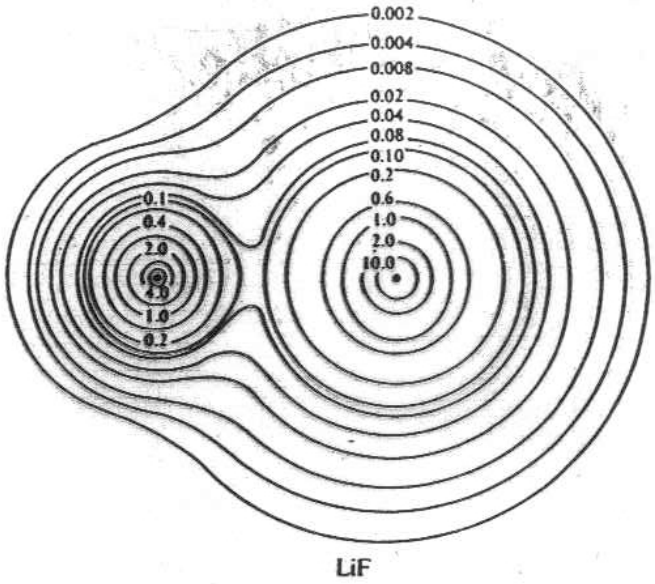
$Li^{\delta+}$ $H^{\delta-}$ ή (+ −)

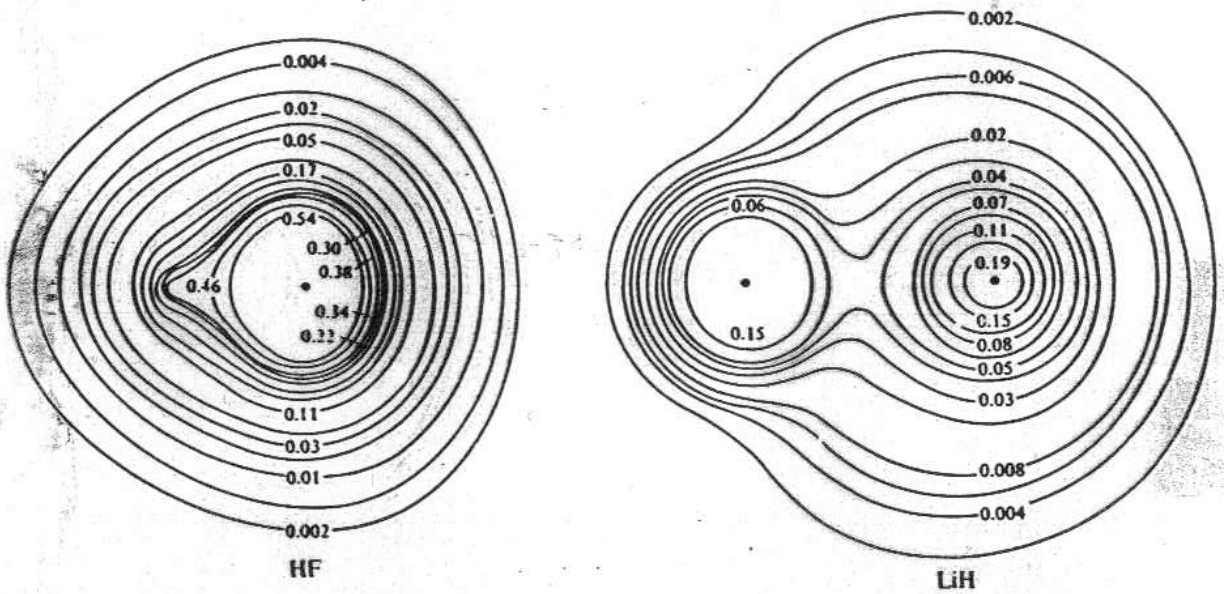
Energy
2s
σ*
σ
1s
Li
LiH
H


Energy
σ*
1s
Non-bonding
2p
σ
Non-bonding
2s
H
HF
F

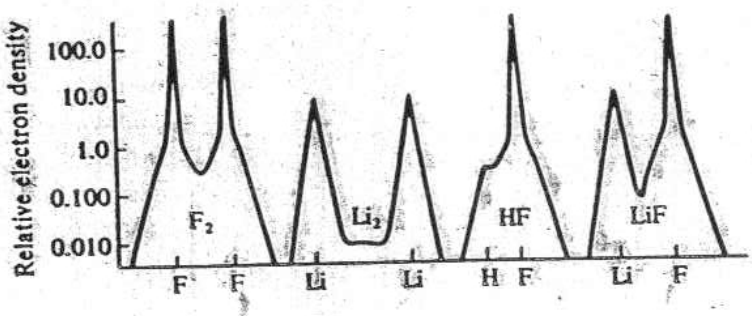

z
1s
H
2p
F
(a)
x
anti-
bonding
z
bonding
1s
H
2p
F
(b)

Energy
2s
σ*
Non-bonding
σ
2p
Li
LiF
F
Non-bonding
2s



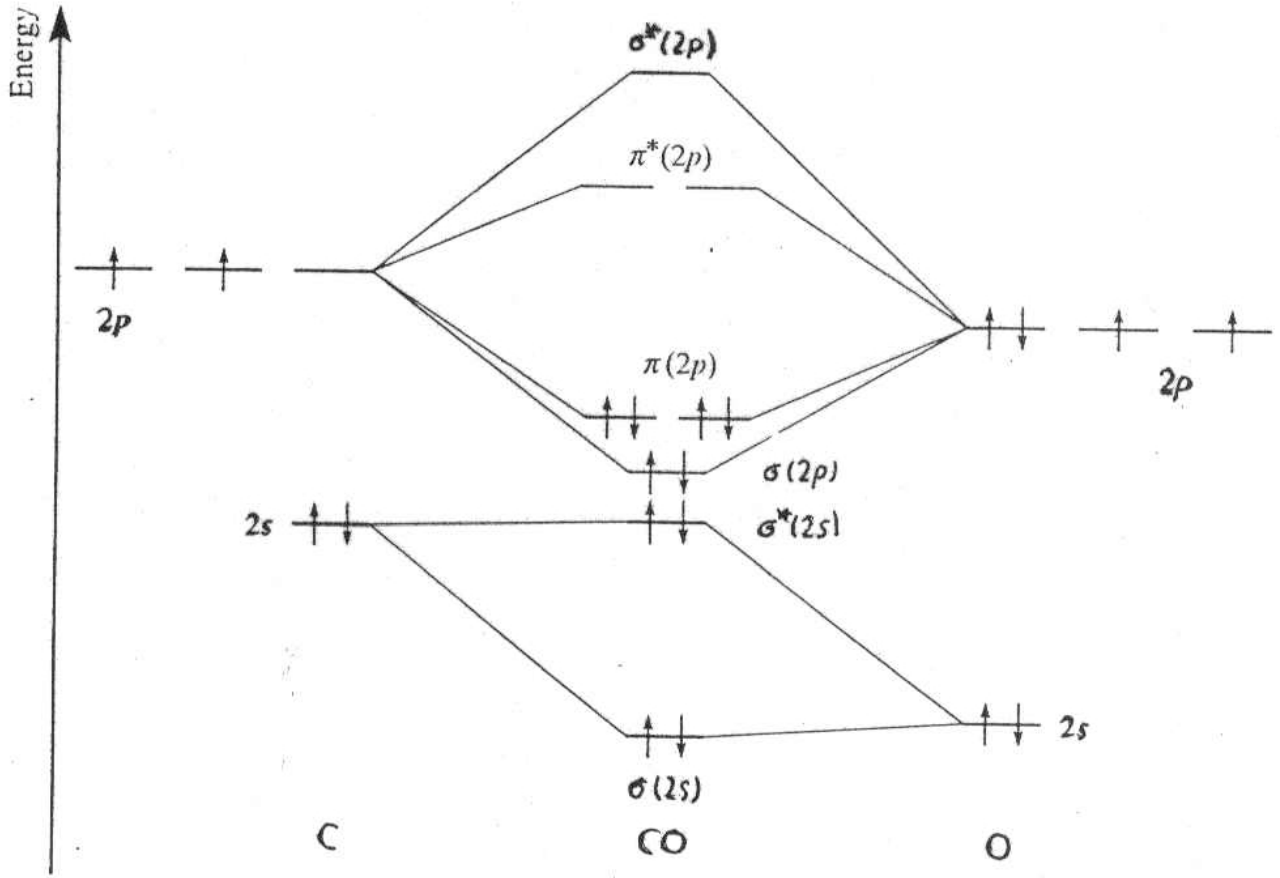


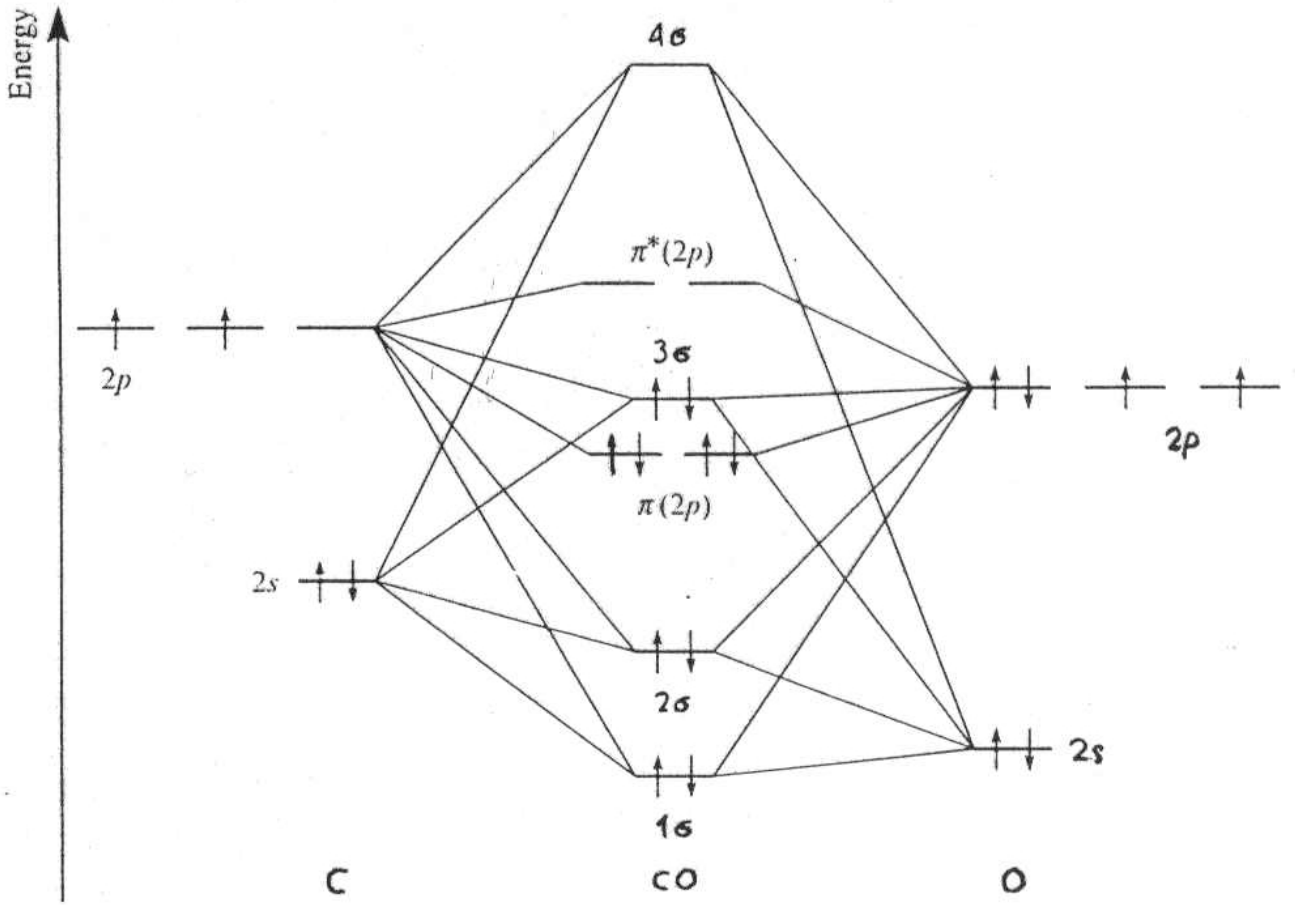
Electron density contours for LiF, HF, and LiH molecules. All molecules drawn to the same scale. The inner contours of F in HF and Li in LiH have been omitted for clarity. [From Bader R. F. W.; Keaveny, I.; Cade, P. E. *J. Chem. Phys.* **1967**, *47*, 3381–3402; Bader, R. F. W.; Bandrauk, A. D. *J. Chem. Phys.* **1968**, *49*, 1653–1655. Reproduced with permission.]



Total electron density profiles of simple molecules along the internuclear axis. [From Ransil, B. J.; Sinai, J. J. *J. Chem. Phys.* **1967**, *46*, 4050. Reproduced with permission.]

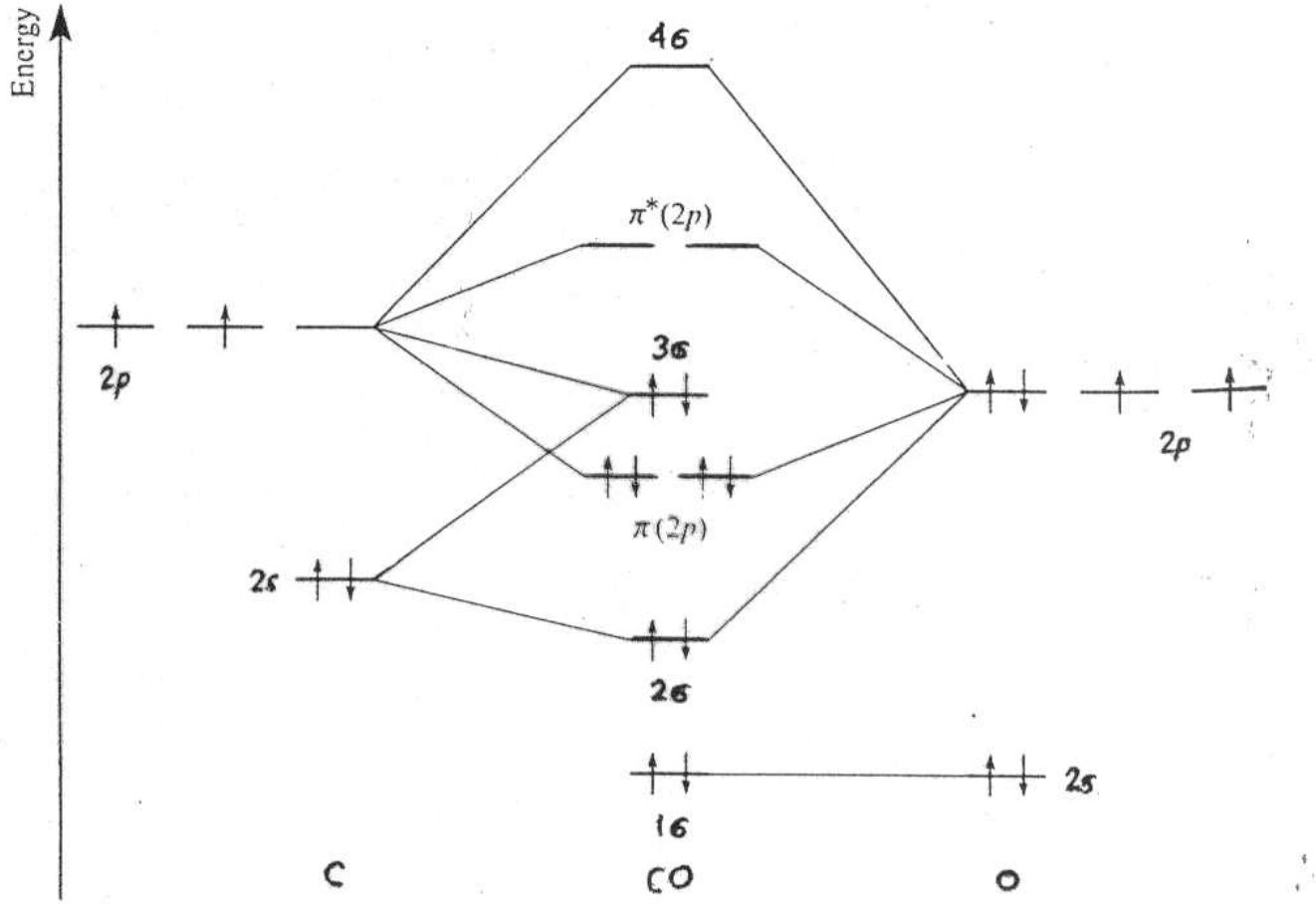
An MO diagram for the formation of CO which allows only overlap between $2s$(C) and $2s$(O) and between $2p$(C) and $2p$(O) atomic orbitals.

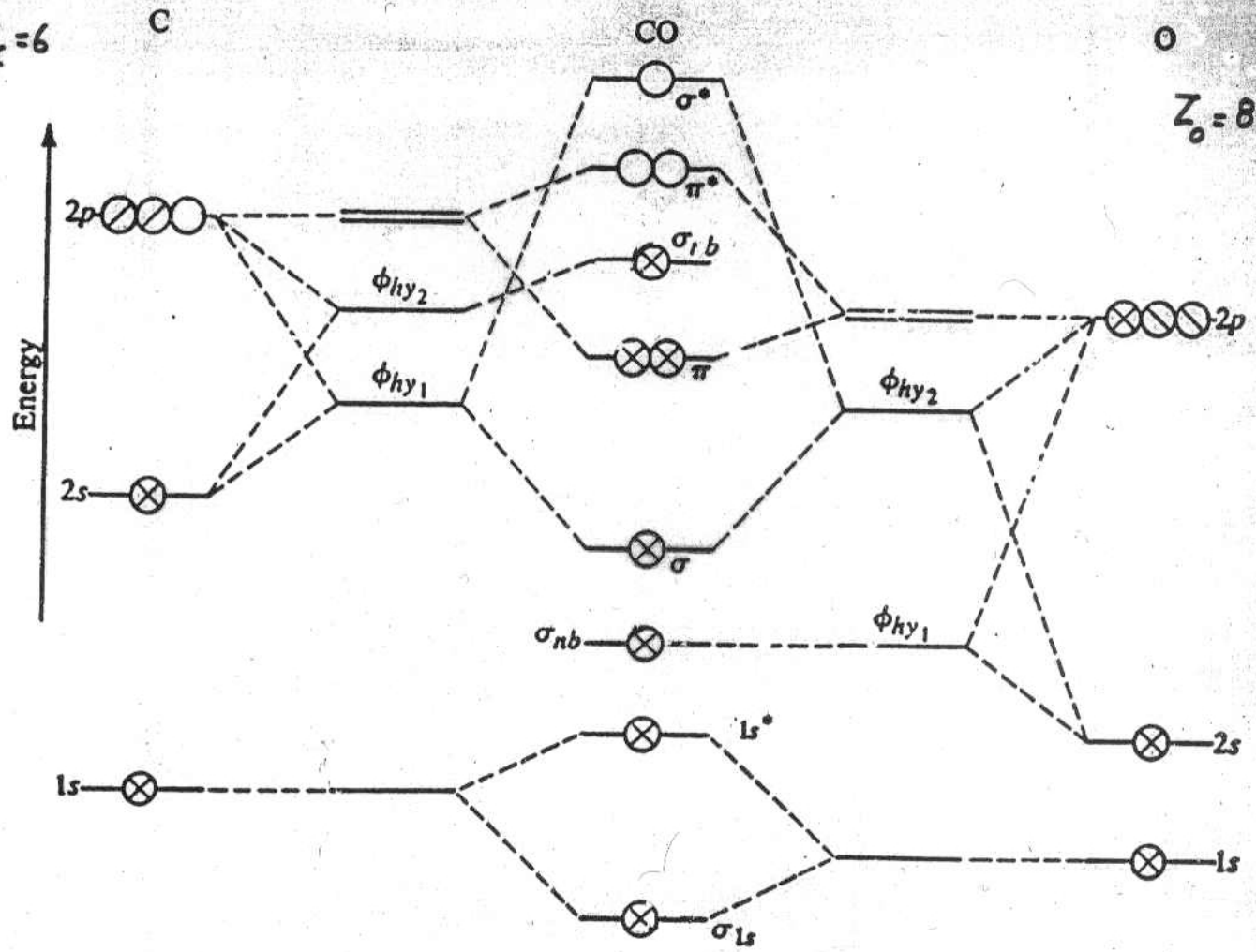




4.14 An MO diagram for the formation of CO which allows for orbital mixing between the $\sigma(2s)$ and $\sigma(2p)$ and between the $\sigma^*(2s)$ and $\sigma^*(2p)$.

4.15 An MO diagram for CO which allows for the effects of orbital mixing but also recognizes the fact that not all the AOs will make major contributions to all the σ- MOs. A major change in going from Figure 4.14 to 4.15 is that the 1σ and 3σ MOs become non-bonding. This is actually an over-simplification.

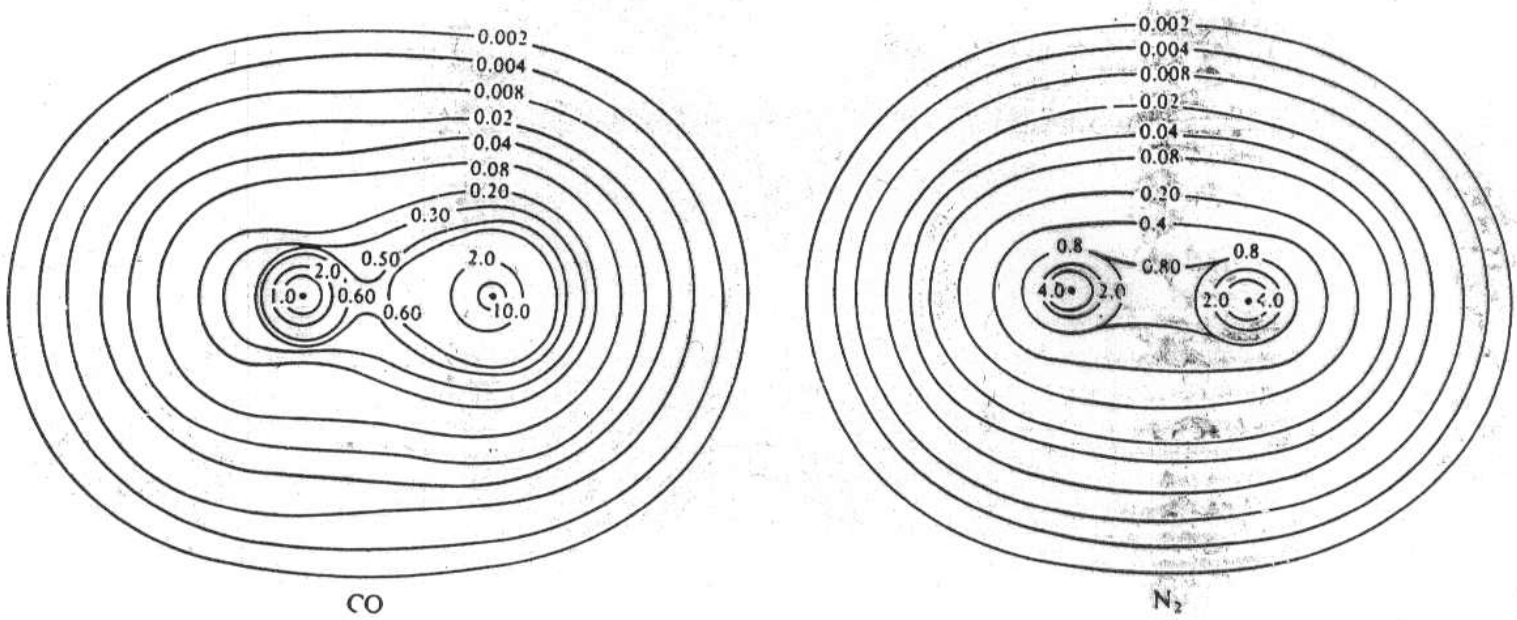




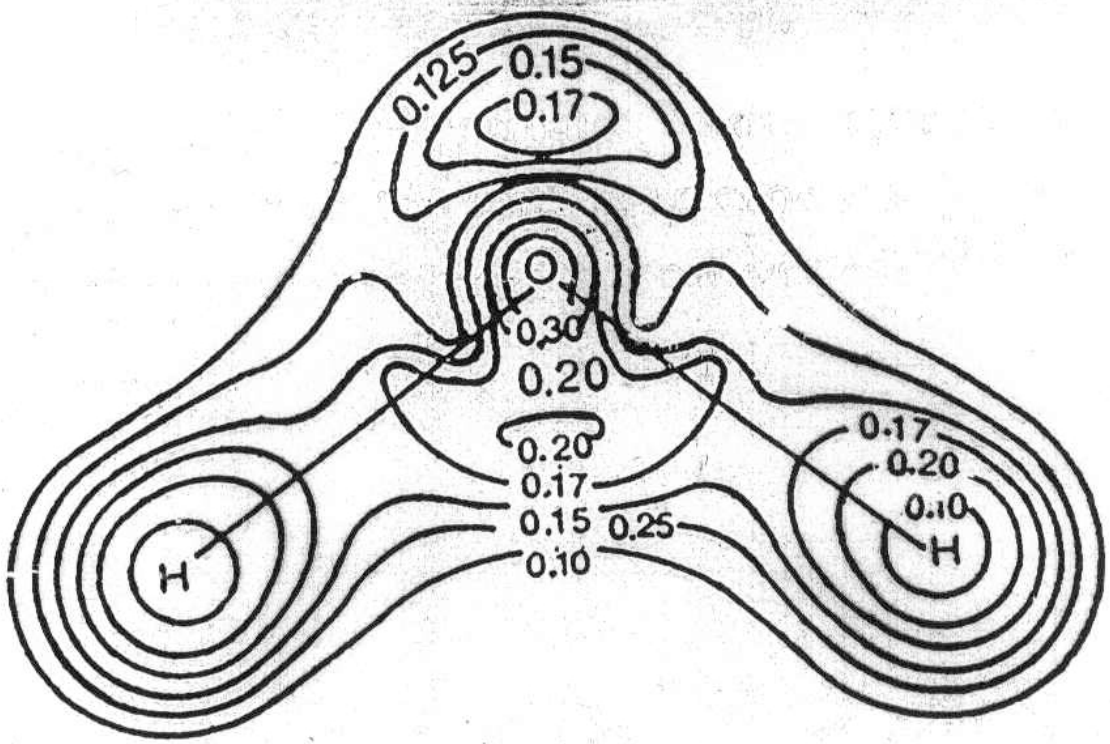
The MO energy-level diagram for CO. (Adapted with permission from M. Orchin and H. H. Jaffé, *Symmetry, Orbitals, and Spectra,* Wiley-Interscience, New York, 1971, p. 47, copyright © 1971.)

$$\text{Τ.Δ} = \frac{8-2}{2} = \frac{6}{2} = 3$$

$:C \overset{(-)}{\equiv} O \overset{(+)}{:}$



(a) Total electron density contours for the carbon monoxide molecule. The carbon atom is on the left. (b) Total electron density contours for the dinitrogen molecule. [From Bader, R. F. W.; Bandrauk, A. D. *J. Chem. Phys.* **1968**, *49*, 1653. Reproduced with permission.]



Σχ. 3.12. Διάγραμμα, που εμφανίζει την κατανομή της ηλεκτρονικής πυκνότητας στο μόριο του νερού (H_2O)