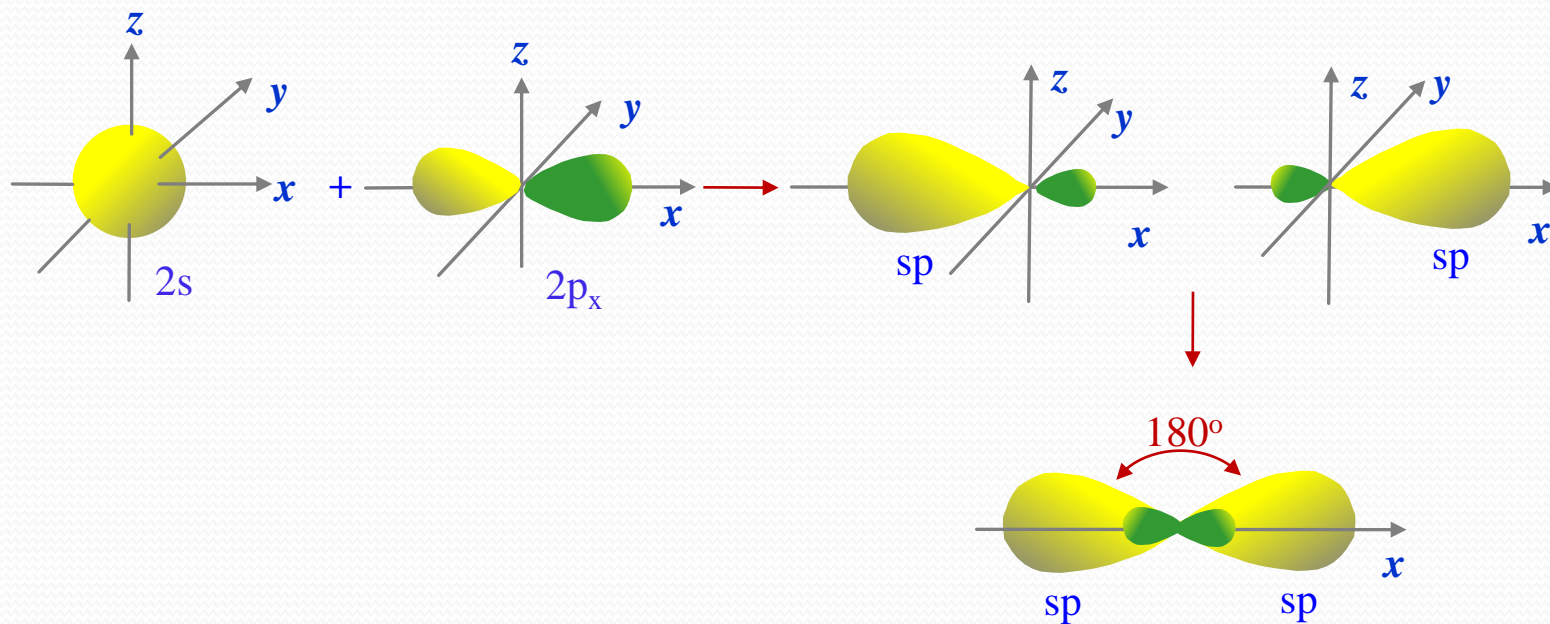
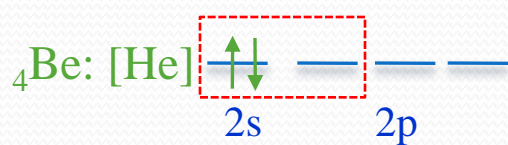
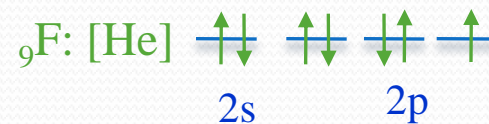
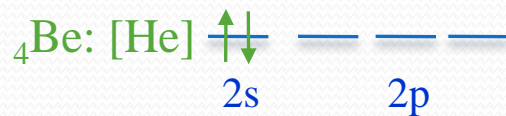


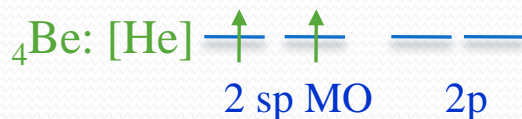
$2s + 2p_x \rightarrow 2$ tane sp melez orbitali



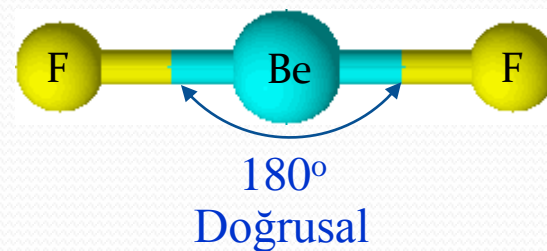
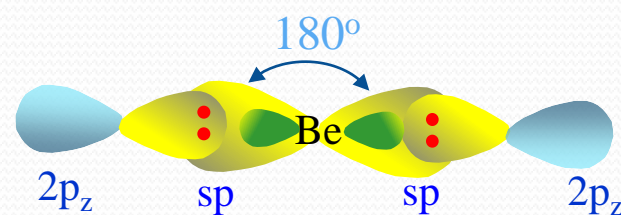
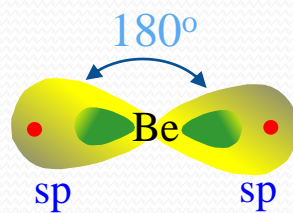


Temel Hal

E_d



Melez Hal



- Her bir orbital, kendi dalga fonksiyonu (ψ) ile tanımlanabilir.
- İki atomik orbitalin dalga fonksiyonları ψ_{2s} ve ψ_{2p}
- Aynı doğrultuda uzayda yer alan iki melez orbitalin dalga fonksiyonu ise ψ_{sp} olsun.
- ψ_{sp} , bu iki atomik dalga fonksiyonunun *doğrusal birleşimiyle* elde edilir.

$$\psi_{sp} = C_1 \psi_{2s} + C_2 \psi_{2px}$$

- Farklı C_1 ve C_2 katsayıları ile iki farklı birleşim mümkündür.

$$\psi_{sp}(1) = \frac{1}{\sqrt{2}} \psi_{2s} + \frac{1}{\sqrt{2}} \psi_{2px}$$

$$\psi_{sp}(1) = \frac{1}{\sqrt{2}} \psi_{2s} - \frac{1}{\sqrt{2}} \psi_{2px}$$

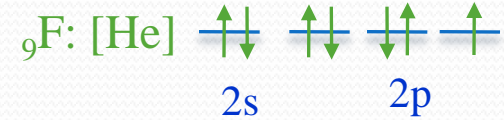
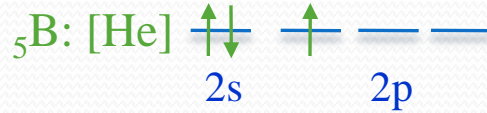
- Eşitlikteki $\frac{1}{\sqrt{2}}$ katsayısı, iki dalga fonksiyonun normalizasyonundan kaynaklanır ve melez orbitallerin oluşumuna ilgili atomik orbitallerin katkısını gösterir.
- Bu şekilde atomik orbitallerin dalga fonksiyonlarının birleşimine veya harmanlanmasına, *melezleşme* denir.
- sp melez orbitalinin dilimleri büyük olduğundan kendisini oluşturan 2s ve 2p atomik orbitallerine oranla, F atomunun 2p orbitali ile daha etkin girişim yapar ve daha kuvvetli bağ oluşturur.

❖ Çeşitli orbitallerin girişim sonucu verdiği bağların yaklaşık kuvvetleri

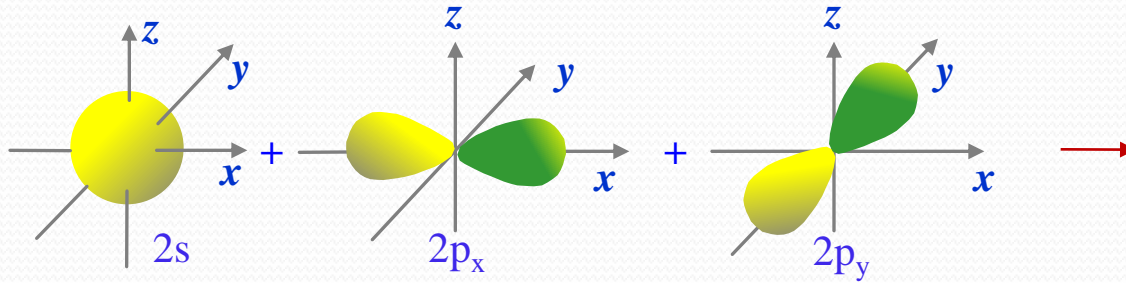
Orbital	Bağlı bağ kuvveti
s	1,00
p	1,73
sp	1,93
sp ²	1,99
sp ³	2,00

➤ Dalga fonksiyonu, ancak tek elektronlu sistemler için tam olarak çözülebildiğinden, tablodaki bağlı değerler yaklaşık çözümlerle hesaplanmıştır.

sp² Melezleşmesi



2s + 2p_x + 2p_y → 3 tane sp² melez orbitali

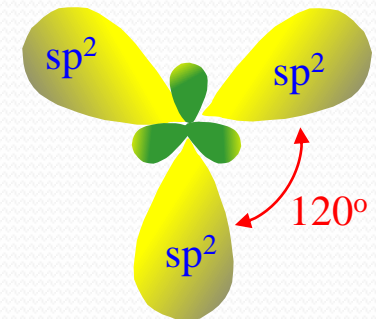
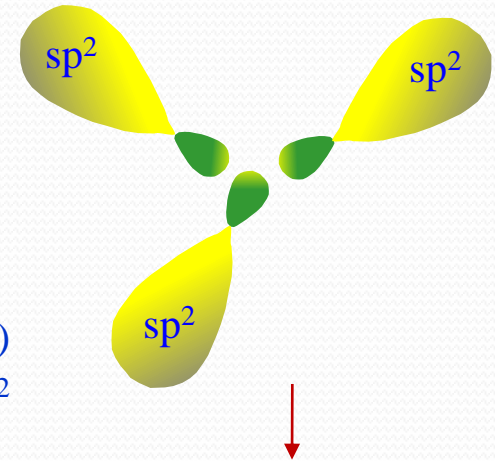


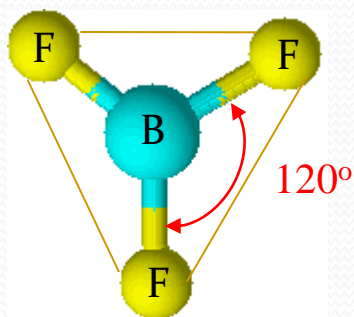
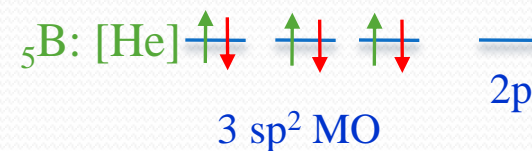
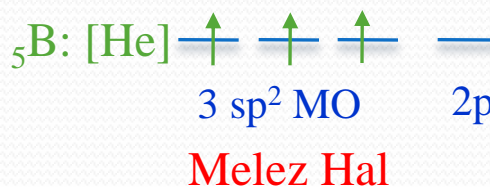
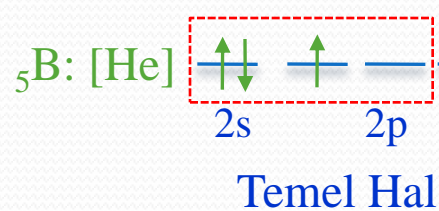
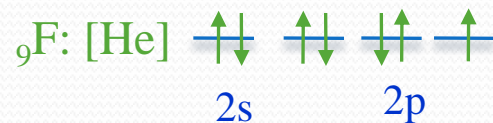
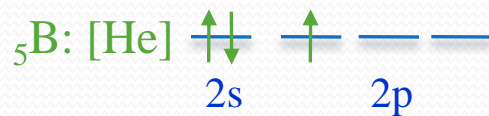
➤ B atomunun 2s ve 2p orbitallerinden herhangi iki (2p_x, 2p_y) atomik orbitalinin dalga fonksiyonlarının doğrusal birleşimi üç sp² melez orbitali verir.

$$\Psi_{sp^2}(1) = \frac{1}{\sqrt{3}} \Psi_{2s} + \frac{2}{\sqrt{6}} \Psi_{2p_x}$$

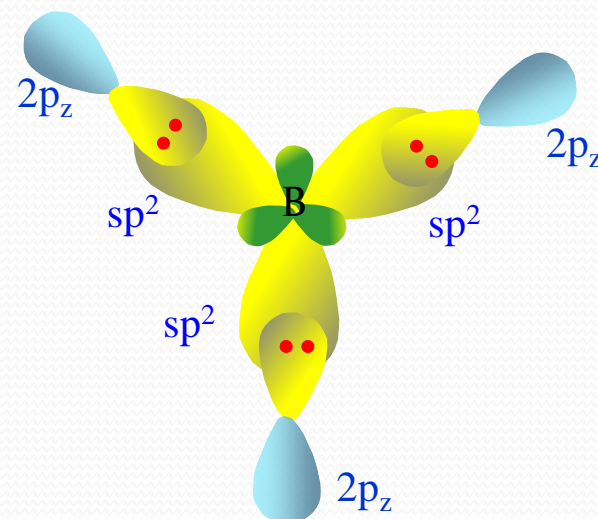
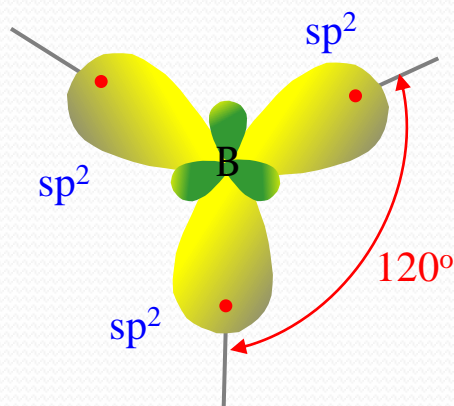
$$\Psi_{sp^2}(2) = \frac{1}{\sqrt{3}} \Psi_{2s} + \frac{2}{\sqrt{6}} \Psi_{2p_x} + \frac{1}{\sqrt{2}} \Psi_{2p_y}$$

$$\Psi_{sp^2}(3) = \frac{1}{\sqrt{3}} \Psi_{2s} + \frac{2}{\sqrt{6}} \Psi_{2p_x} - \frac{1}{\sqrt{2}} \Psi_{2p_y}$$

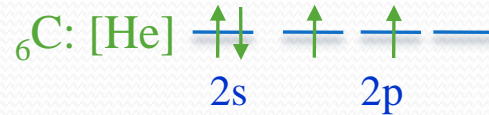




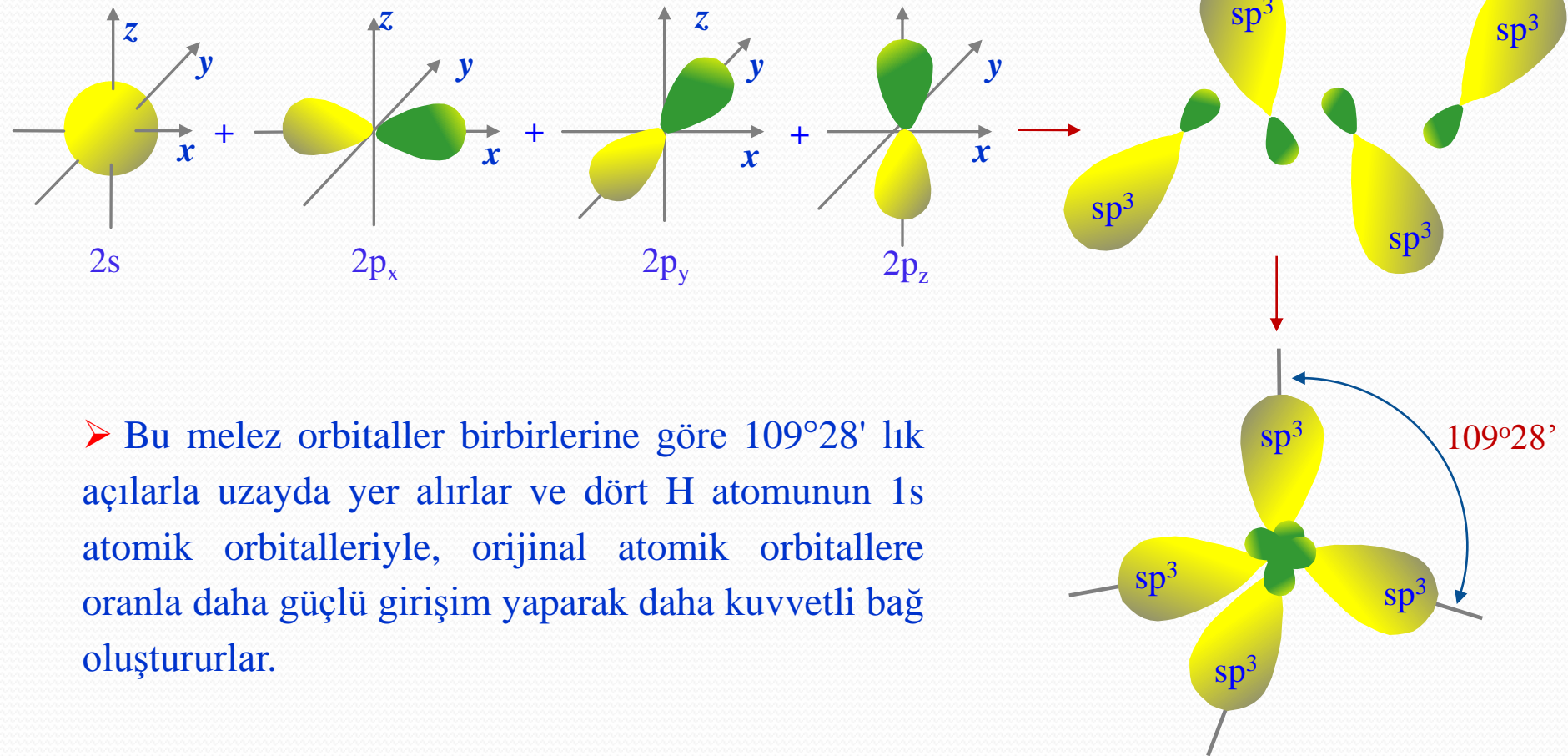
Üçgen düzlem



sp³ melezleşmesi



$2s + 2p_x + 2p_y + 2p_z \rightarrow 4 \text{ tane } sp^3 \text{ melez orbitali}$



➤ Bu melez orbitaller birbirlerine göre 109°28' lık açılarla uzayda yer alırlar ve dört H atomunun 1s atomik orbitalleriyle, orijinal atomik orbitallere oranla daha güçlü girişim yaparak daha kuvvetli bağ oluştururlar.

➤ Melezleşme, atomik orbitallerin dalga fonksiyonlarının doğrusal birleşimi ile de gösterilebilir.

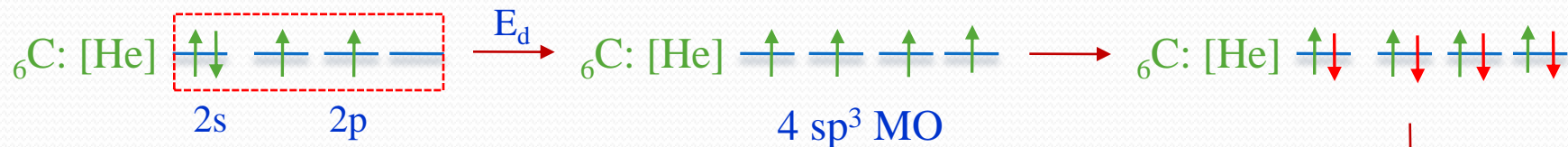
$$\Psi_{sp^3}(1) = \frac{1}{2}\Psi_{2s} + \frac{1}{2}\Psi_{2p_x} + \frac{1}{2}\Psi_{2p_y} + \frac{1}{2}\Psi_{2p_z}$$

$$\Psi_{sp^3}(2) = \frac{1}{2}\Psi_{2s} + \frac{1}{2}\Psi_{2p_x} - \frac{1}{2}\Psi_{2p_y} - \frac{1}{2}\Psi_{2p_z}$$

$$\Psi_{sp^3}(3) = \frac{1}{2}\Psi_{2s} - \frac{1}{2}\Psi_{2p_x} + \frac{1}{2}\Psi_{2p_y} - \frac{1}{2}\Psi_{2p_z}$$

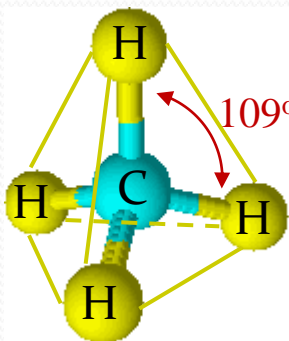
$$\Psi_{sp^3}(4) = \frac{1}{2}\Psi_{2s} - \frac{1}{2}\Psi_{2p_x} - \frac{1}{2}\Psi_{2p_y} + \frac{1}{2}\Psi_{2p_z}$$

➤ Bu dalga fonksiyonun her biri, oluşan dört sp^3 melez orbitalinden birini tanımlar.

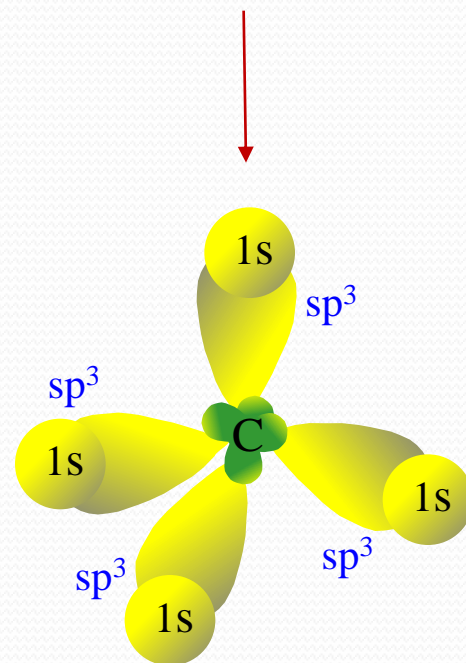
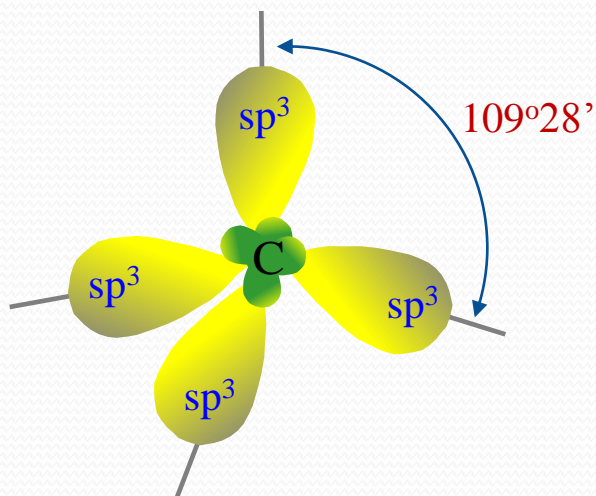


Temel Hal

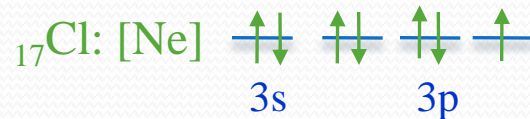
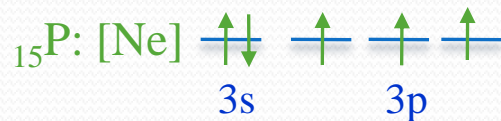
Melez Hal



TETRAHEDRAL

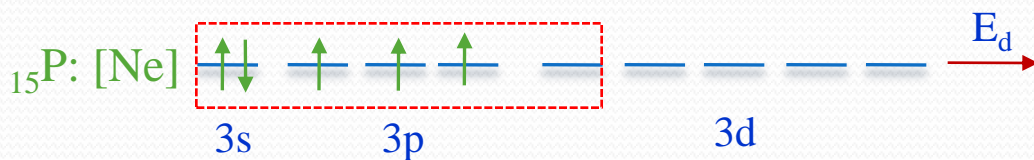


sp^3d melezleşmesi

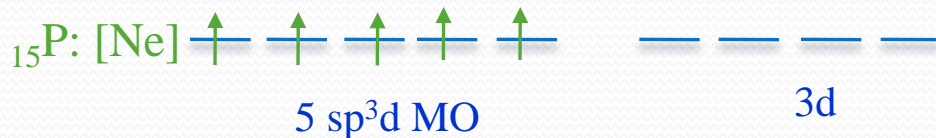


$2s + 2p_x + 2p_y + 2p_z + 3d_{z^2} \rightarrow 5$ tane sp^3d melez orbitali

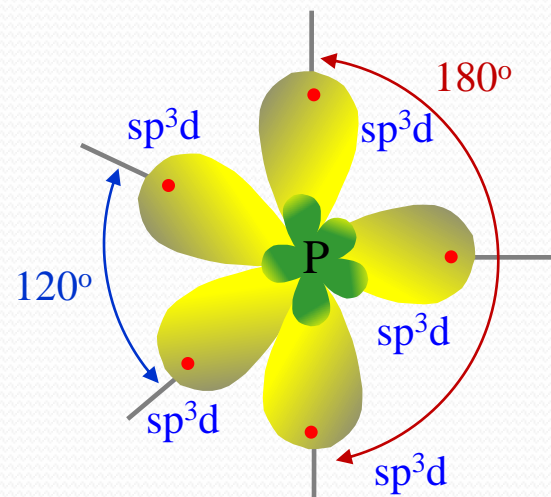
➤ PCl_5 molekülünün bağları, P atomunun 3s, 3p ve 3d atomik orbitallerinin kaynaşması ile oluşan sp^3d melez orbitalleri ile açıklanabilir.

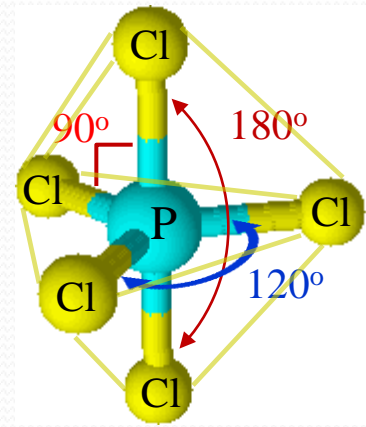
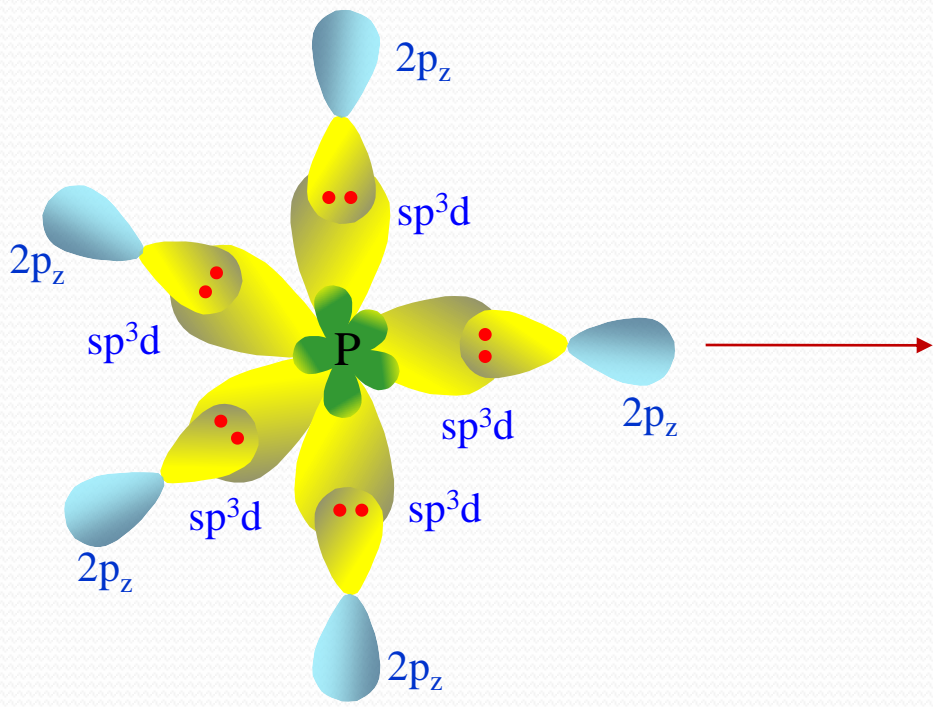
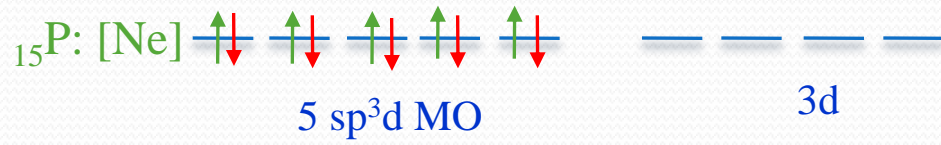


Temel Hal



Melez Hal





ÜÇGEN ÇİFTPİRAMİT

Pentahalojenürler

- Fosfor pentahalojenürlerde (PX_5), fosfor atomu sp^3d melezleşmesi yapar ve molekül üçgen çift piramit geometriye sahiptir.
- Pentahalojenürler, trihalojenürlerden daha az termik kararlılığa sahiptir.
- PCl_5 molekülü gaz fazında karardır. Katı fazda, $[PCl_4]^+[PCl_6]^-$ şeklinde iyonlar halinde bulunur.
- $PBr_5 \rightarrow [PBr_4]^+[PBr_6]^-$
- $PI_5 \rightarrow [PI_4]^+I^-$ şeklinde katı fazda iyonik halde bulunur.

