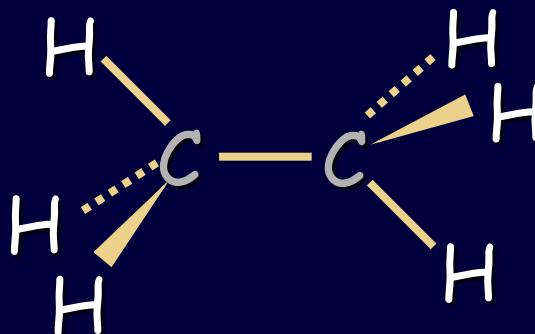
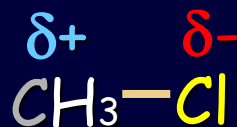


Yapı ve Bağlanma

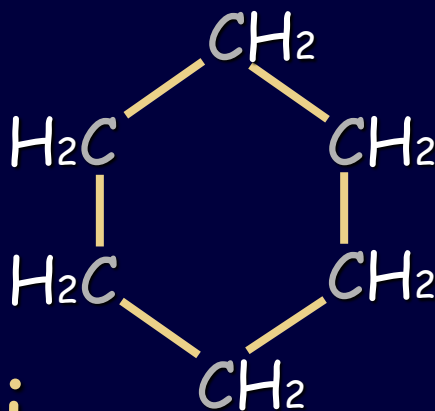
Alkanlar



Haloalkanlar

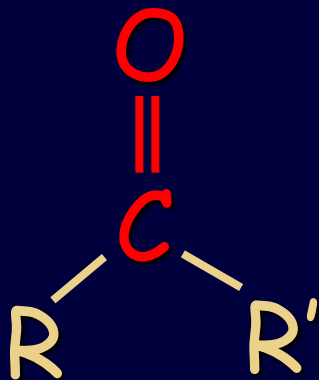
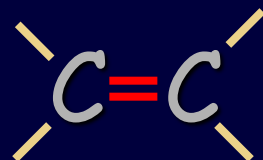
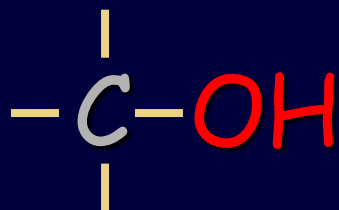


Sikloalkanlar



Stereoizomeri

Fonksiyonlu (işlevsel) Gruplar



Bağlanma



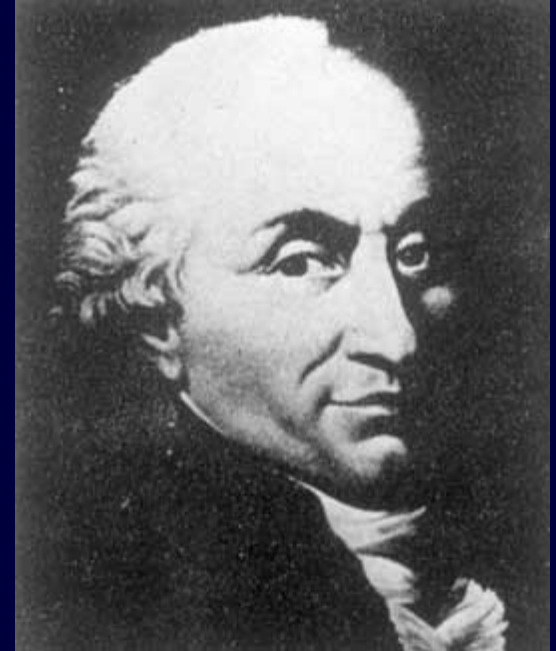
"Kurallar":

1. Zıt yükler birbirini çeker (Coulomb Yasası).

Coulomb Yasası

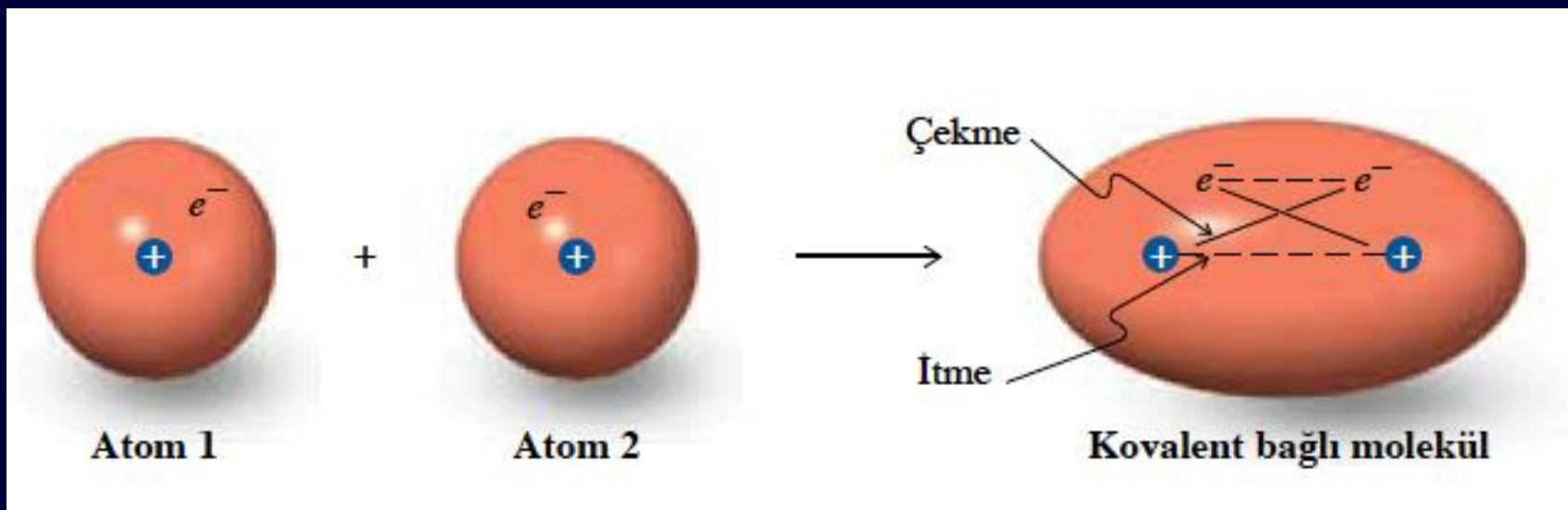
$$\text{Çekim kuvveti} = \text{sabit} \times \frac{(+)\text{ yük} \times (-)\text{ yük}}{\text{uzaklık}^2}$$

2. Elektronlar uzayda dağılır (delokalizasyon).
3. Asal gaz dizilişi tercih edilir.



1736-1806

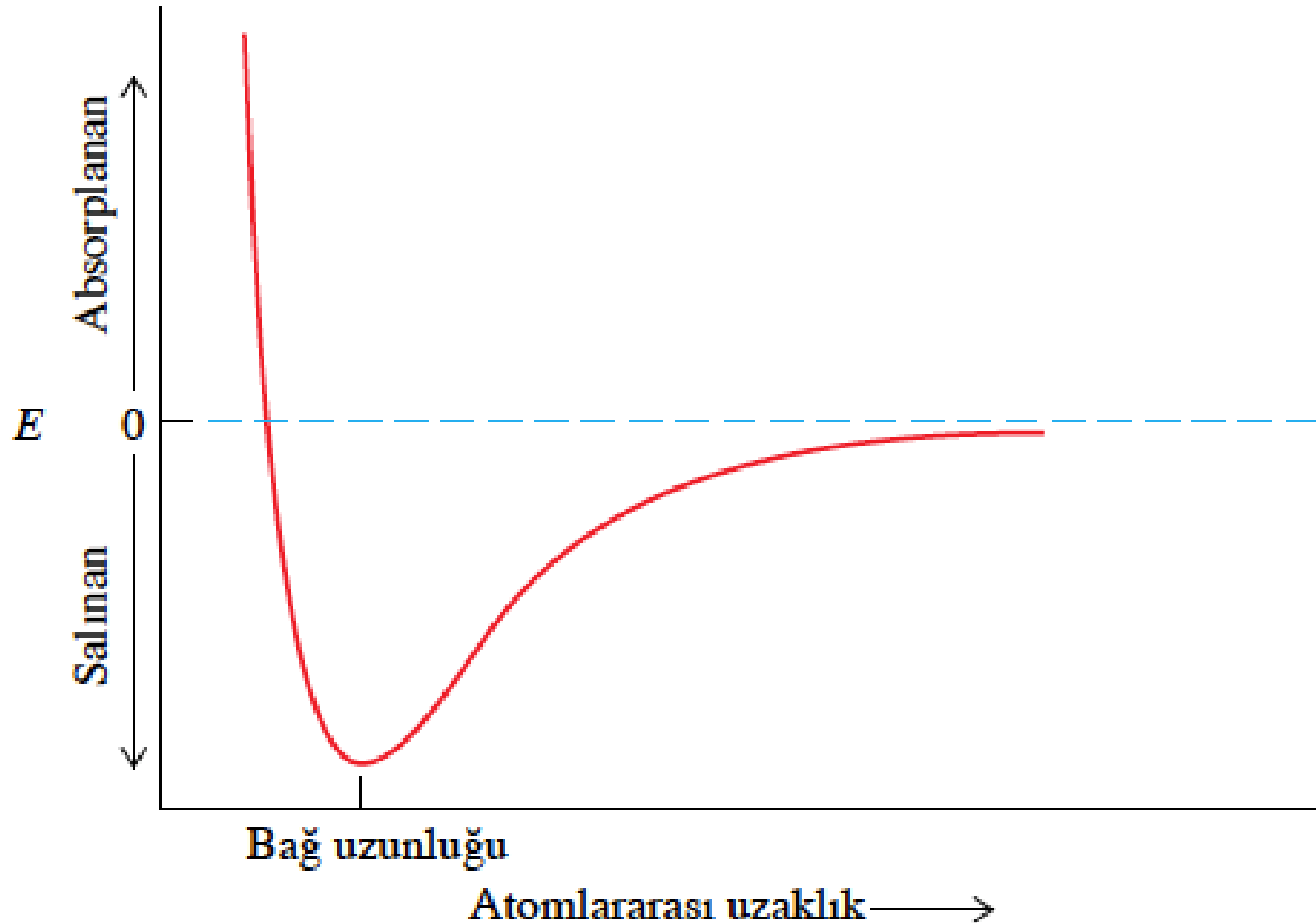
Kovalent Bağ: Elektronları Paylaşma



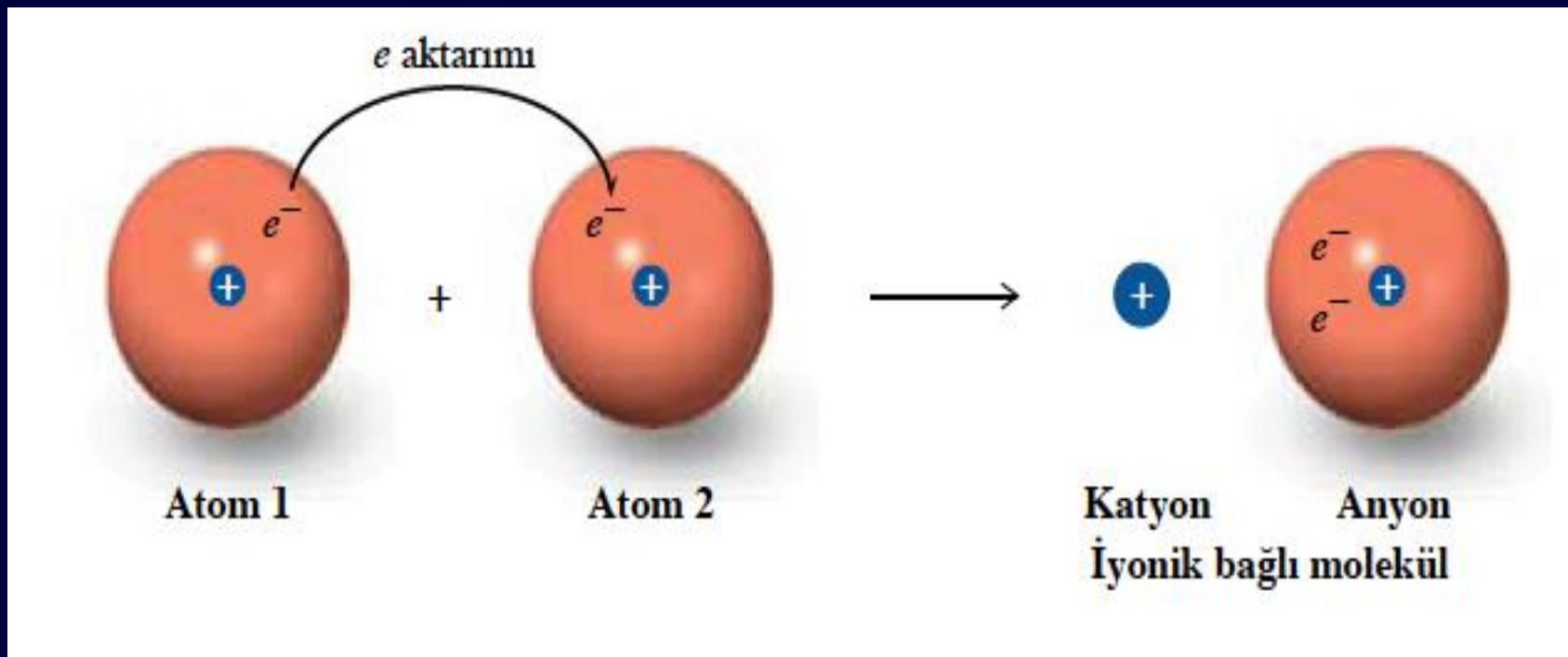
Boyutlar: Çekirdek çapı $\sim 10^{-15}$ m } Beş kat
Elektron yörüngesi $\sim 10^{-10}$ m } büyüklük
farkı

Kütle oranı: proton / elektron = ~ 1800

Çekirdeklerarası Potansiyel



İyonik Bağ: Elektron Paylaşımı “Yok”



Elektronu kim verir, kim alır?

Periyodik Çizelge Bölümü

Duet

Çizelge 1-1	Kısmi Periyodik Çizelge							
Periyot							Halojenler	Soygazlar
Birinci	H ¹							He ²
İkinci	Li ^{2,1}	Be ^{2,2}	B ^{2,3}	C ^{2,4}	N ^{2,5}	O ^{2,6}	F ^{2,7}	Ne ^{2,8}
Üçüncü	Na ^{2,8,1}	Mg ^{2,8,2}	Al ^{2,8,3}	Si ^{2,8,4}	P ^{2,8,5}	S ^{2,8,6}	Cl ^{2,8,7}	Ar ^{2,8,8}
Dördüncü	K ^{2,8,8,1}						Br ^{2,8,18,7}	Kr ^{2,8,18,8}
Beşinci							I ^{2,8,18,18,7}	Xe ^{2,8,18,18,8}

Not: Üst indisler atomun temel durumdaki elektron dağılımlarını belirtmektedir.

Değerlik elektronları

Oktet

itme



çekme



Table 1-2 Electronegativities of Selected Elements

Increasing electronegativity

Artma

			H 2.2					
Li 1.0	Be 1.6	B 2.0		C 2.6	N 3.0	O 3.4		F 4.0
Na 0.9	Mg 1.3	Al 1.6		Si 1.9	P 2.2	S 2.6		Cl 3.2
K 0.8								Br 3.0
								I 2.7

Azalma

Increasing electronegativity

Note: Values established by L. Pauling and updated by A. L. Allred (see Journal of Inorganic and Nuclear Chemistry, 1961, 17, 215).



:

0.3

<

0.3 - 2.0

<

2.0

Kovalent

Polar Kovalent

İyonik

Molekül Şekilleri

Değerlik elektronları çiftleri itmesi
(VSEPR) tarafından kontrol edilir

İki atomlular: doğrusal $\text{H}:\text{H}$ $\text{Li}:\text{H}$ $:\ddot{\text{F}}:\ddot{\text{F}}:$

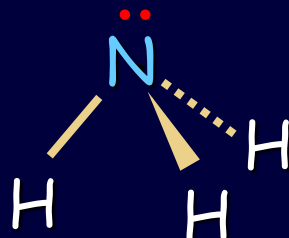
Üç atomlular: doğrusal (yani kırık değil)

bu $:\ddot{\text{F}}:\text{Be}:\ddot{\text{F}}:$ $:\ddot{\text{F}}:\text{Be}:\ddot{\text{F}}:$ Bu değil

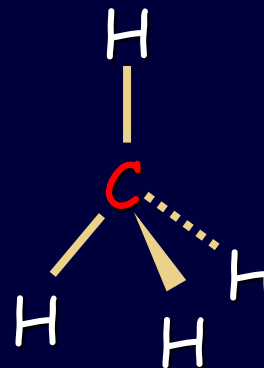
VEYA kırık olabilir, elektron çiftleri VARSA; $\text{H}:\ddot{\text{O}}:\text{H}$

Dört atomlular: üçgen düzlemsel $:\ddot{\text{Cl}}:\text{B}:\ddot{\text{Cl}}:$

VEYA piramit, elektron çiftleri varsa;



Beş atomlular: tetrahedral;



Geçiş metallere olduğu gibi, daha fazla elektron varsa, oktahedral gibi diğer şekillerde mümkündür.

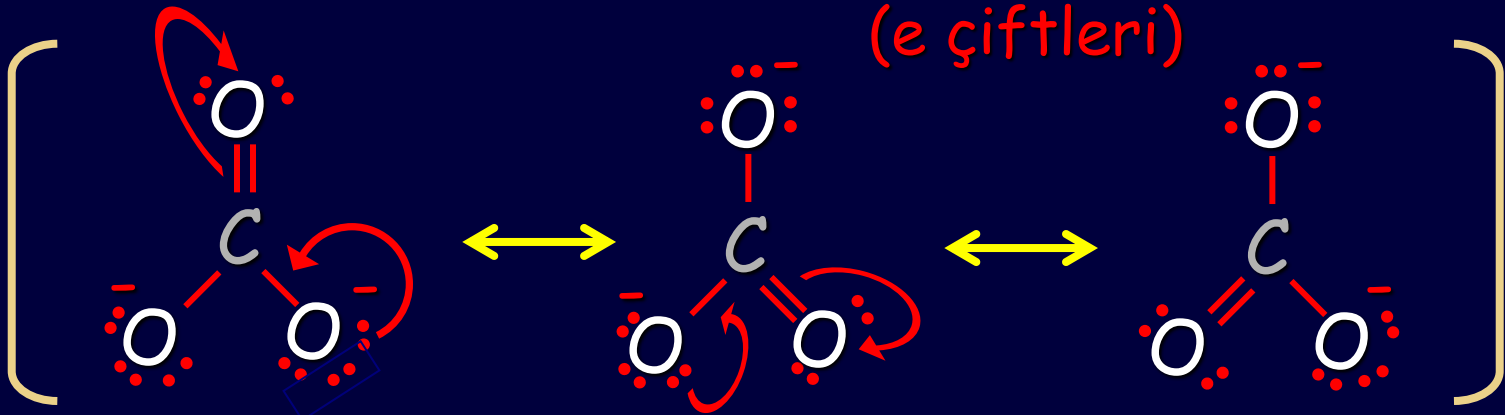
Rezonans

Bir molekül için birkaç farklı oktet yapısı yazılabilir: **Rezonans yapıları**

Molekül bu yapıların çakışmasıdır

A yapısı \longleftrightarrow B yapısı

Elektronların hareketi (e çiftleri)

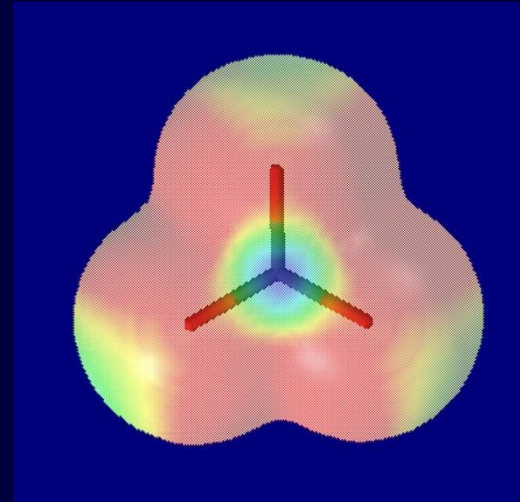
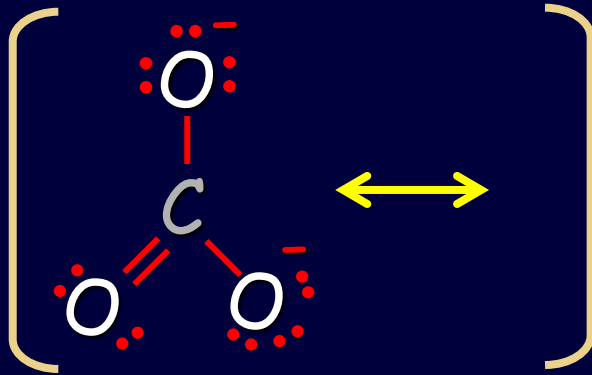


Karbonat, CO_3^{2-} . Bütün yapılar eşittir

Rezonans Yapıları

Karbonat iyonu delokalizedir

Simetrik olarak!



Elektrostatik Potansiyel haritası:

Kırmızı = kısmen **elektronca zengin**

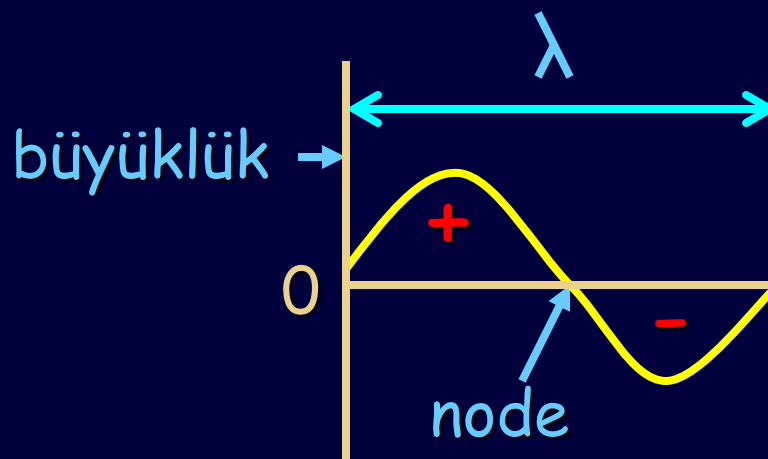
Mavi = kısmen **elektronca fakir**

Orbitaller

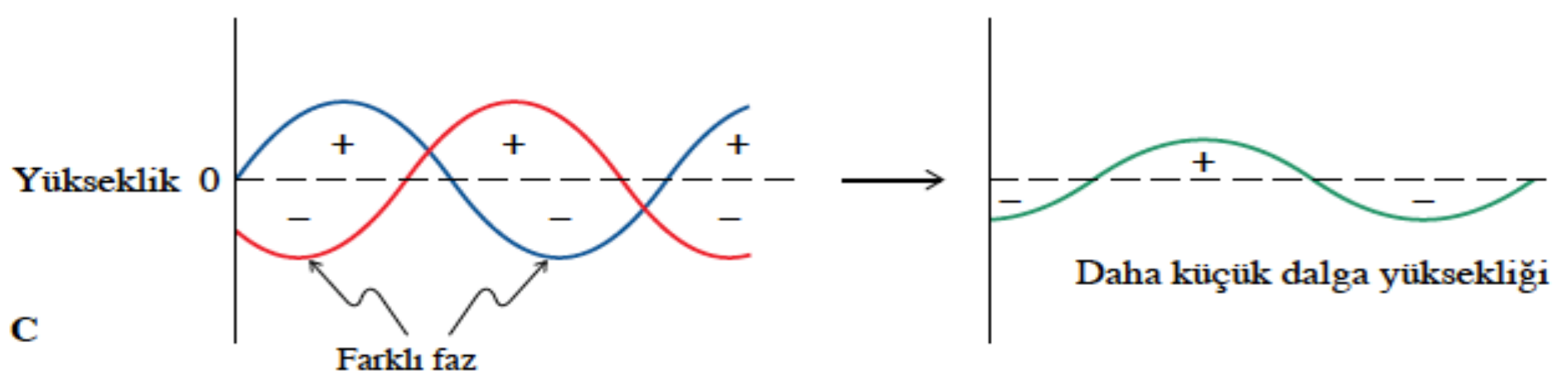
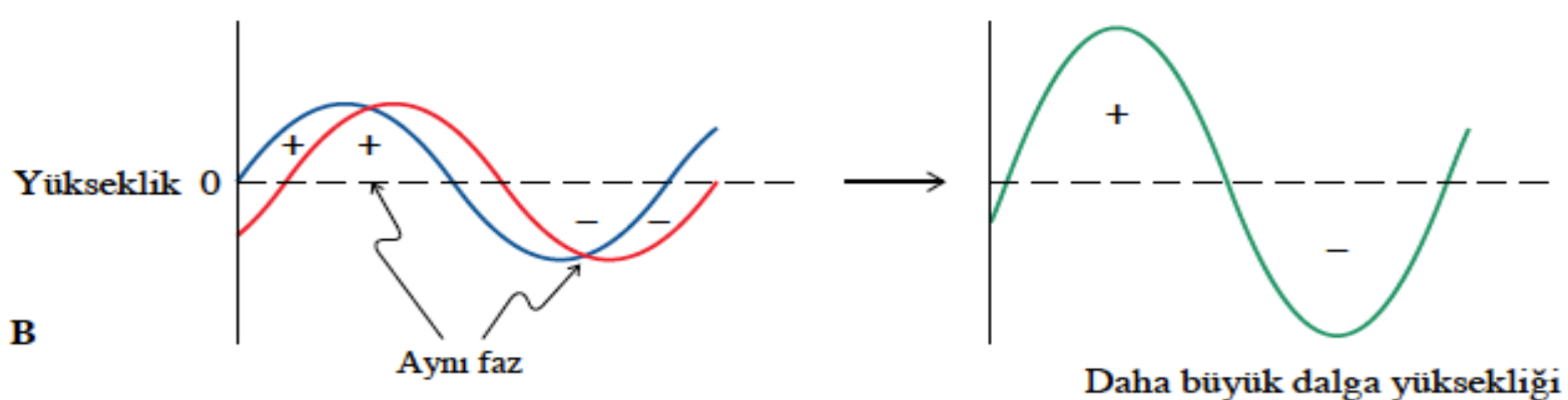
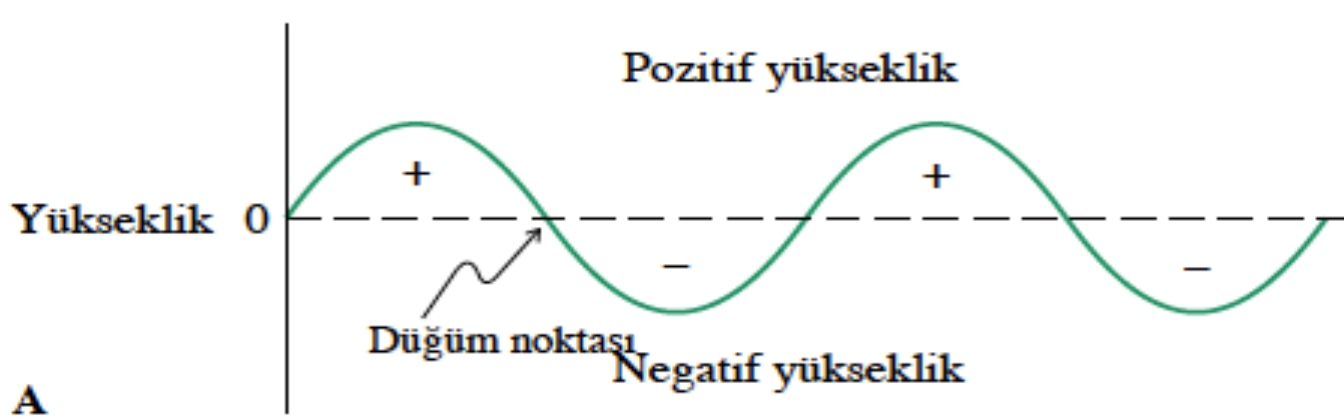
Küresel (üç-boyutlu) şekil.

Mekanik dalga kuramına ters (gitar teli, lastik bant)

İki-boyutlu
dalga



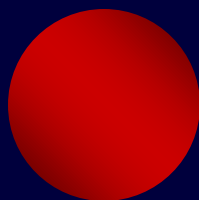
+/- = işaret, yük değil



En önemli orbitaller (bizim için):

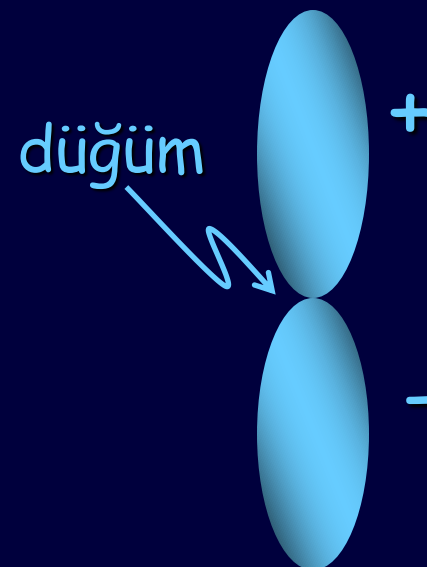
s Orbitali

"top"



p Orbitali

küresel
"sekiz"

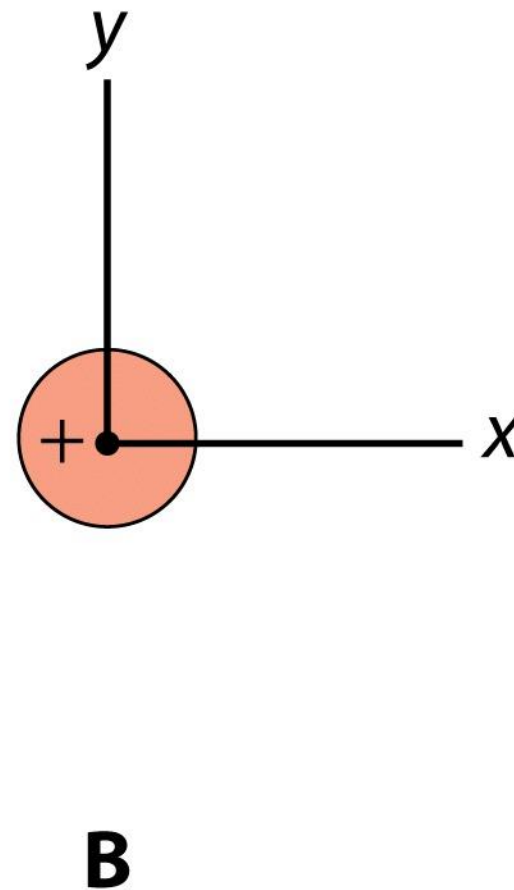
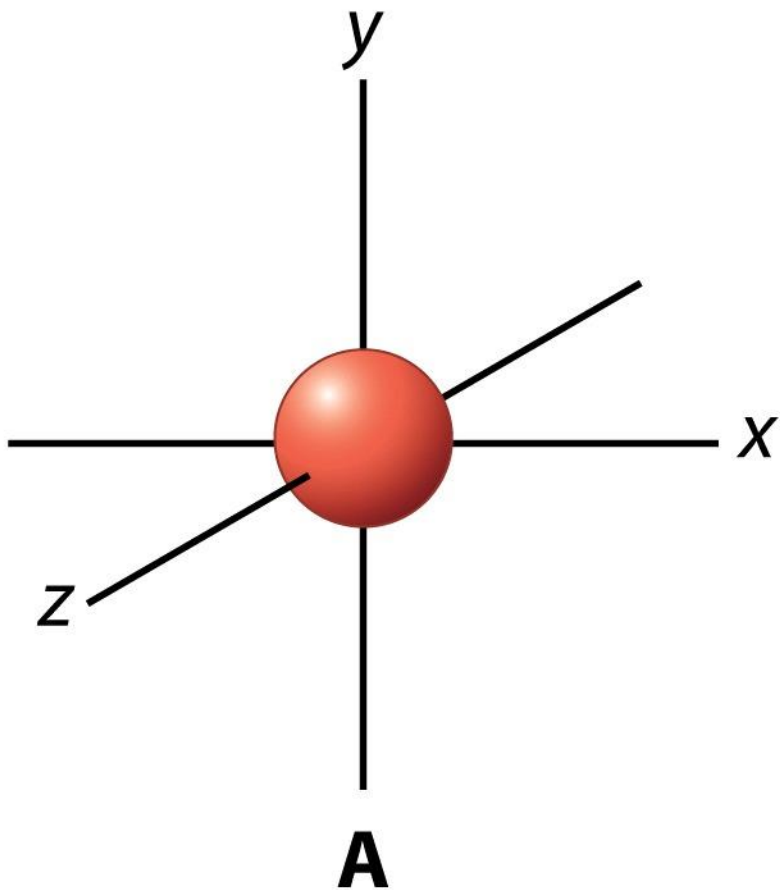


Gerçek çözümler: $1s, 2s, 2p_x, 2p_y, 2p_z,$
 $3s, 3p_x, 3p_y, 3p_z,$ gibi.

klasik kabuk modeli
ile ilişkilendirilir

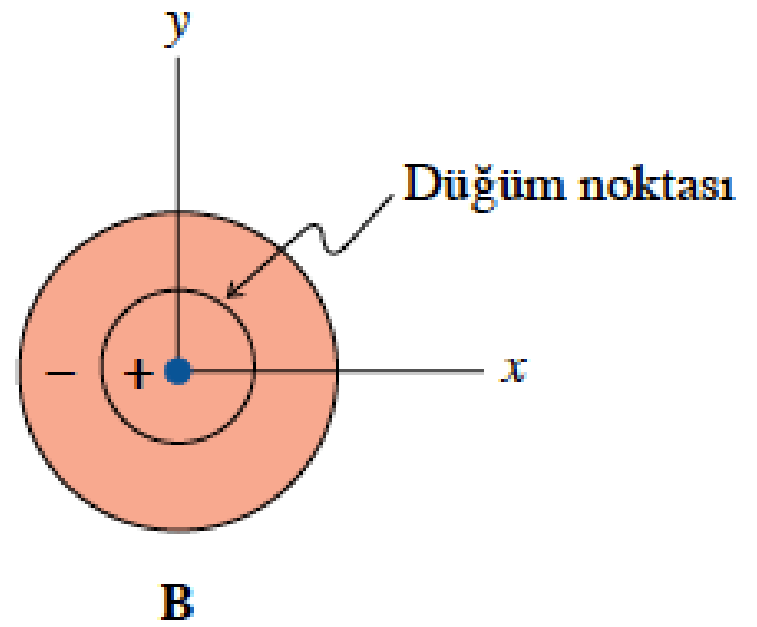
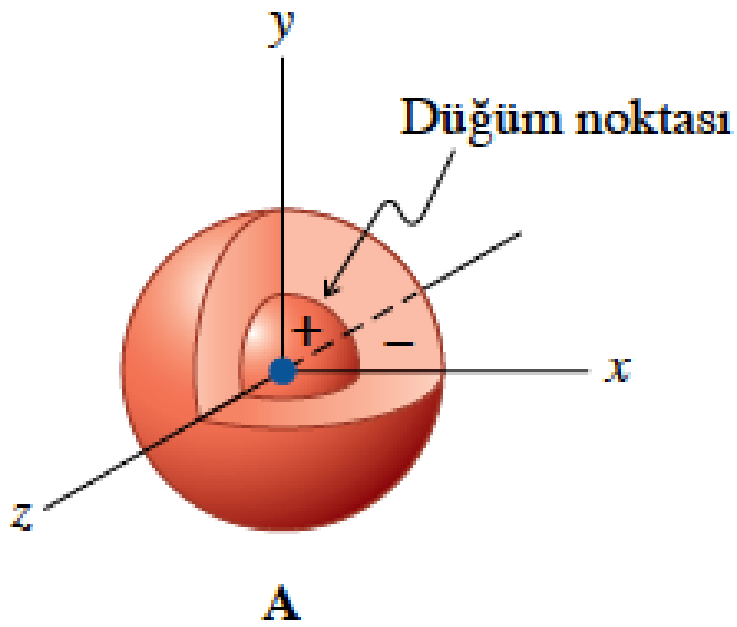
(artan enerji)

1s Orbitali

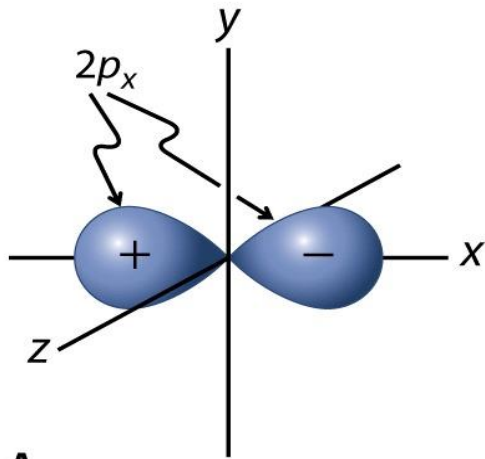


s-Orbital

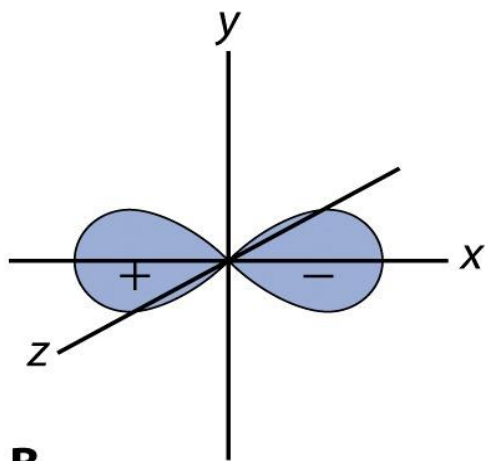
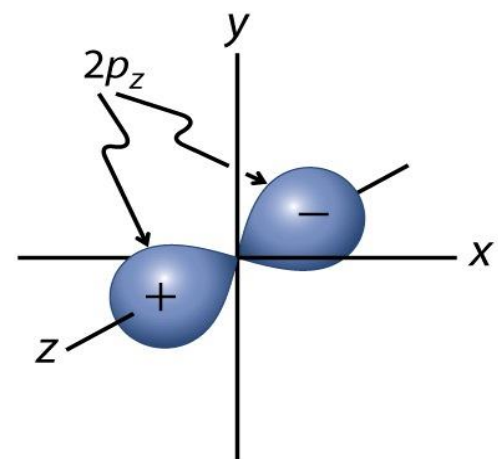
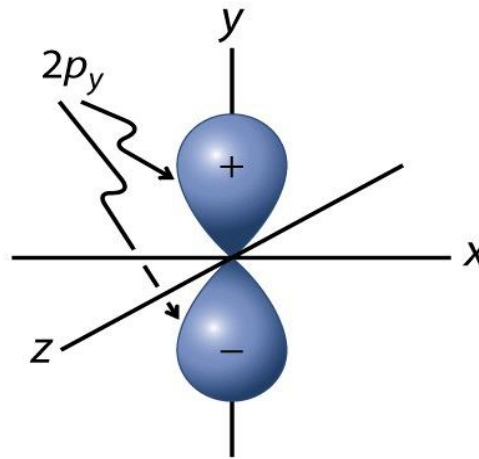
2s Orbitali



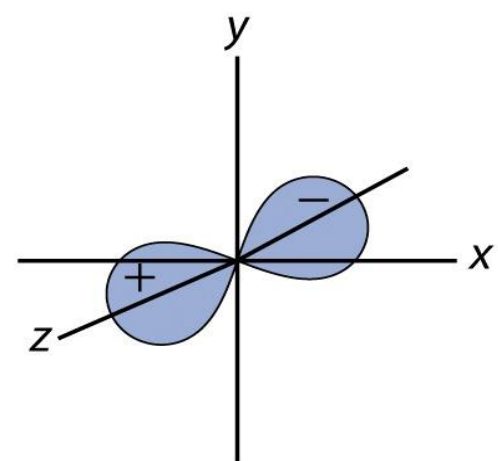
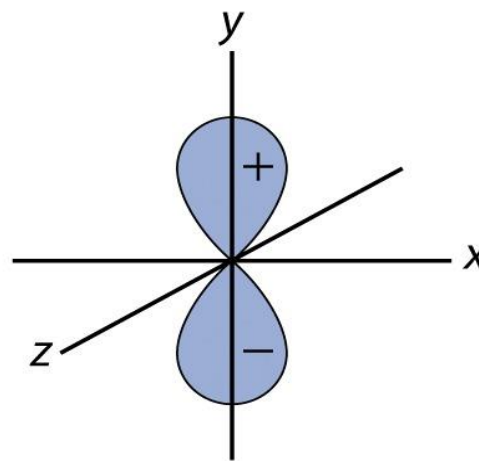
2p Orbitalleri



A



B

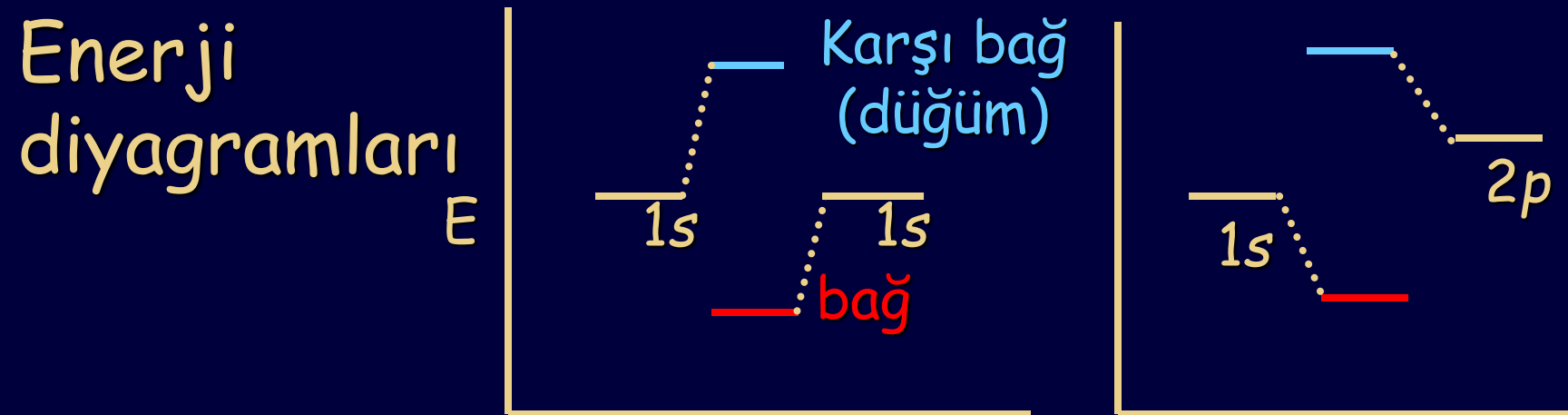


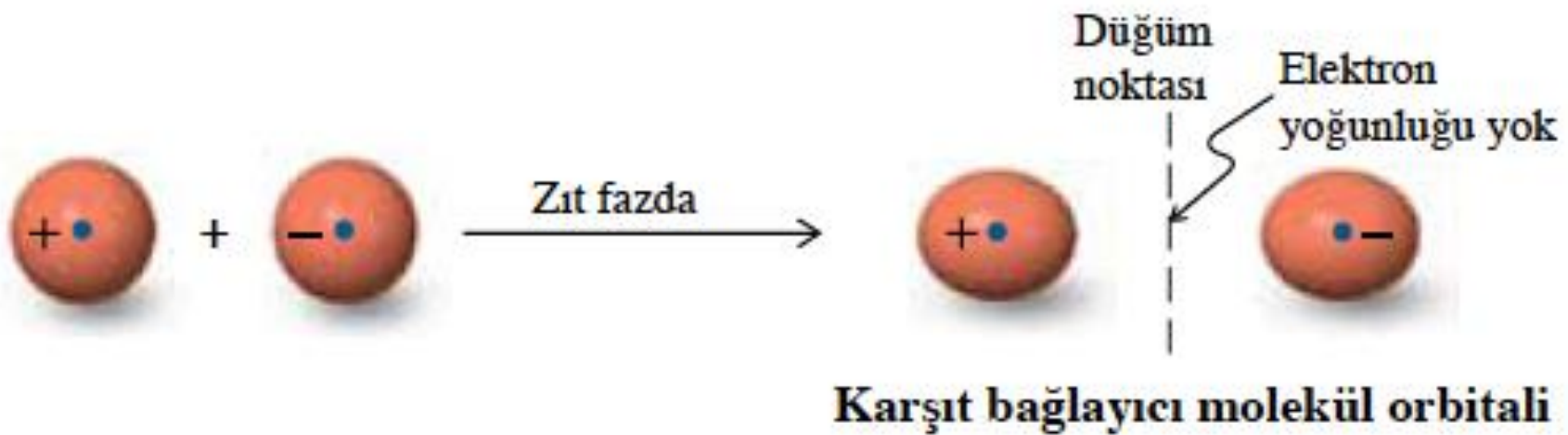
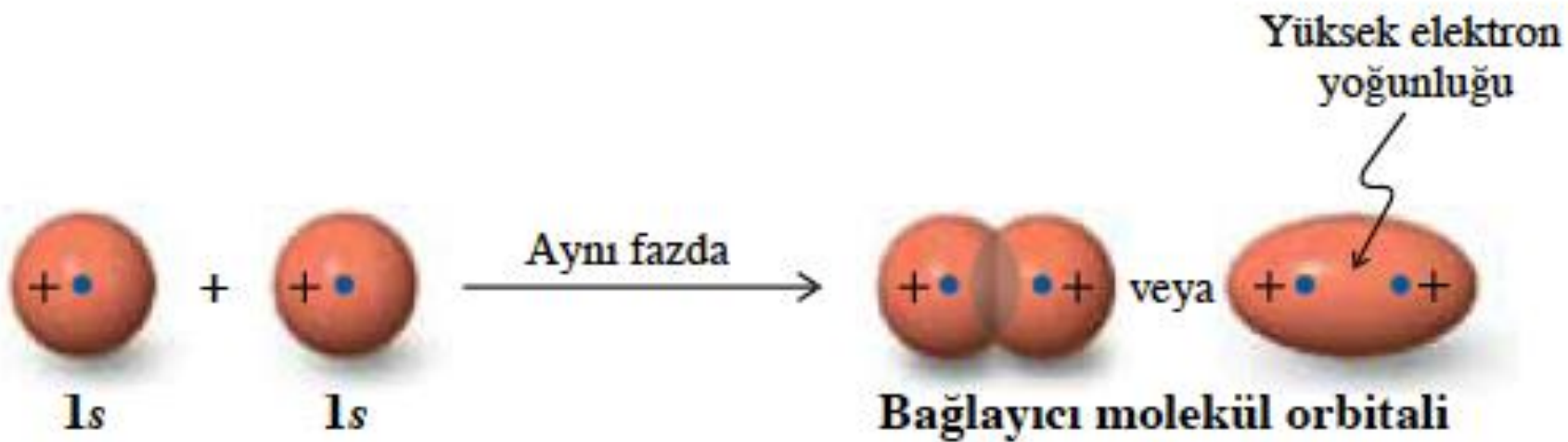
Bağlanma

Bağlanma **moleküler orbitalleri** vermek üzere atomik orbitallerin örtüşmesinden meydana gelir.

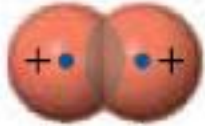
Aynı fazda örtüşme → moleküler **bağlanma**

Zıt fazda örtüşme → **karşıbağ** moleküler orbital





Orbital Örtüşme Çeşitleri



1s 1s

σ bağı,
H-H daki gibi

A



1s 2p

σ bağı,
H-F deki gibi

B

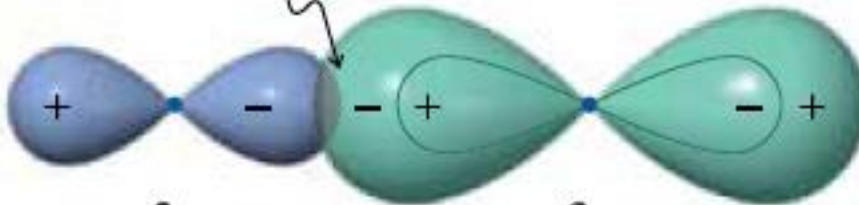


2p 2p

σ bağı,
F-F deki gibi

C

Göreceli olarak daha yayılmış:
zayıf örtüşme



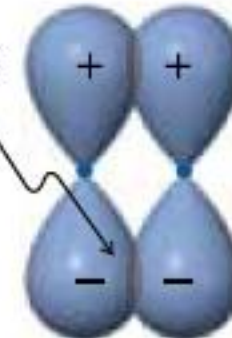
2p

3p

σ bağı,
F-Cl deki gibi

D

Paralel yönlenme:
zayıf örtüşme



2p 2p

π bağı,
H₂C=CH₂ deki gibi

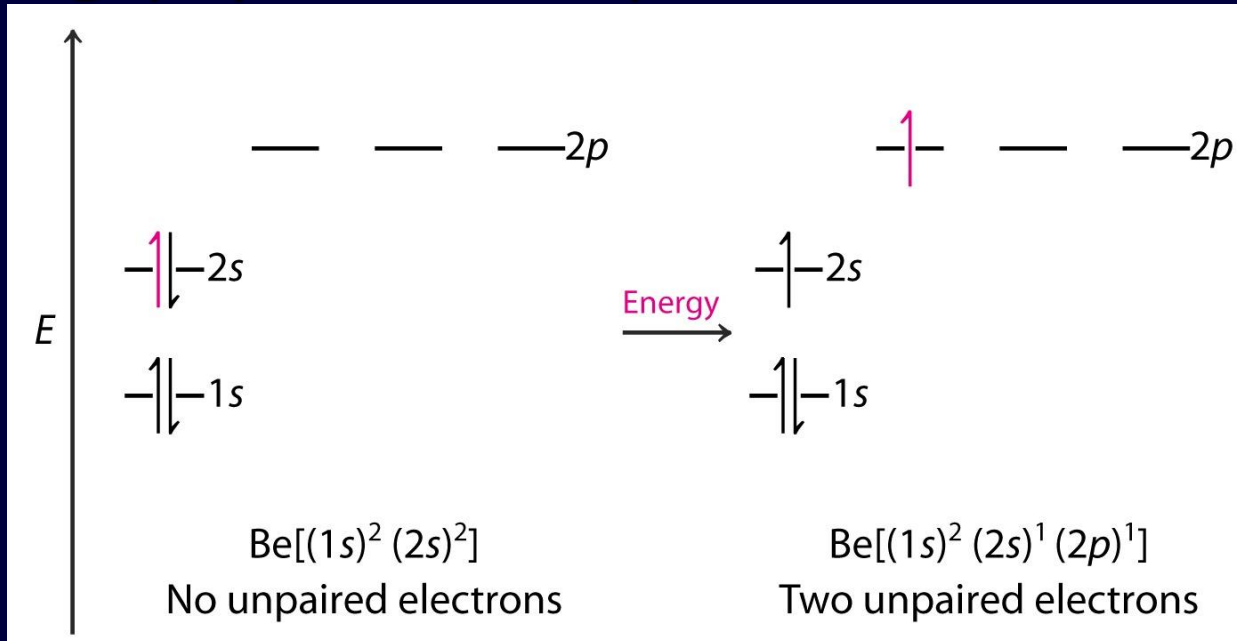
E

Hibritleşme ve şekil

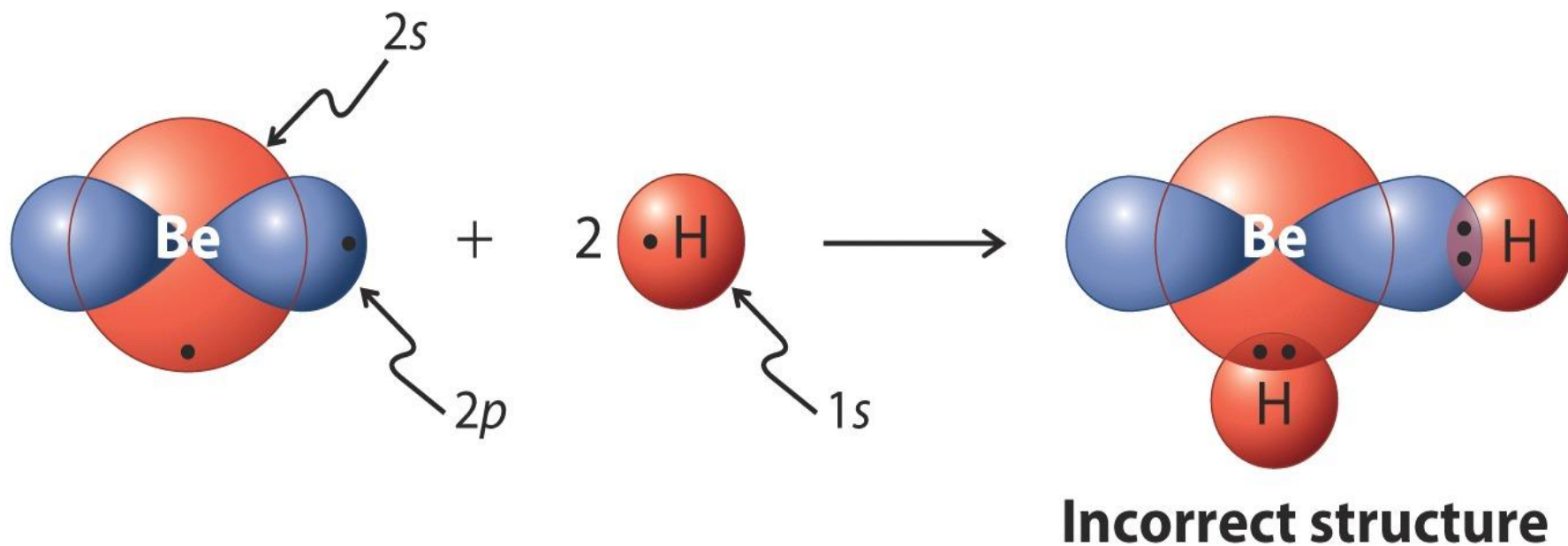
Li : H $2s + 1s$ şekil yok

δ^- -H : Be : H δ^+ doğrusaldır; fakat Be atomunun kabuğu doludur $(1s)^2(2s)^2$!

Nasıl bağ yapar? Boş p orbitalini kullanır:

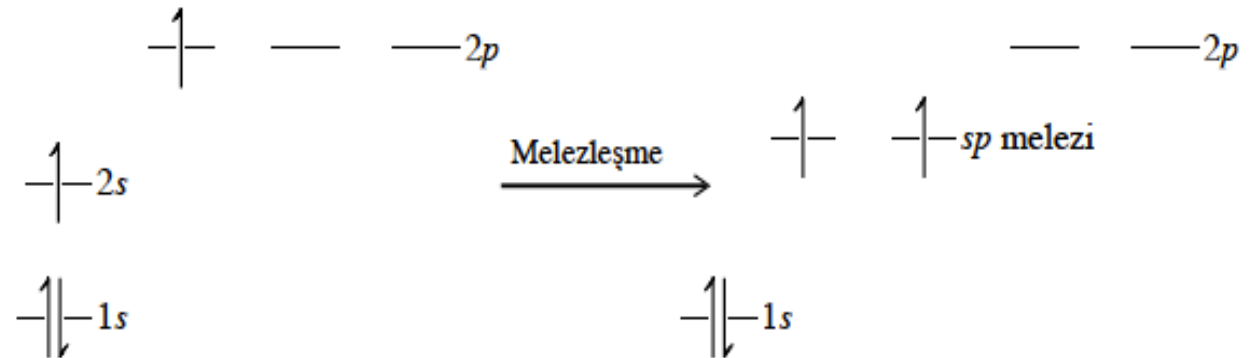
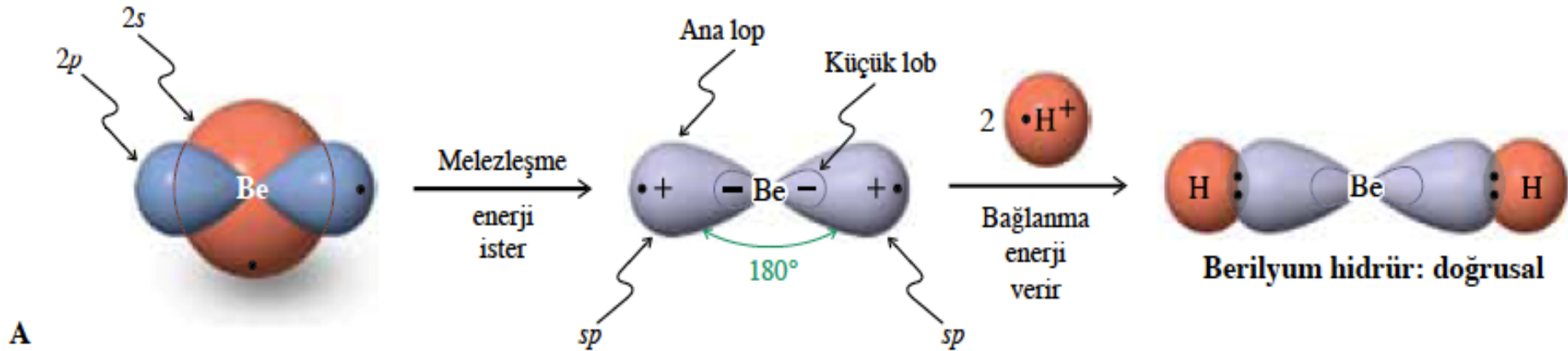


Bu durum bağ yapabilir, fakat,
yanlış yapıya gider:



Orbitalerin "Hibritleşmesi" uygun çözüm

Atomlar arası örtüşme 2s ve bir 2p orbitallerinin, iki yeni hibrit moleküler orbitaller oluşturmasıdır: **linear** bir düzenlenme ile $s + p \rightarrow$ iki **sp** hibritleri:



B

Diğer atomlararası örtüşme olasılıkları
(hibritleşme):

$s + p + p \rightarrow 3 \text{ } sp^2$ trigonal

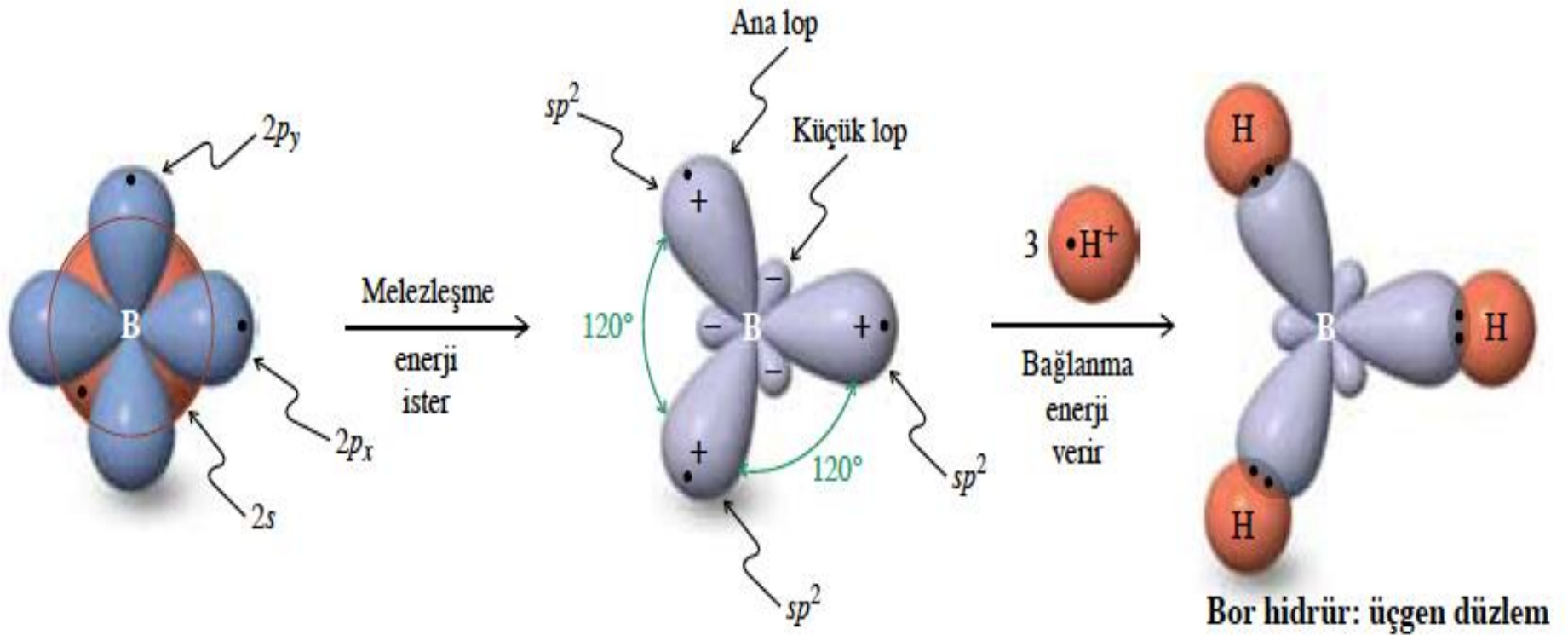
$s + p + p + p \rightarrow 4 \text{ } sp^3$ tetrahedral

$s + 3 p + d \rightarrow 5 \text{ } sp^3d$ üçgen bipiramit

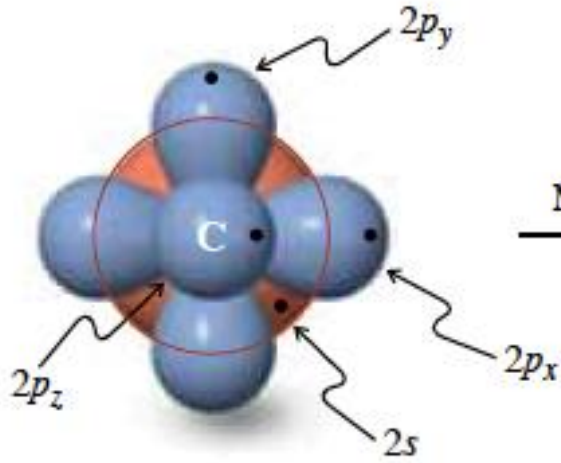
$s + 3 p + 2d \rightarrow 6 \text{ } sp^3d^2$ oktahedral

Not: n sayıda atomik orbital $\rightarrow n$ sayıda yeni orbital

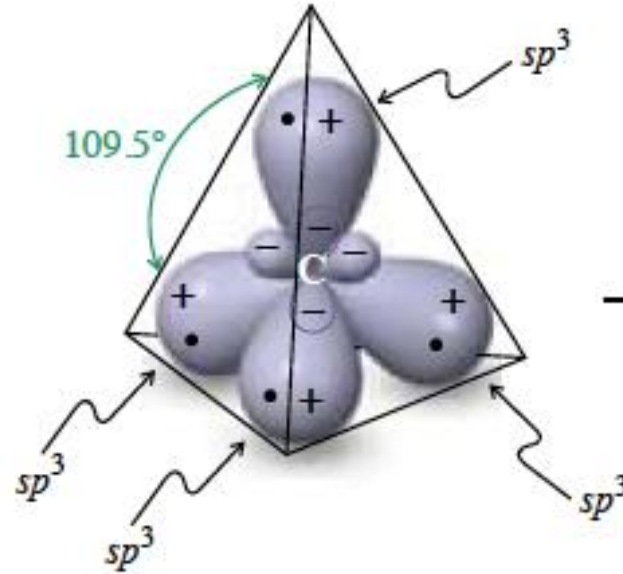
Örnek: BH_3 Trigonal (üçgen düzlemsel) hibritleşme



Metan: Tetrahedral Hibritleşme



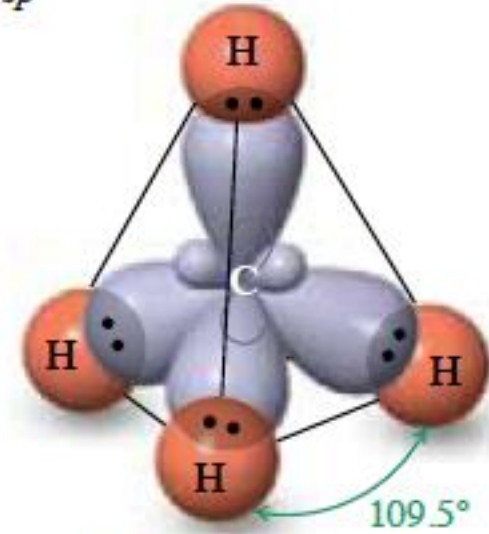
Melezleşme
enerji
ister



sp³-Hibrit
orbitaler

4 •H⁺

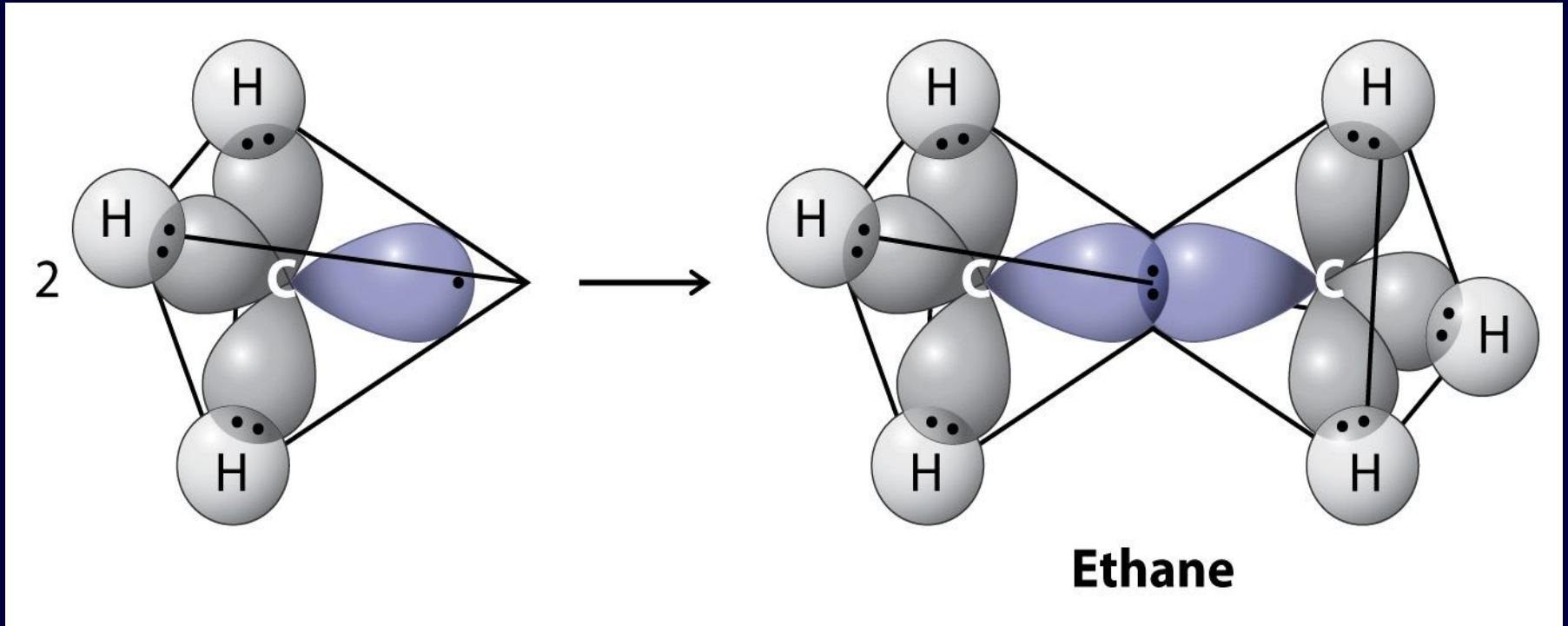
Bağlanma
enerji
verir



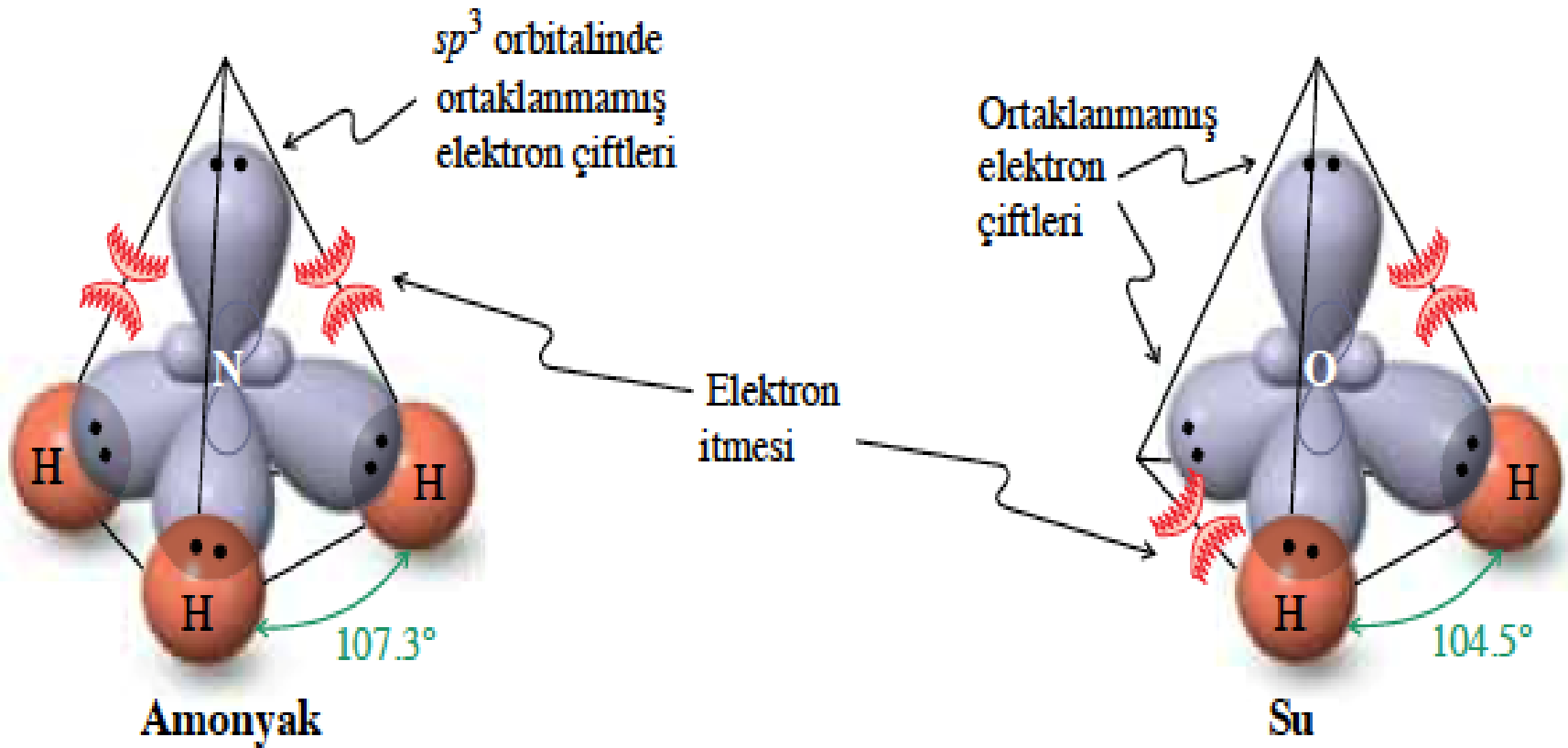
Metan: dörtyüzlü

Metan

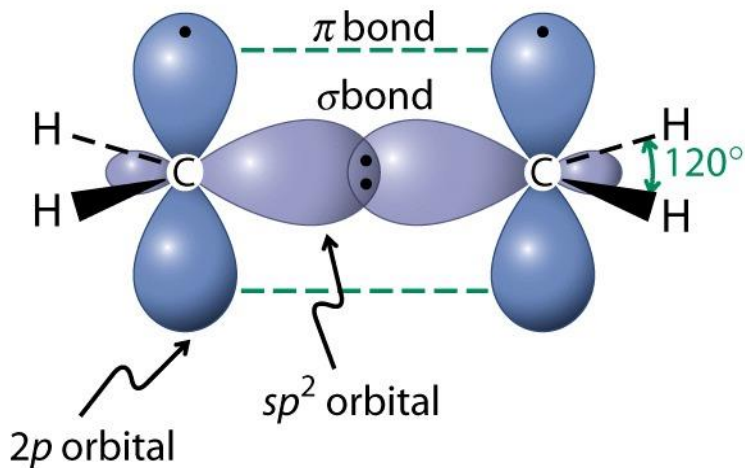
Etan: iki sp^3 Hibrit Orbitalinin Örtüşmesi



Farklı sp^3 Hibritleşmeleri: NH_3 ve H_2O

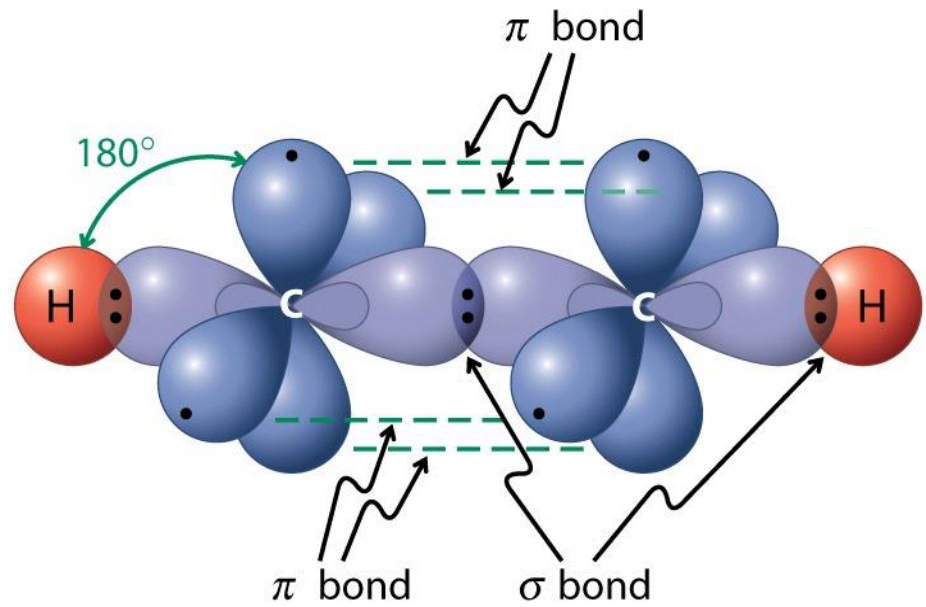


İkili ve Üçlü Bağlar:



Ethene

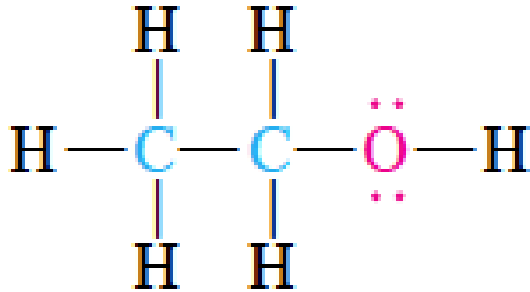
Eten



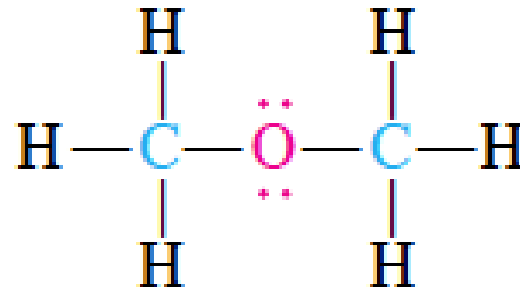
Ethyne

Etin

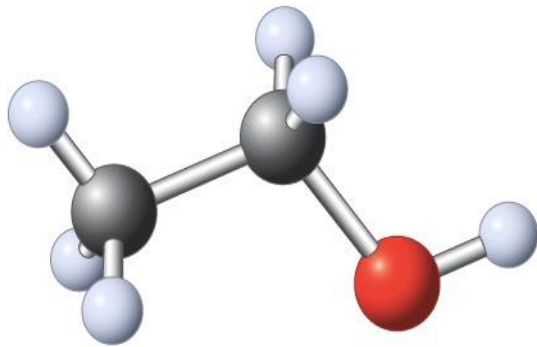
Molekül Modelleri:



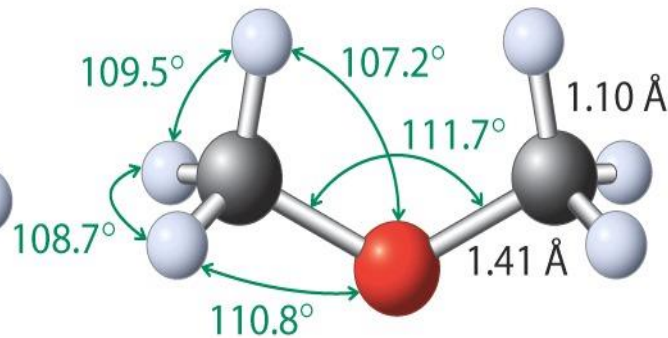
Etanol
(k.n. 78.5°C)



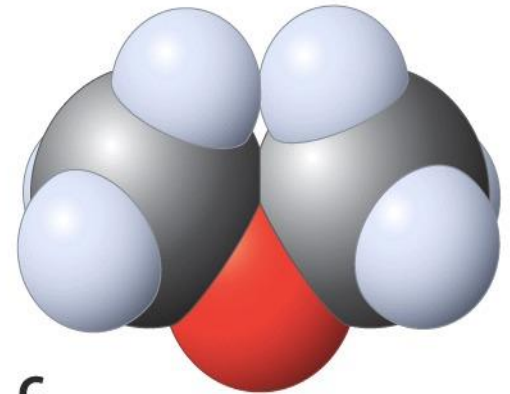
Metoksimetan
(Dimetil eter)
(k.n. -23°C)



A



B



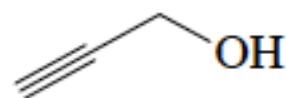
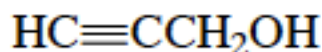
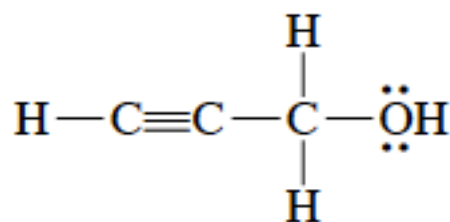
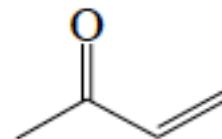
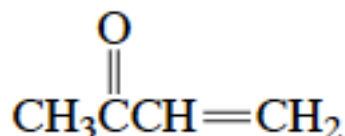
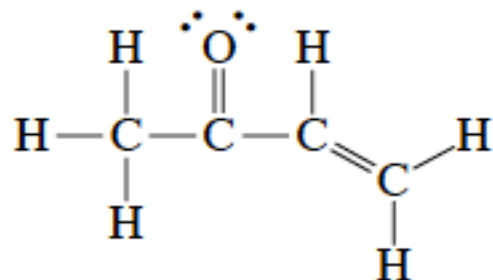
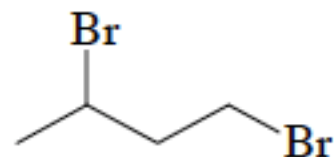
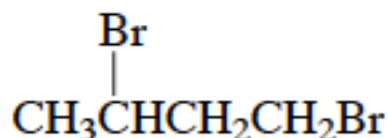
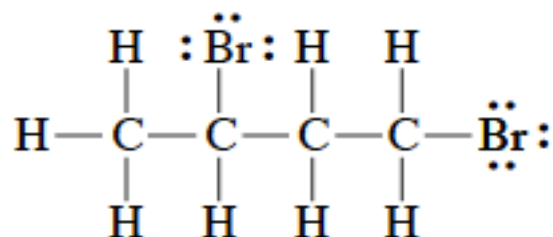
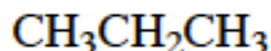
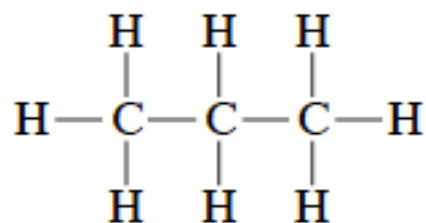
C

Molekül yapılarını göstermek için çeşitli çizim türleri kullanılır

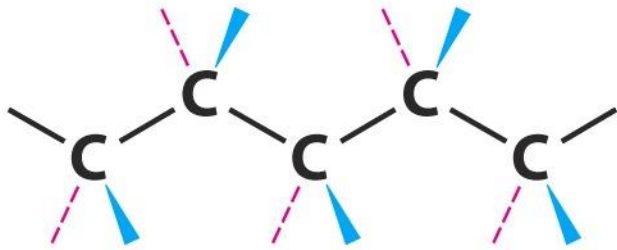
Kekulé

Sıkıştırılmış

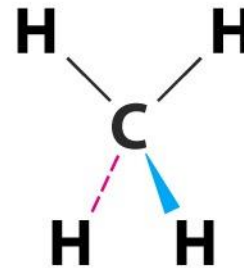
Çizgi Formülleri



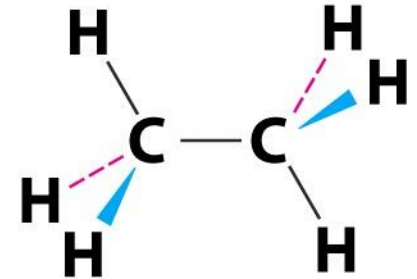
Kesikli(kırmızı)-Kamalı(mavi) Çizgi Gösterimi



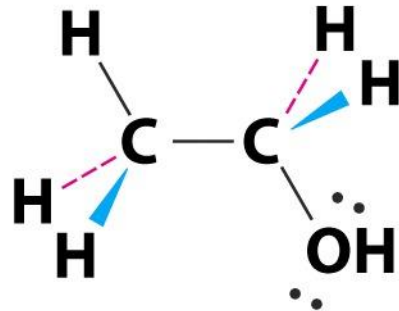
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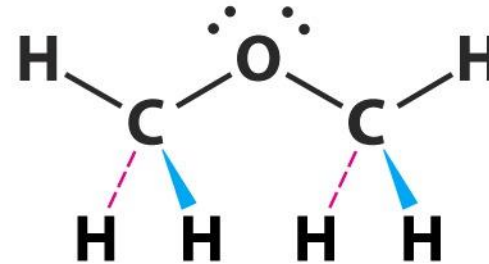
B



C



D



E