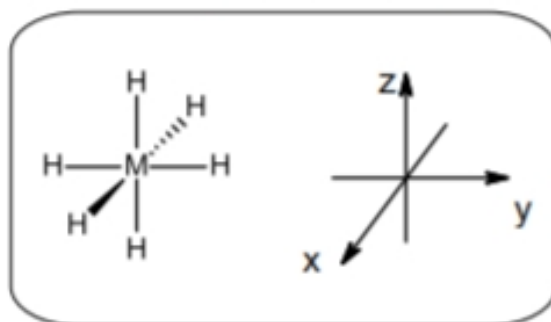
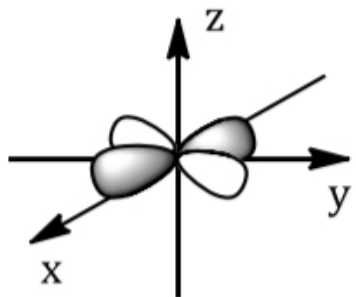


Méthode des fragments appliquée aux complexes octaédriques de métaux de transition

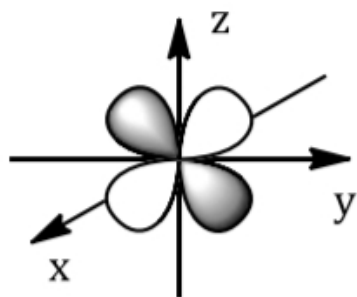
- Fragment 1 : Centre métallique M
- Fragment 2 : Ensemble des six ligands « H » disposés aux sommets de l'octaèdre.



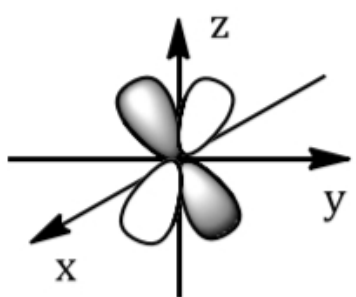
Système d'axes choisi



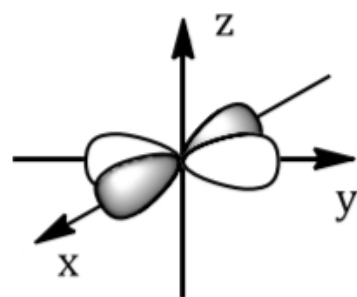
$(n-1)d_{xy}$



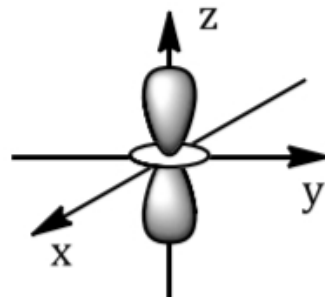
$(n-1)d_{yz}$



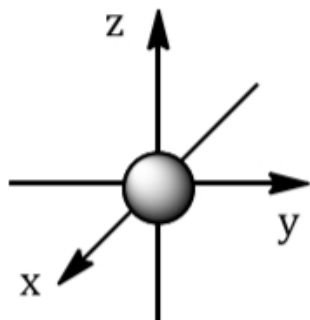
$(n-1)d_{xz}$



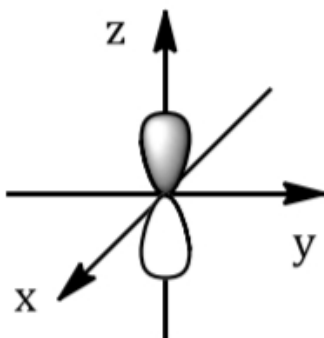
$(n-1)d_{x^2-y^2}$



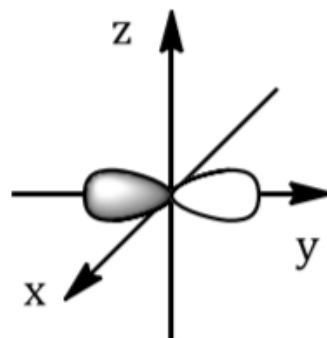
$(n-1)d_{z^2}$



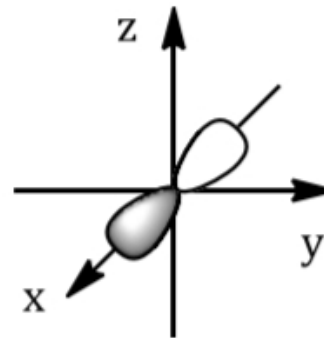
ns



np_z



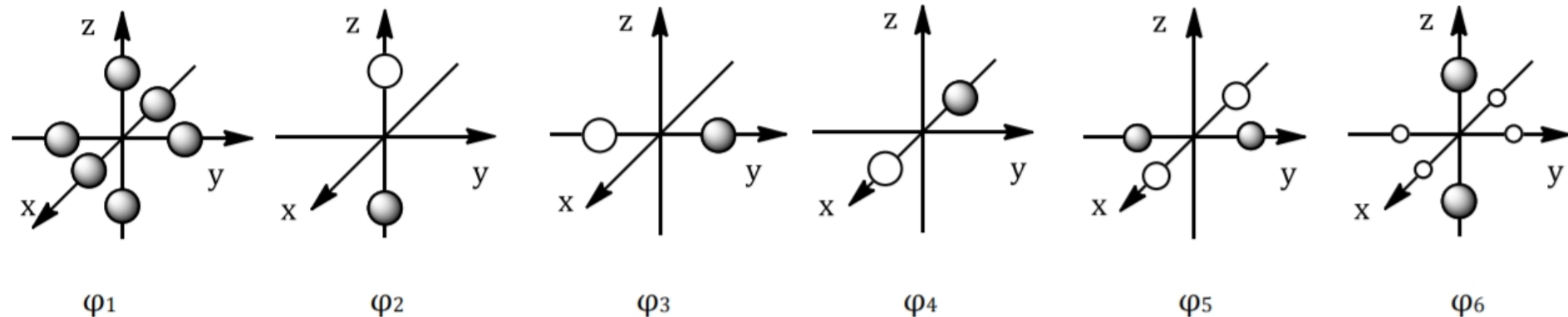
np_y



np_x

	ns	(n-1)d _{xy}	(n-1)d _{yz}	(n-1)d _{xz}	(n-1)d _{z²}	(n-1)d _{x²-y²}	np _x	np _y	np _z
Plan (xy)	S	S	A	A	S	S	S	S	A
Plan (yz)	S	A	S	A	S	S	A	S	S
Plan (xz)	S	A	A	S	S	S	S	A	S
Rotation (x)	S	A	S	A	S	S	S	A	A
Rotation (y)	S	A	A	S	S	S	A	S	A
Rotation (z)	S	S	A	A	S	S	A	A	S

Les OM du fragment H_6 sont représentées ci-dessous :

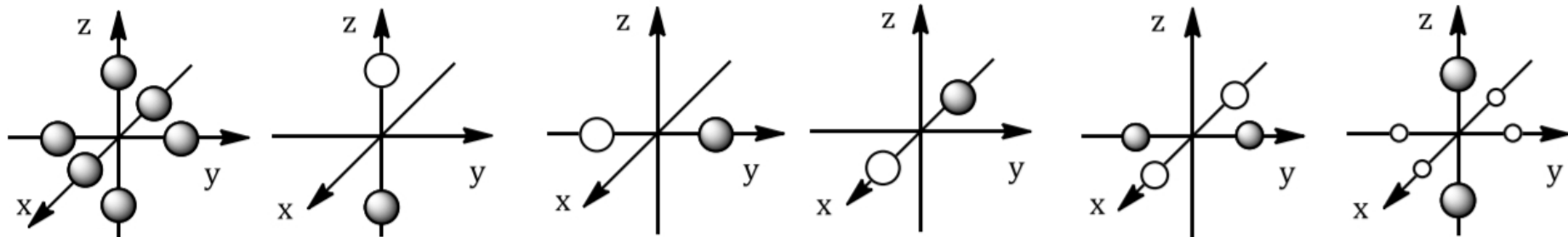
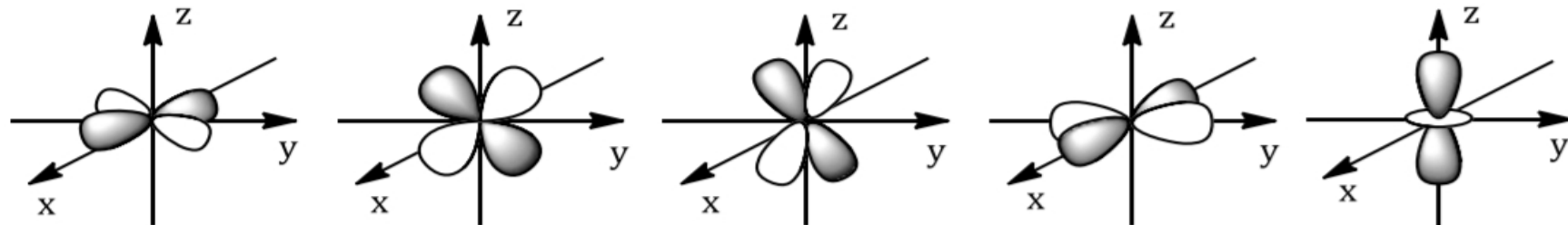
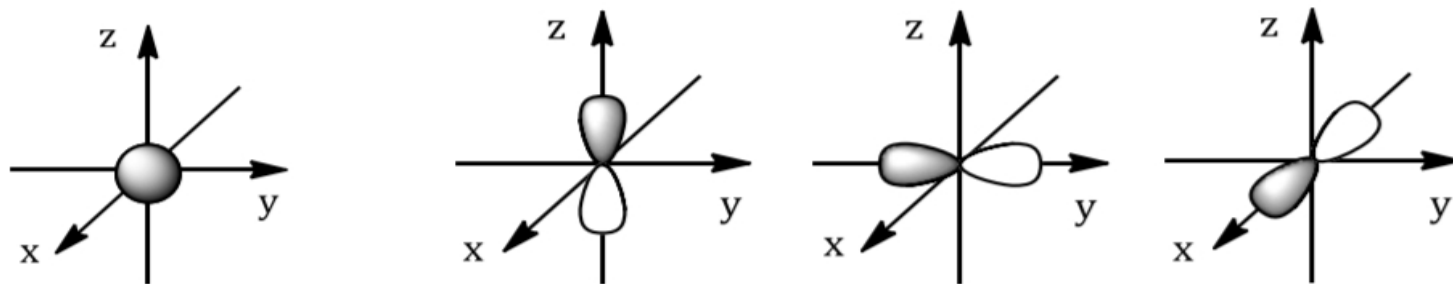


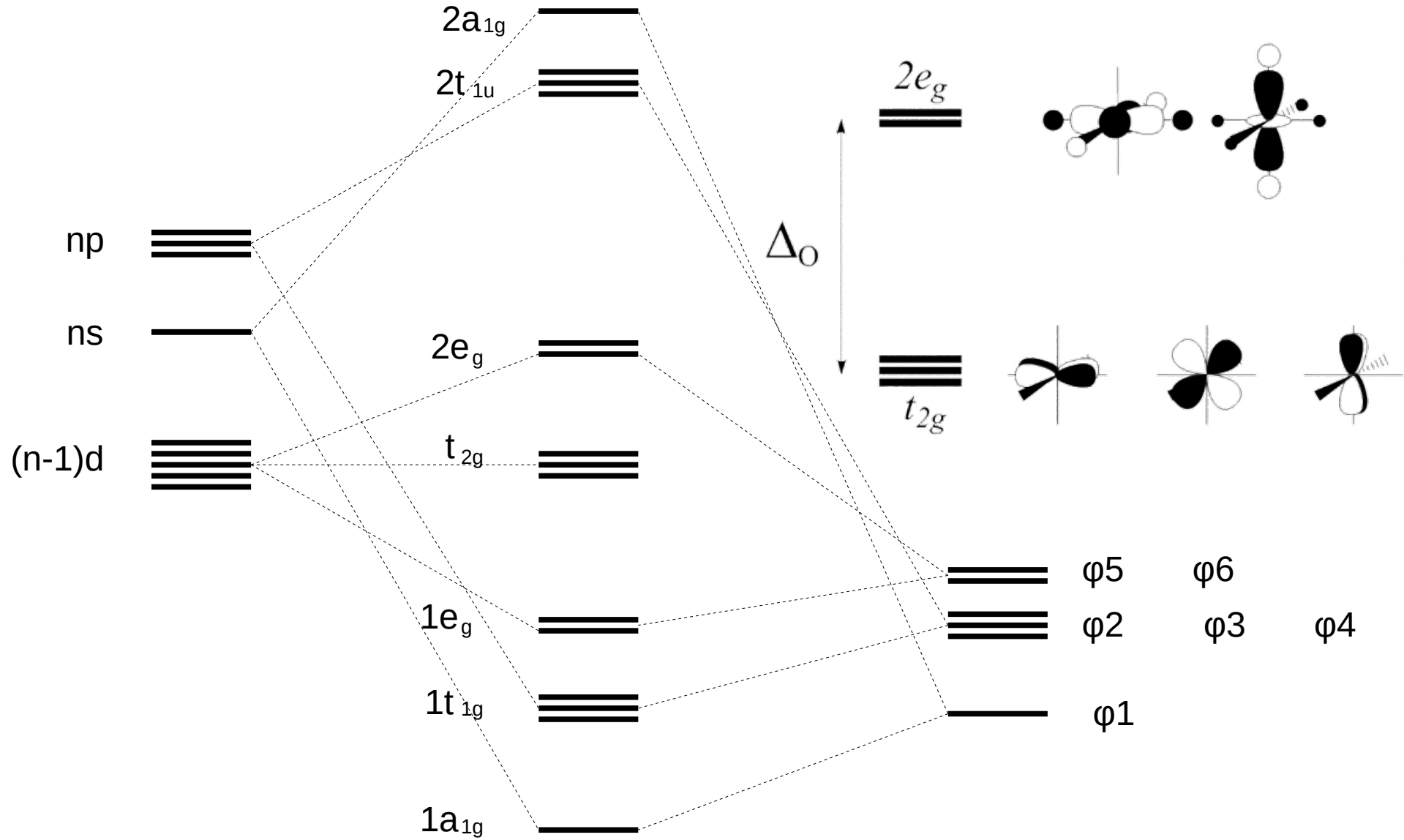
	ϕ_1	ϕ_2	ϕ_3	ϕ_4	ϕ_5	ϕ_6
Plan (xy)						
Plan (yz)						
Plan (xz)						
Rotation (M_x)						
Rotation (M_y)						
Rotation (M_z)						

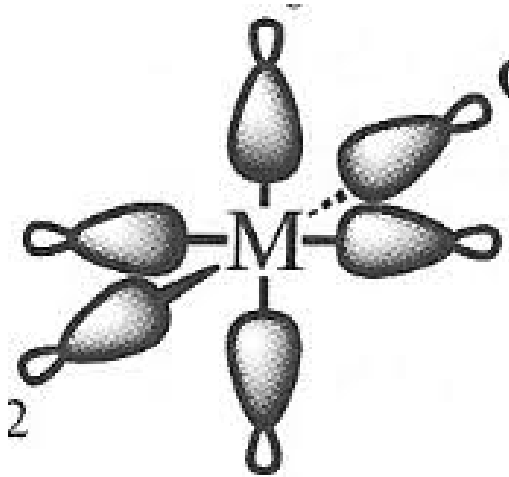
	φ_1	φ_2	φ_3	φ_4	φ_5	φ_6
Plan (xy)	S	A	S	S	S	S
Plan (yz)	S	S	S	A	S	S
Plan (xz)	S	S	A	S	S	S
Rotation (Mx)	S	A	A	S	S	S
Rotation (My)	S	A	S	A	S	S
Rotation (Mz)	S	S	A	A	S	S

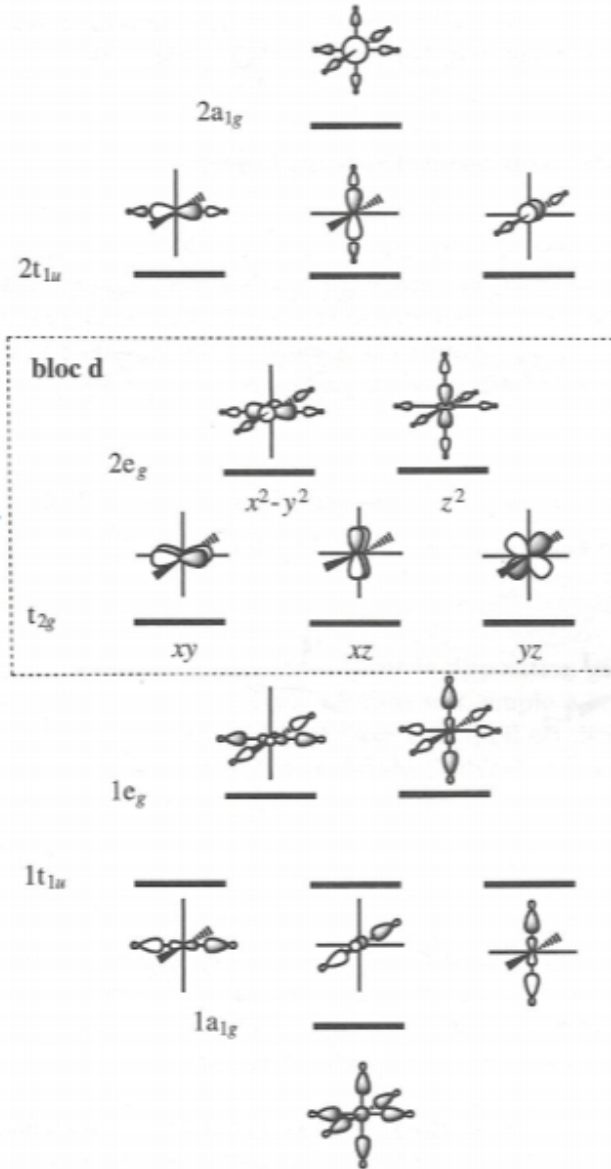
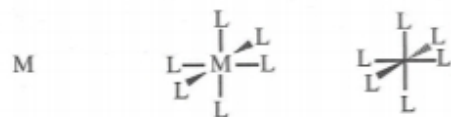
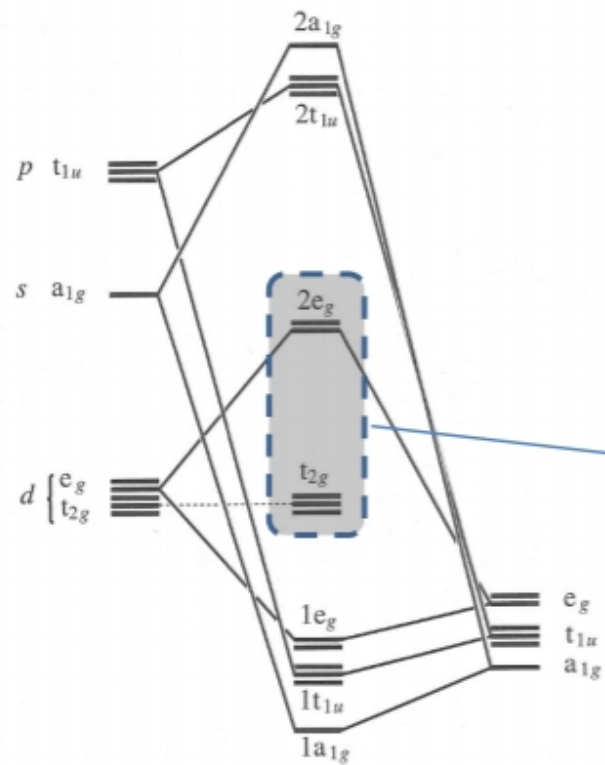
	ns	(n-1)d _{xy}	(n-1)d _{yz}	(n-1)d _{xz}	(n-1)d _{z²}	(n-1)d _{x²-y²}	np _x	np _y	np _z
Plan (xy)	S	S	A	A	S	S	S	S	A
Plan (yz)	S	A	S	A	S	S	A	S	S
Plan (xz)	S	A	A	S	S	S	S	A	S
Rotation (x)	S	A	S	A	S	S	S	A	A
Rotation (y)	S	A	A	S	S	S	A	S	A
Rotation (z)	S	S	A	A	S	S	A	A	S

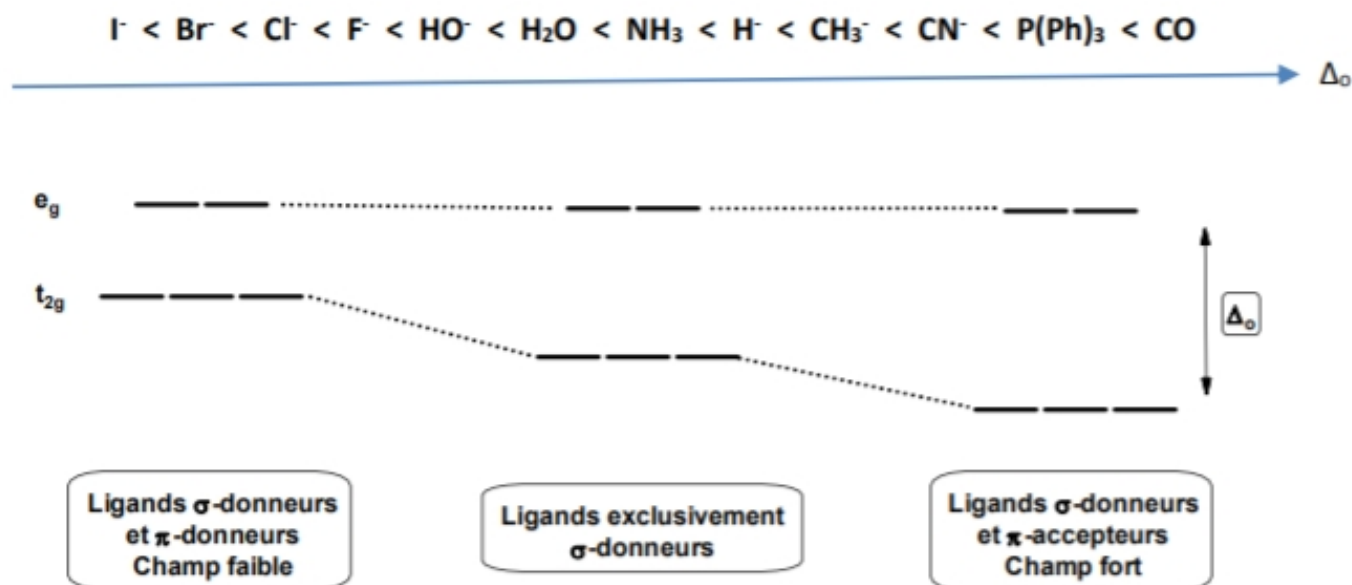
	φ_1	φ_2	φ_3	φ_4	φ_5	φ_6
Plan (xy)	S	A	S	S	S	S
Plan (yz)	S	S	S	A	S	S
Plan (xz)	S	S	A	S	S	S
Rotation (Mx)	S	A	A	S	S	S
Rotation (My)	S	A	S	A	S	S
Rotation (Mz)	S	S	A	A	S	S


 φ_1
 φ_2
 φ_3
 φ_4
 φ_5
 φ_6

 $(n-1)d_{xy}$
 $(n-1)d_{yz}$
 $(n-1)d_{xz}$
 $(n-1)d_{x^2-y^2}$
 $(n-1)d_{z^2}$

 ns
 np_z
 np_y
 np_x









Deux complexes impliquant l'ion Ti^{3+} , $[Ti(H_2O)_6]^{3+}$ et $[TiF_6]^{3-}$, absorbent dans le visible. Les longueurs d'onde absorbées pour la promotion d'un électron du niveau inférieur vers le niveau supérieur du bloc d valent 492 et 546 nm. Attribuer à chaque complexe « sa » longueur d'onde

