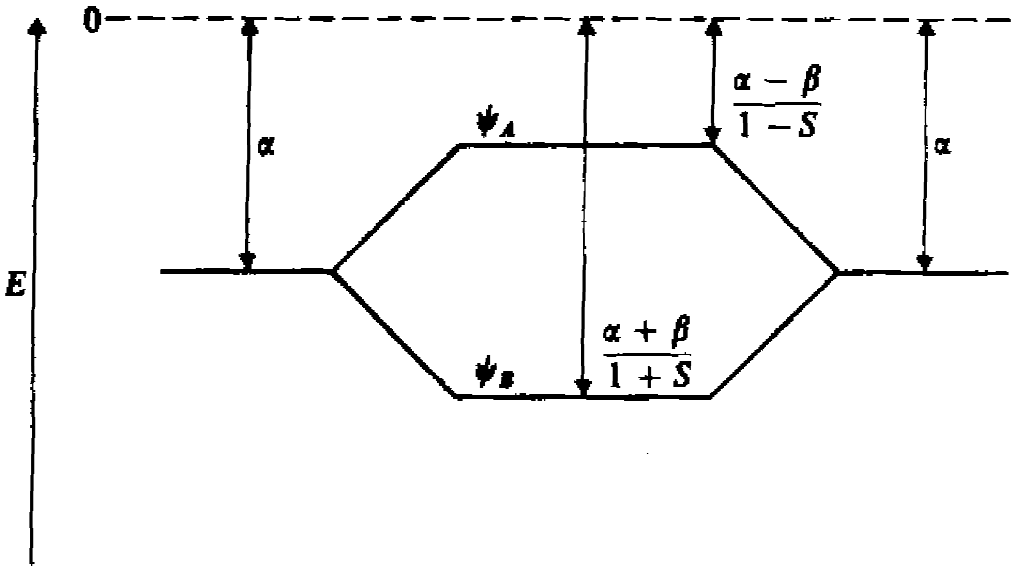
MO Diagram for Dihydrogen - Like Molecules



Species	Electron configuration	Bond order
H_2^+	$(1s\sigma_B)^1$	$\frac{1}{2}$
H_2	$(1s\sigma_B)^2$	1
HHe	$(1s\sigma_B)^2(1s\sigma^*)^1$	$\frac{1}{2}$
He_2	$(1s\sigma_B)^2(1s\sigma^*)^2$	0

Diatomic Species of the First Row Elements

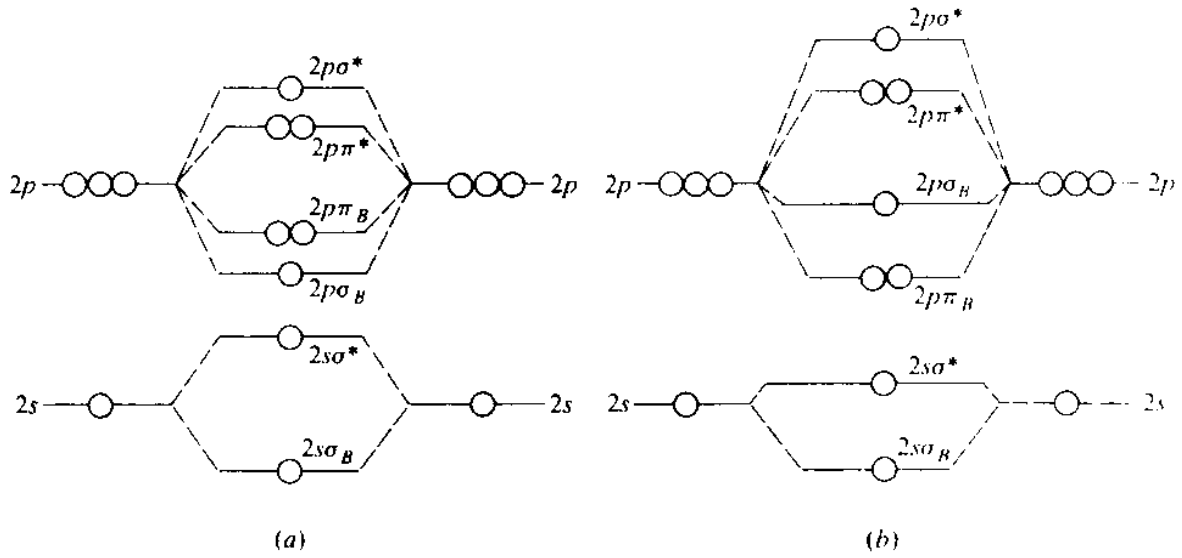


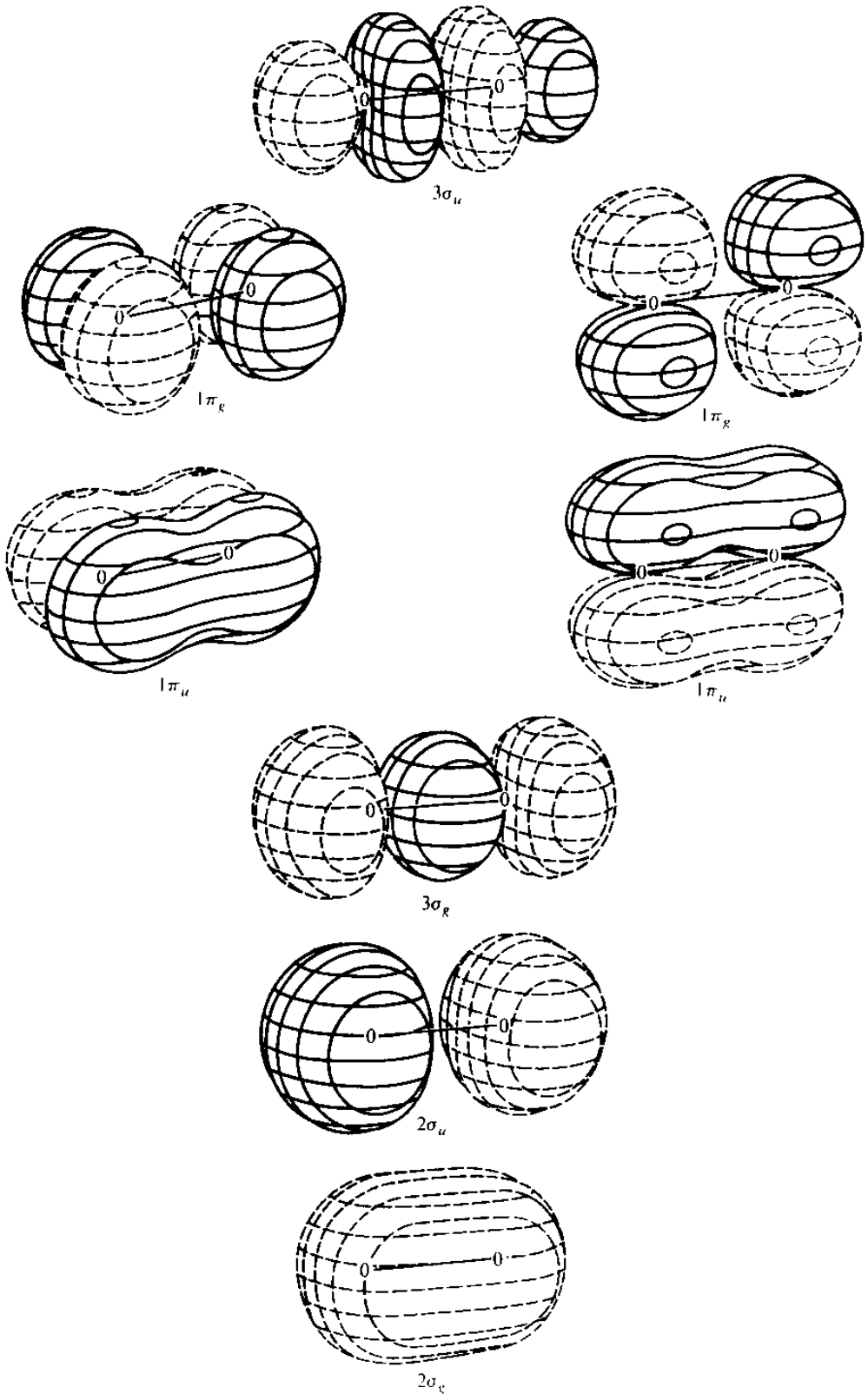
FIGURE 4.7
Valence-shell energy level disgrams for a homonuclear diatomic molecule containing first-row atoms. (*a*) corresponds to no interaction between 2*s* and 2*p* levels; (*b*) corresponds to substantial 2*s*-2*p* interaction.

Diatomic species of first-row elements

Species	Valence electron configuration	Unpaired electrons	Bond order	D, kcal mol^{-1}†	r, Å
Li_2	$(s\sigma_B)^2$	0	1	26	2.67
Be_2	$(s\sigma_B)^2(s\sigma^*)^2$	0	0		
B_2	$(s\sigma_B)^2(s\sigma^*)^2(p\pi_B)^2$	2	1	71	1.59
C_2	$(s\sigma_B)^2(s\sigma^*)^2(p\pi_B)^4$	0	2	142	1.31
N_2	$(s\sigma_B)^2(s\sigma^*)^2(p\pi_B)^4(p\sigma_B)^2$	0	3	226	1.10
O_2	$(s\sigma_B)^2(s\sigma^*)^2(p\sigma_B)^2(p\pi_B)^4(p\pi^*)^2$	2	2	119	1.21
O_2^-	$(s\sigma_B)^2(s\sigma^*)^2(p\sigma_B)^2(p\pi_B)^4(p\pi^*)^3$	1	1.5	....	1.33
F_2	$(s\sigma_B)^2(s\sigma^*)^2(p\sigma_B)^2(p\pi_B)^4(p\pi^*)^4$	0	1	38	1.42
Ne_2	$(s\sigma_B)^2(s\sigma^*)^2(p\sigma_B)^2(p\pi_B)^4(p\pi^*)^4(p\sigma^*)^2$	0	0		

† 1 kcal = 4.1840 kJ

Contour Surfaces of O_2 Molecular Orbitals



X-Ray Difference Electron Density Map for Tricyanocyclopropane

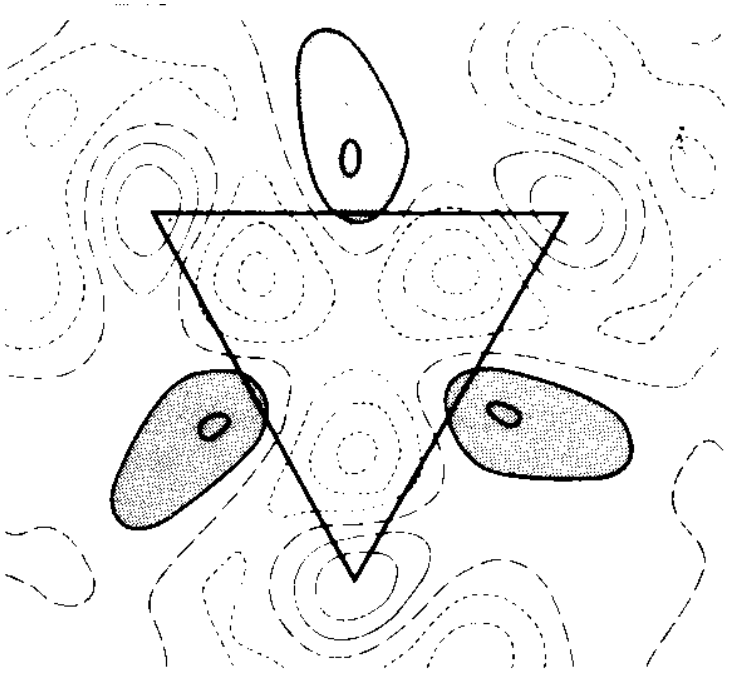


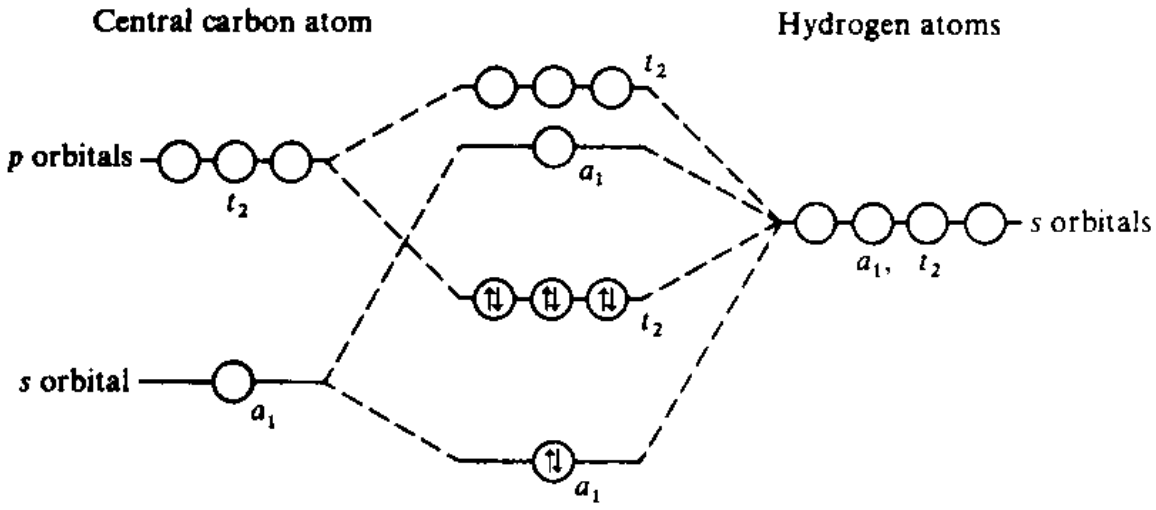
FIG. 8.4. Difference density map for tricyanocyclopropane in the C_3 plane. The important overlap regions have been emphasized by shading.

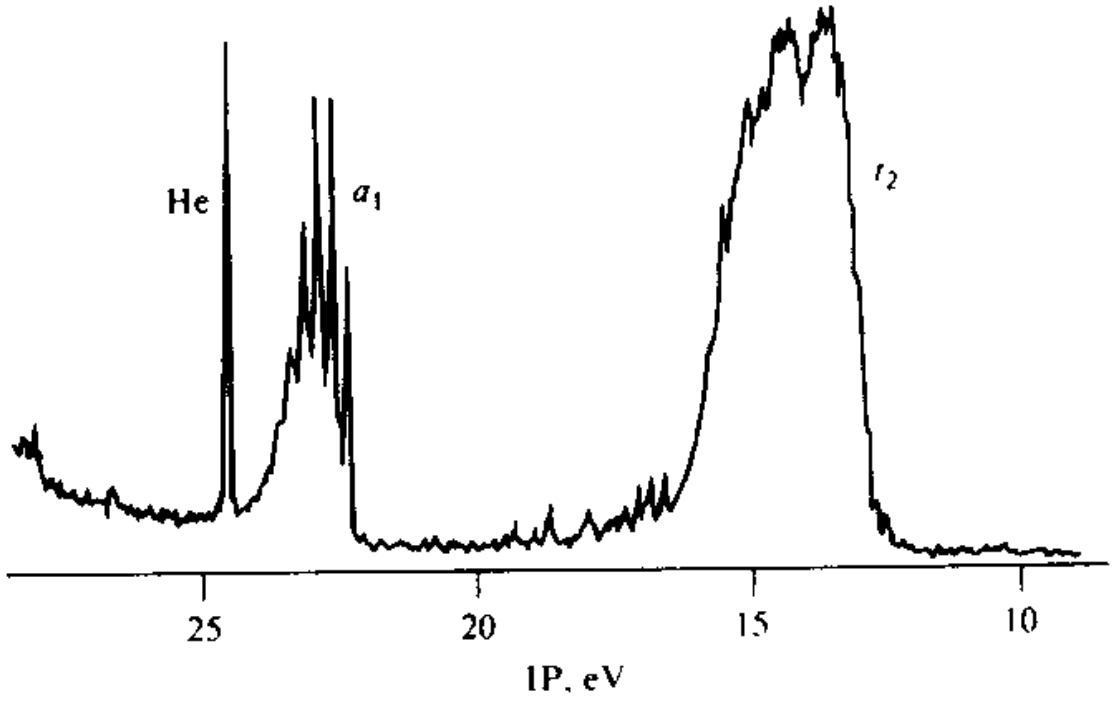
Character Tables - Point Groups C_{2v} and T_d

C_{2v}	E	C_2	$\sigma_v(xz)$	$\sigma_v'(yz)$	
A_1	1	1	1	1	z, x^2, y^2, z^2
A_2	1	1	−1	−1	xy
B_1	1	−1	1	−1	x, xz
B_2	1	−1	−1	1	y, yz

T_d	E	$8C_3$	$3C_2$	$6S_4$	$6\sigma_d$	
A_1	1	1	1	1	1	$x^2 + y^2 + z^2$
A_2	1	1	1	−1	−1	
E	2	−1	2	0	0	$(2z^2 - x^2 - y^2, x^2 - y^2)$
T_1	3	0	−1	1	−1	
T_2	3	0	−1	−1	1	$(x, y, z), (xy, xz, yz)$

Molecular Orbitals of Methane (CH_4) and Photon Electron Spectrum

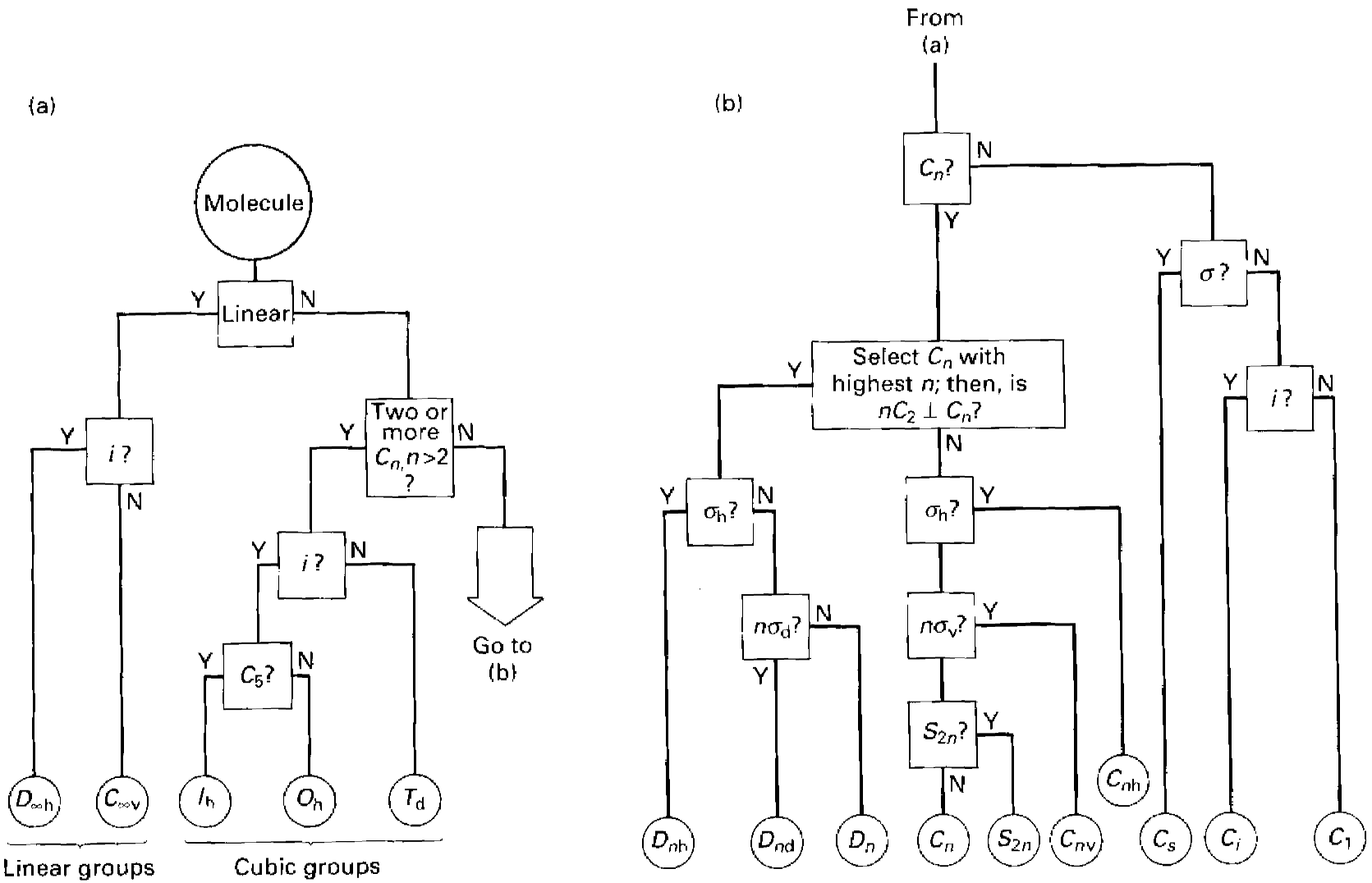




LINEAR POINT GROUPS

$C_{\infty v}$	E	$2C_\infty^\phi$	$\cdots$	$\infty\sigma_v$		
$A_1 \equiv \Sigma^+$	1	1	$\cdots$	1	z	$x^2 + y^2, z^2$
$A_2 \equiv \Sigma^-$	1	1	$\cdots$	-1	R_z	
$E_1 \equiv \Pi$	2	$2\cos\Phi$	$\cdots$	0	$(x, y), (R_x, R_y)$	(xz, yz)
$E_2 \equiv \Delta$	2	$2\cos 2\Phi$	$\cdots$	0		$(x^2 - y^2, xy)$
$E_3 \equiv \Phi$	2	$2\cos 3\Phi$	$\cdots$	0		
$\cdots$	$\cdots$	$\cdots$	$\cdots$	$\cdots$		

$D_{\infty h}$	E	$2C_\infty^\phi$	$\cdots$	$\infty\sigma_v$	i	$2S_\infty^\phi$	$\cdots$	∞C_2		
Σ_g^+	1	1	$\cdots$	1	1	1	$\cdots$	1		$x^2 + y^2, z^2$
Σ_g^-	1	1	$\cdots$	-1	1	1	$\cdots$	-1	R_z	
Π_g	2	$2\cos\Phi$	$\cdots$	0	2	$-2\cos\Phi$	$\cdots$	0	(R_x, R_y)	(xz, yz)
Δ_g	2	$2\cos 2\Phi$	$\cdots$	0	2	$2\cos 2\Phi$	$\cdots$	0		$(x^2 - y^2, xy)$
$\cdots$	$\cdots$	$\cdots$	$\cdots$	$\cdots$	$\cdots$	$\cdots$	$\cdots$	$\cdots$		
Σ_u^+	1	1	$\cdots$	1	-1	-1	$\cdots$	-1	z	
Σ_u^-	1	1	$\cdots$	-1	-1	-1	$\cdots$	1		
Π_u	2	$2\cos\Phi$	$\cdots$	0	-2	$2\cos\Phi$	$\cdots$	0	(x, y)	
Δ_u	2	$2\cos 2\Phi$	$\cdots$	0	-2	$-2\cos 2\Phi$	$\cdots$	0		
$\cdots$	$\cdots$	$\cdots$	$\cdots$	$\cdots$	$\cdots$	$\cdots$	$\cdots$	$\cdots$		


(a)
Molecule
Linear
Y
N
i ?
Two or more C_n, $n>2$?
C_5?
Go to (b)
$D_{\infty h}$
$C_{\infty v}$
I_h
O_h
T_d
Linear groups
Cubic groups
(b)
From (a)
C_n?
Select C_n with highest n; then, is $nC_2 \perp C_n$?
σ ?
σ_h?
$n\sigma_d$?
$n\sigma_v$?
S_{2n}?
D_{nh}
D_{nd}
D_n
C_n
S_{2n}
C_{nv}
C_{nh}
C_s
C_i
C_1