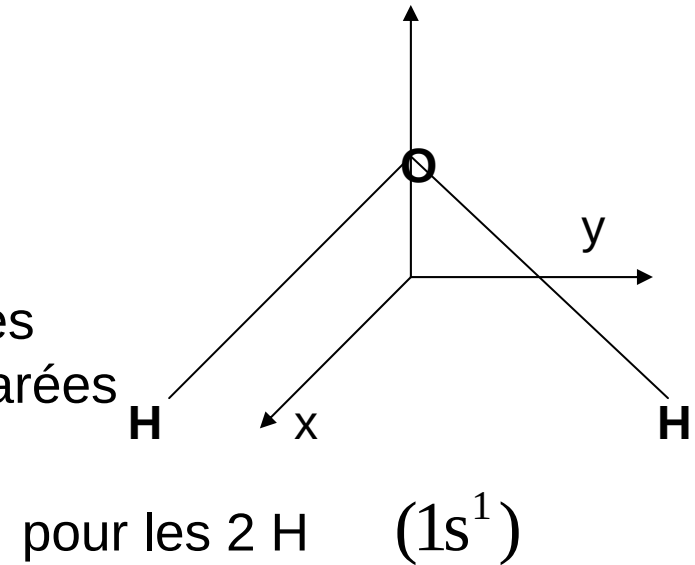
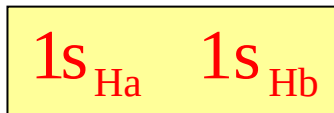


Molécules polyatomiques

H₂O:

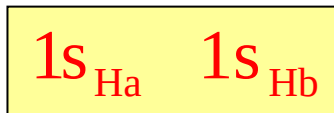
Base dite `minimale`: ensemble d'OA des couches occupées dans les atomes séparés



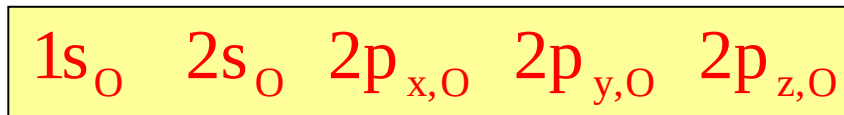
Molécules polyatomiques

H₂O:

Base dite `minimale`: ensemble d'OA des couches occupées dans les atomes séparées



pour les 2 H ($1s^1$)

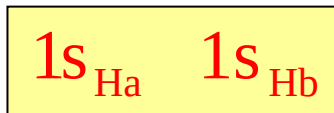


pour O ($1s^2 2s^2 2p^4$)

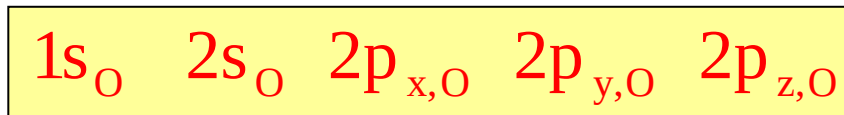
Molécules polyatomiques

H₂O:

Base dite `minimale`: ensemble d'OA des couches occupées dans les atomes séparées



pour les 2 H ($1s^1$)

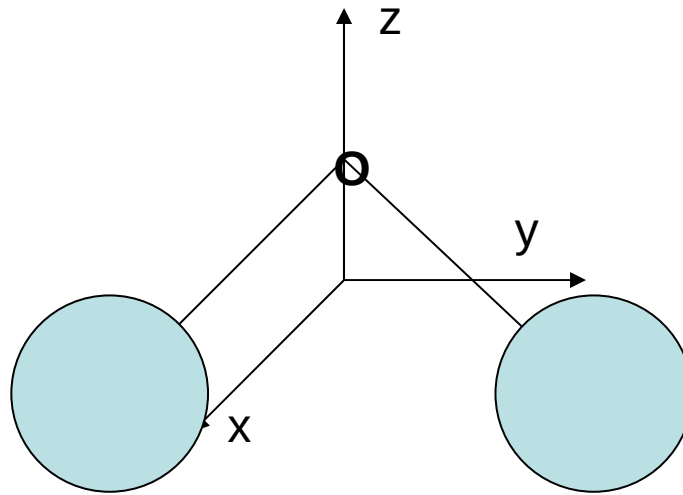


pour O ($1s^2 2s^2 2p^4$)

(**Note**: concept applicable aux molécules AB aussi)

Molécules polyatomiques

H₂O:

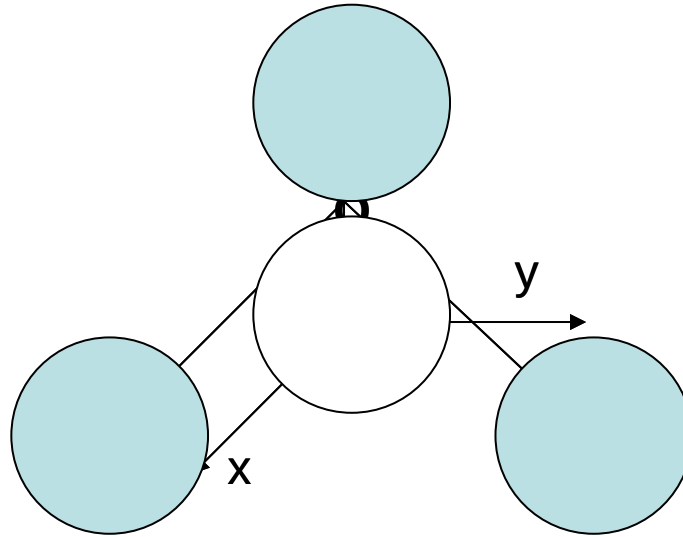


Orbitales de symétrie:

$$1s_{\text{Ha}} + 1s_{\text{Hb}}$$

Molécules polyatomiques

H₂O:



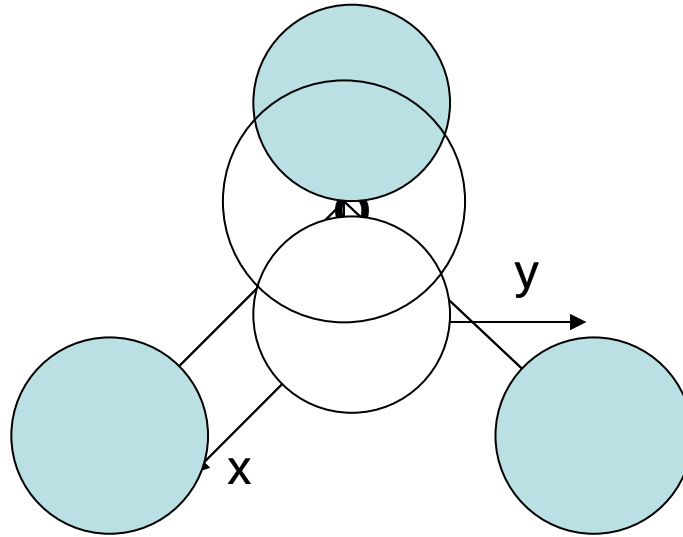
Orbitales de symétrie:

$1s_{\text{Ha}} + 1s_{\text{Hb}}$

$1s_{\text{O}} \quad 2s_{\text{O}} \quad 2p_{z,\text{O}}$

Molécules polyatomiques

H₂O:



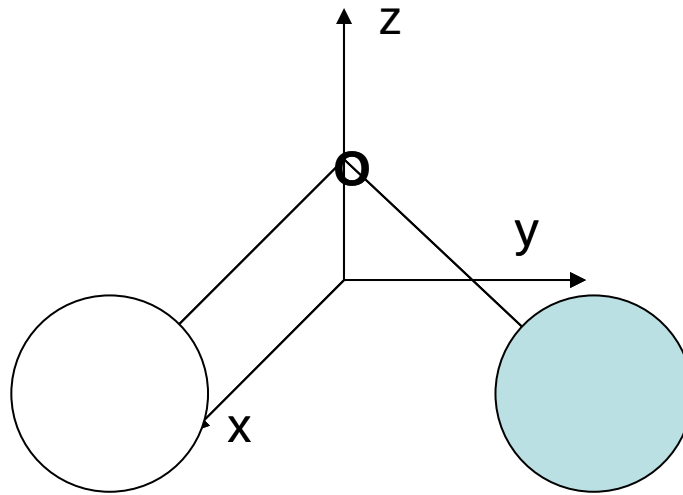
Orbitales de symétrie:

$1s_{\text{Ha}} + 1s_{\text{Hb}}$

$1s_{\text{O}} \quad 2s_{\text{O}} \quad 2p_{z,\text{O}}$

Molécules polyatomiques

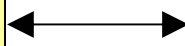
H₂O:



Orbitales de symétrie:

$$1s_{\text{Ha}} + 1s_{\text{Hb}}$$

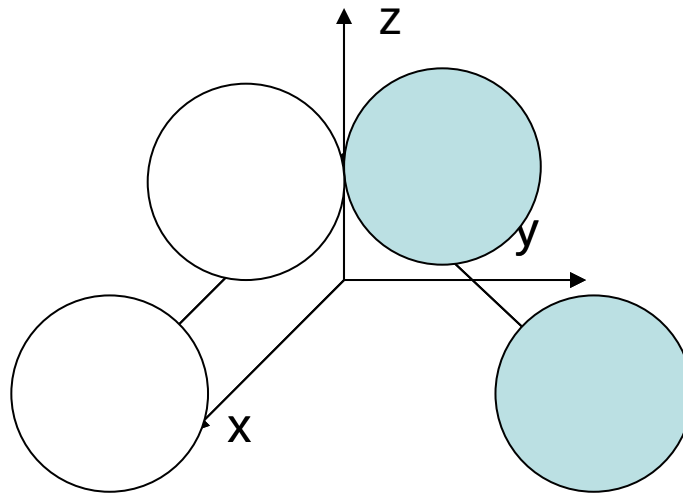
$$1s_{\text{O}} \quad 2s_{\text{O}} \quad 2p_{z,\text{O}}$$



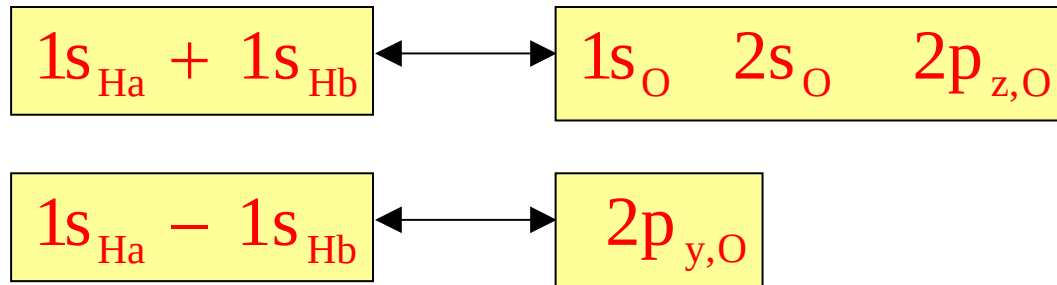
$$1s_{\text{Ha}} - 1s_{\text{Hb}}$$

Molécules polyatomiques

H₂O:

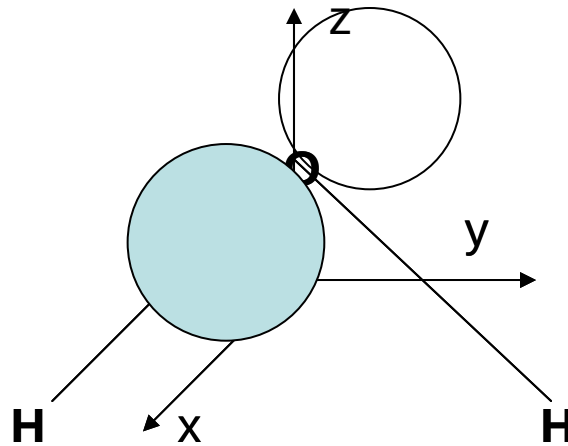


Orbitales de symétrie:

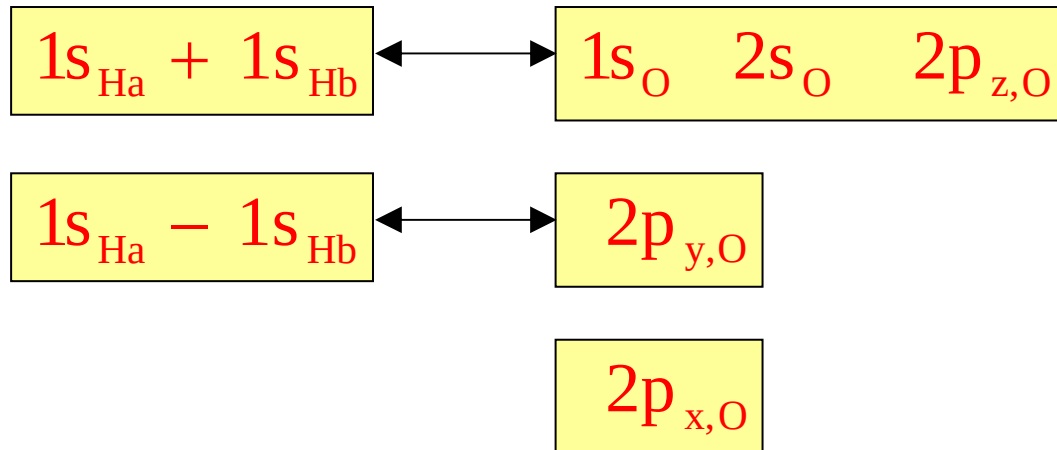


Molécules polyatomiques

H₂O:

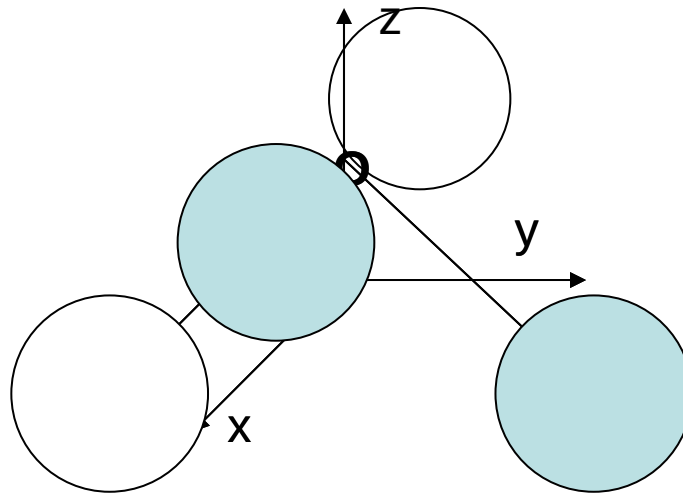


Orbitales de symétrie:

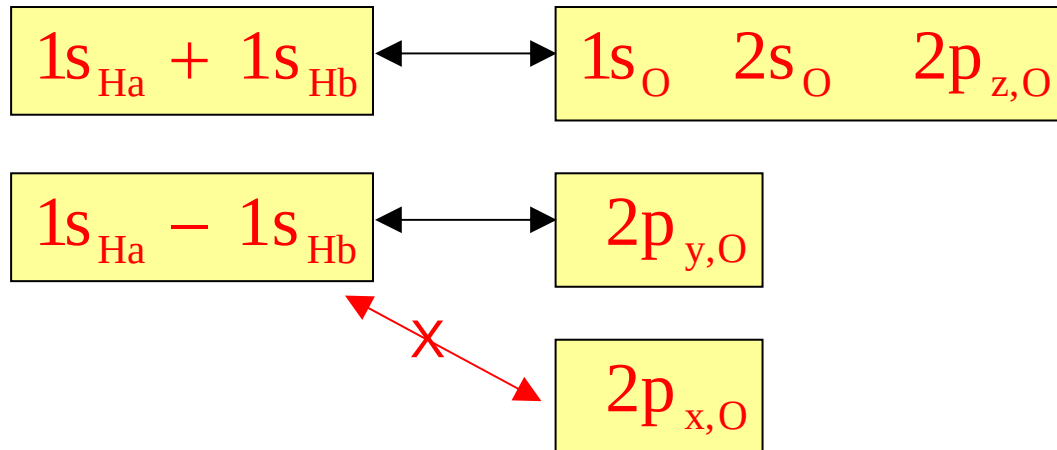


Molécules polyatomiques

H₂O:

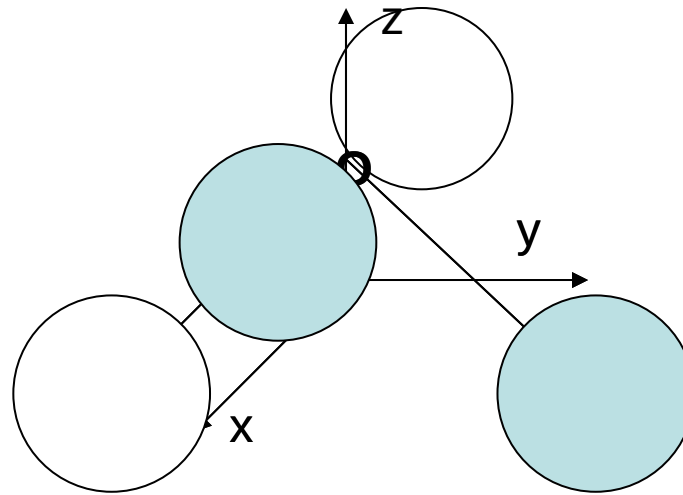


Orbitales de symétrie:



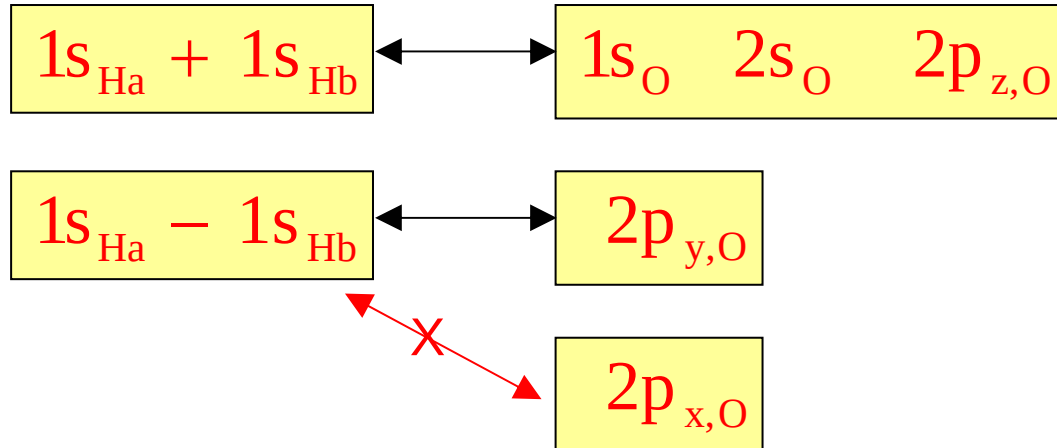
Molécules polyatomiques

H₂O:



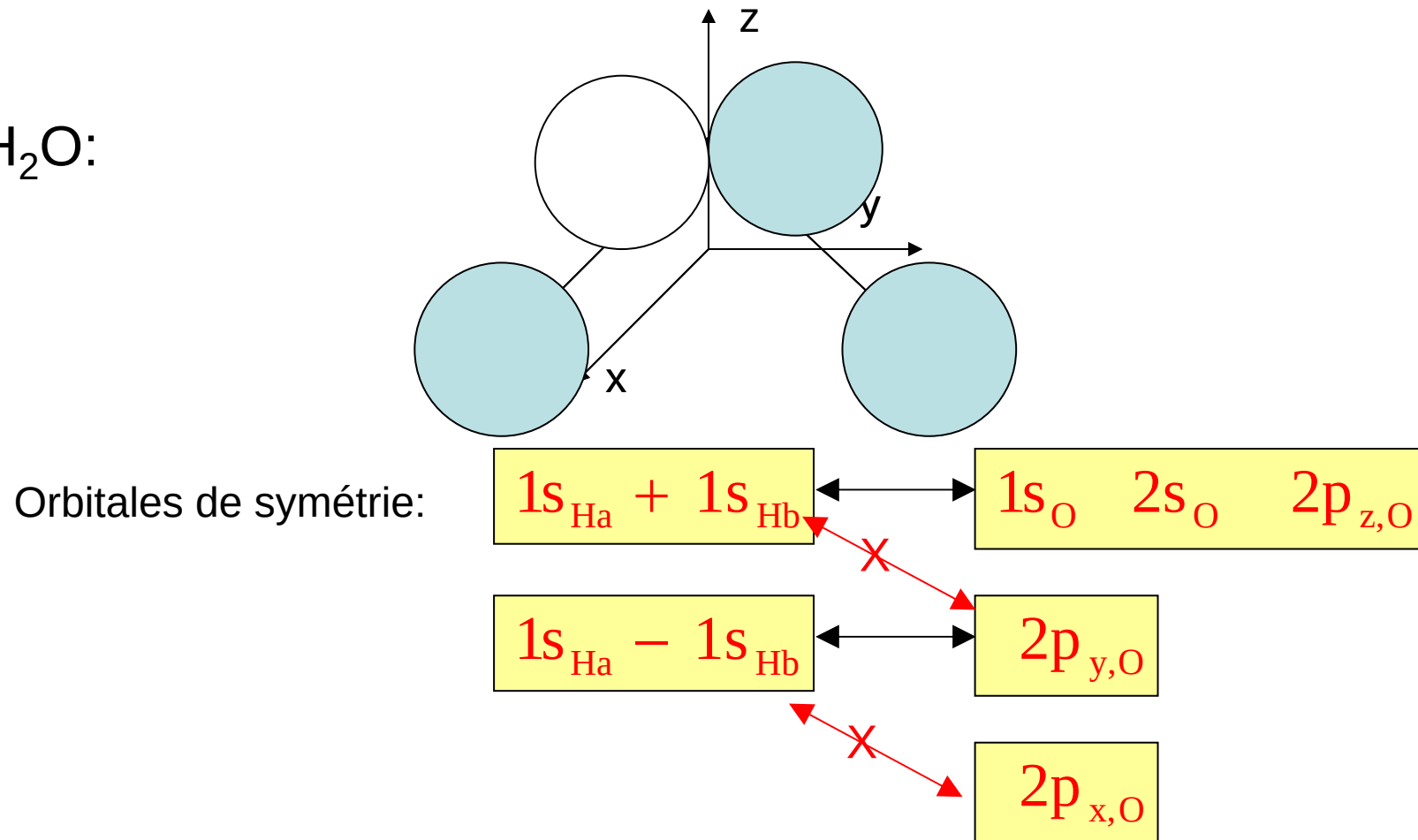
$$S_{AB}=0$$

Orbitales de symétrie:



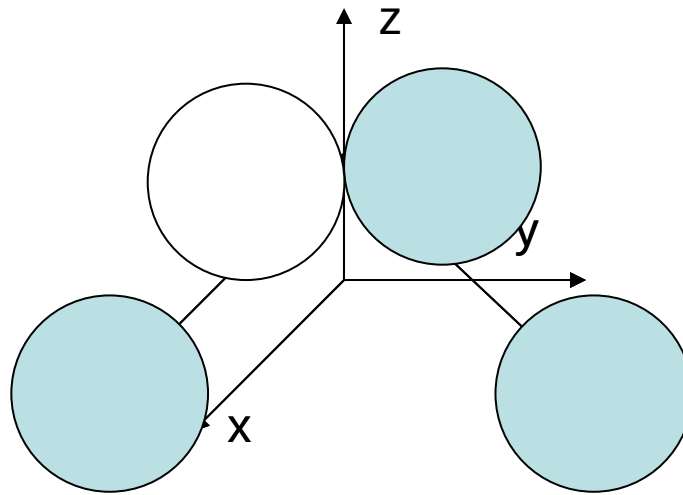
Molécules polyatomiques

H₂O:



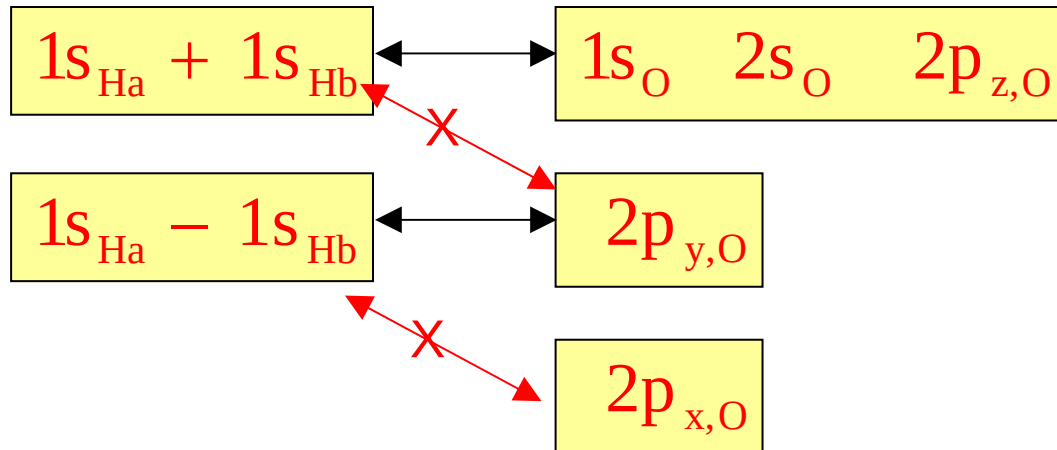
Molécules polyatomiques

H₂O:



$$S_{AB}=0$$

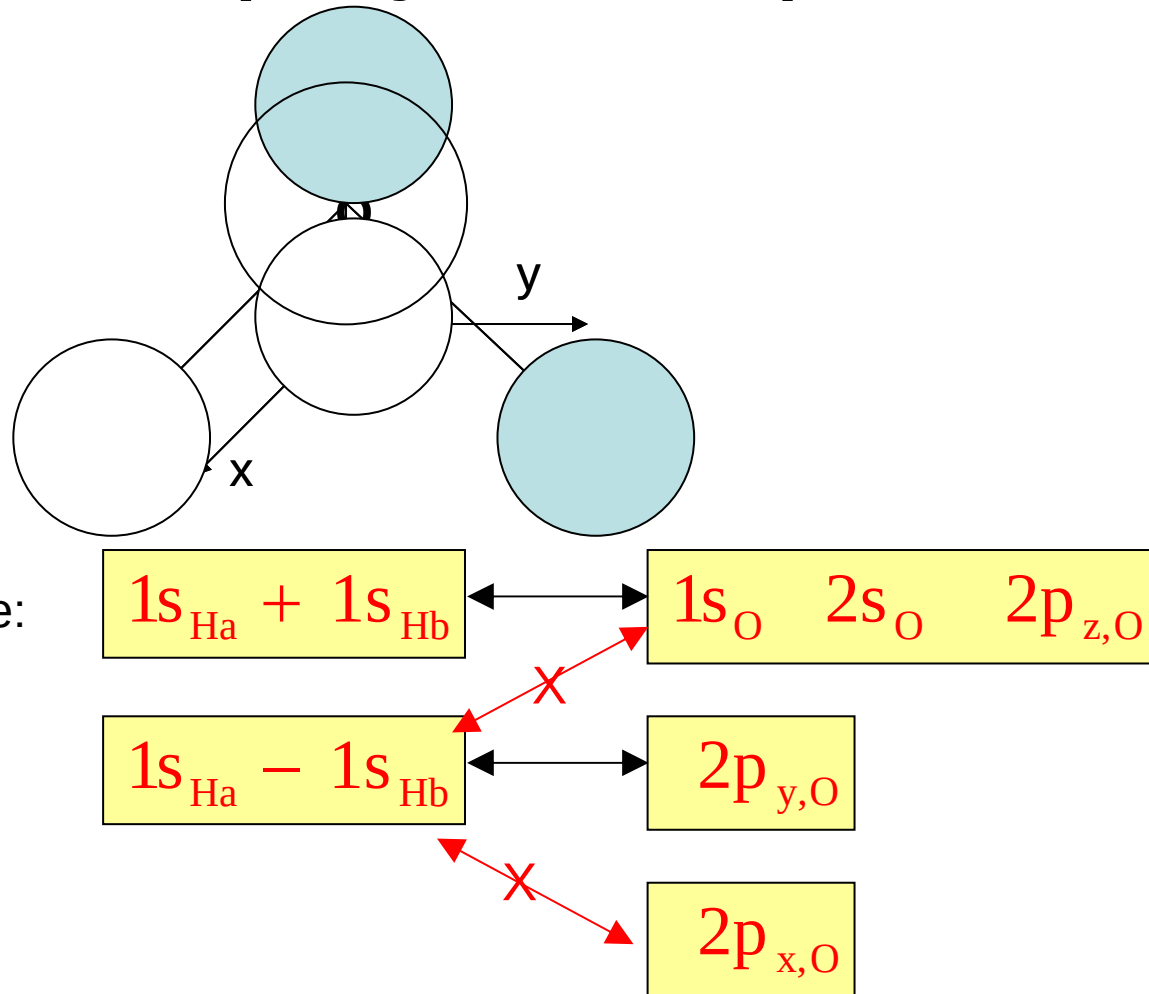
Orbitales de symétrie:



Molécules polyatomiques

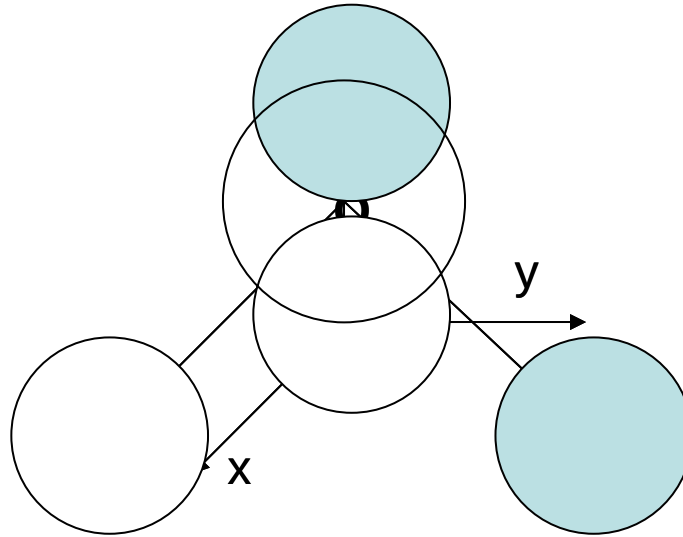
H₂O:

Orbitales de symétrie:



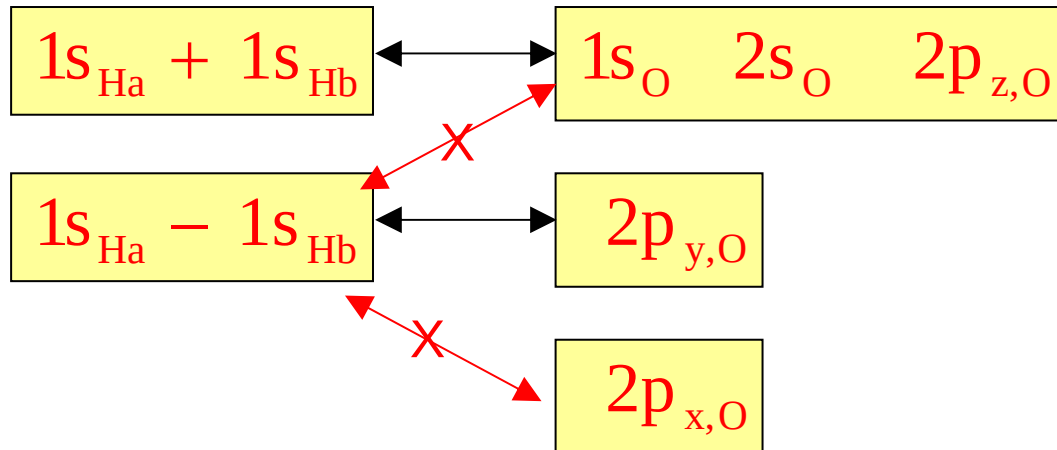
Molécules polyatomiques

H₂O:



$$S_{AB}=0$$

Orbitales de symétrie:



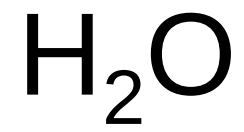
Molécules polyatomiques

H₂O:

Ordre énergétiques des OA :

$$1s_{\text{O}} \ll 2s_{\text{O}} \quad 2p_{z,\text{O}}$$

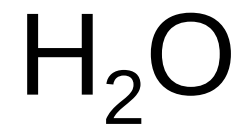
$$1s_{\text{H}} \approx 2s_{\text{O}} \quad 2p_{z,\text{O}}$$



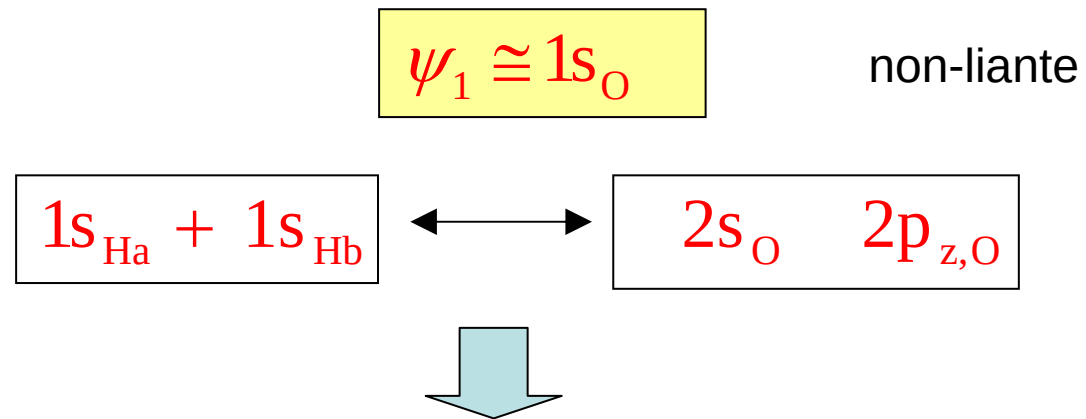
Orbitales moléculaires :

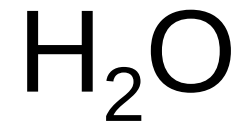
$$\psi_1 \cong 1s_{\text{O}}$$

non-liante



Orbitales moléculaires :

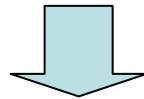
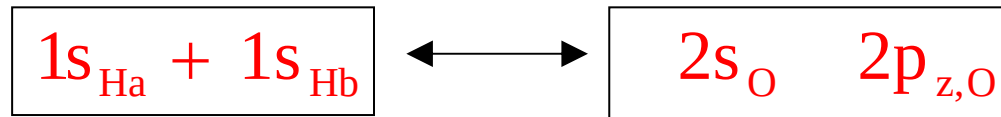




Orbitales moléculaires :

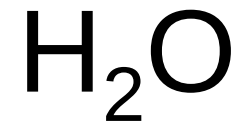
$$\psi_1 \cong 1s_O$$

non-liante



$$\psi_2 \cong (2s_O + 2p_{z,O}) + c(1s_{Ha} + 1s_{Hb})$$

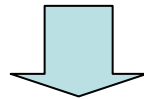
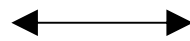
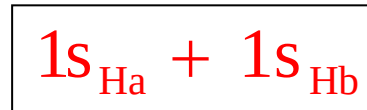
liante



Orbitales moléculaires :

$$\psi_1 \cong 1s_O$$

non-liante

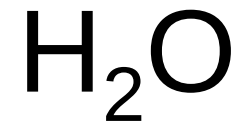


$$\psi_2 \cong (2s_O + 2p_{z,O}) + c(1s_{Ha} + 1s_{Hb})$$

liante

$$\psi_4 \cong (2s_O + 2p_{z,O})$$

non-liante

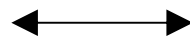


Orbitales moléculaires :

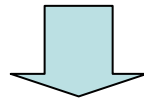
$$\psi_1 \cong 1s_O$$

non-liante

$$1s_{Ha} + 1s_{Hb}$$



$$2s_O \quad 2p_{z,O}$$



$$\psi_2 \cong (2s_O + 2p_{z,O}) + c(1s_{Ha} + 1s_{Hb})$$

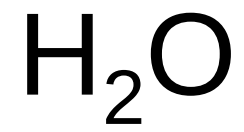
liante

$$\psi_4 \cong (2s_O + 2p_{z,O})$$

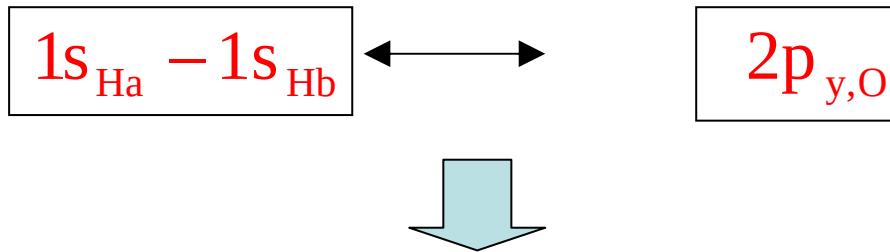
non-liante

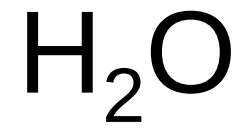
$$\psi_7 \cong (1s_{Ha} + 1s_{Hb}) - c(2s_O + 2p_{z,O})$$

anti-liante

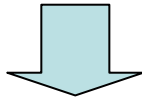
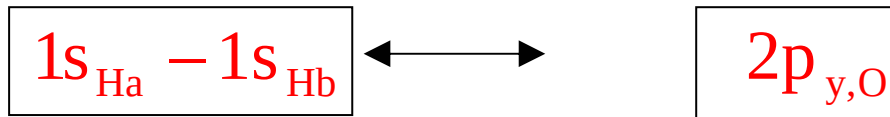


Orbitales moléculaires :



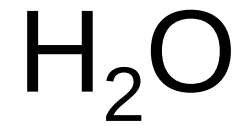


Orbitales moléculaires :

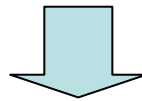
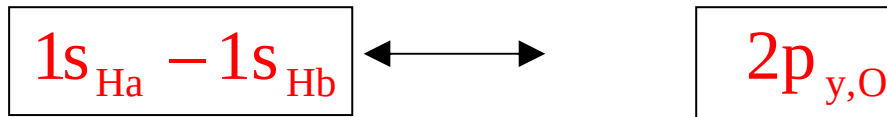


$$\boxed{\psi_3 \cong 2p_{y,\text{O}} + c(1s_{\text{Ha}} - 1s_{\text{Hb}})}$$

liante



Orbitales moléculaires :

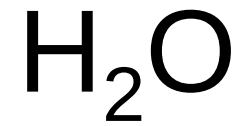


$$\psi_3 \cong 2p_{y,\text{O}} + c(1s_{\text{Ha}} - 1s_{\text{Hb}})$$

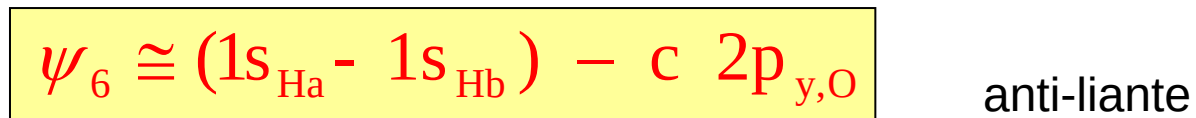
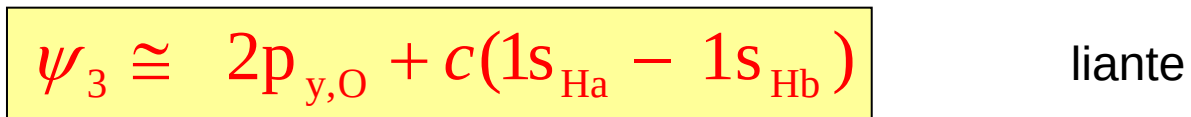
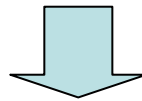
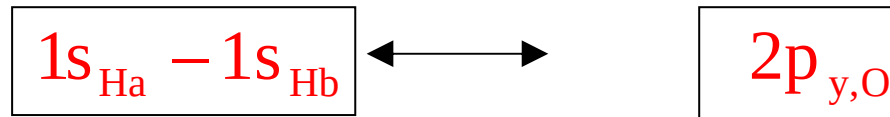
liante

$$\psi_6 \cong (1s_{\text{Ha}} - 1s_{\text{Hb}}) - c 2p_{y,\text{O}}$$

anti-liante



Orbitales moléculaires :



Il reste



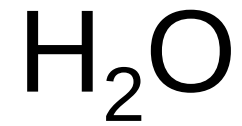


Diagramme de corrélation: (voir notes de cours, fig.4.15)
avec

$$\begin{aligned}\psi_1 &\leftrightarrow 1a_1 \\ \psi_2 &\leftrightarrow 2a_1 \\ \psi_4 &\leftrightarrow 3a_1 \\ \psi_7 &\leftrightarrow 4a_1\end{aligned}$$

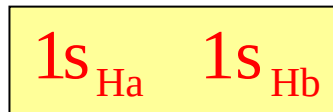
$$\begin{aligned}\psi_3 &\leftrightarrow 1b_2 \\ \psi_6 &\leftrightarrow 2b_2\end{aligned}$$

$$\psi_5 \leftrightarrow 1b_1$$

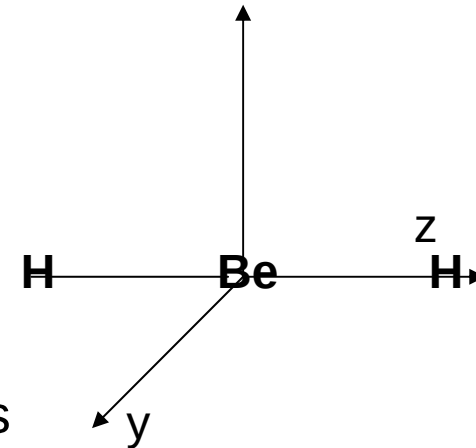
Molécules polyatomiques



Base dite `minimale`: ensemble d'OA des couches occupées dans les atomes séparées



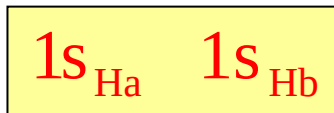
pour les 2 H ($1s^1$)



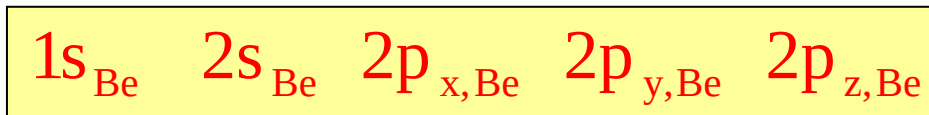
Molécules polyatomiques



Base dite `minimale`: ensemble d'OA des couches occupées dans les atomes séparées



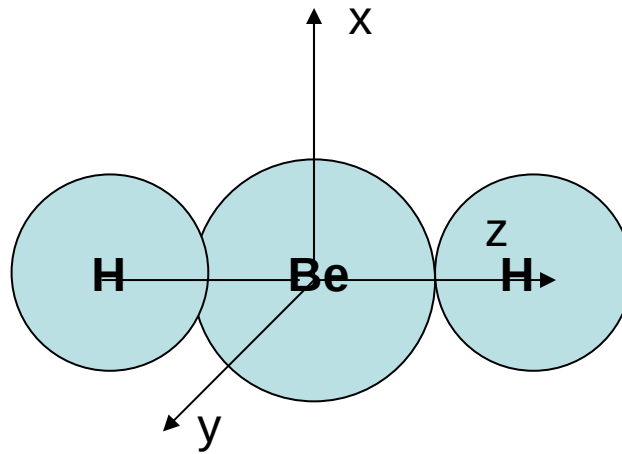
pour les 2 H $(1s^1)$



pour Be $(1s^2 2s^2)$

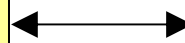
Molécules polyatomiques

BeH₂



Orbitales de symétrie:

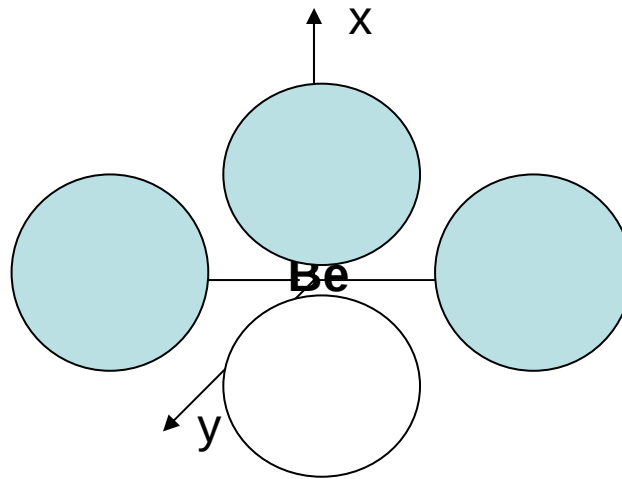
$1s_{\text{Ha}} + 1s_{\text{Hb}}$



$1s_{\text{Be}} \quad 2s_{\text{Be}}$

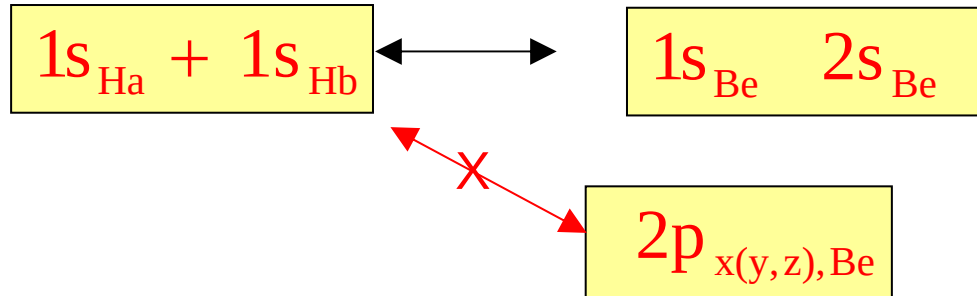
Molécules polyatomiques

BeH₂



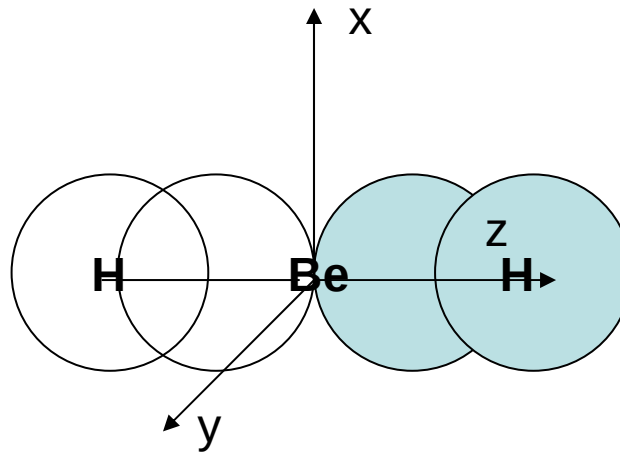
$$S_{AB}=0$$

Orbitales de symétrie:

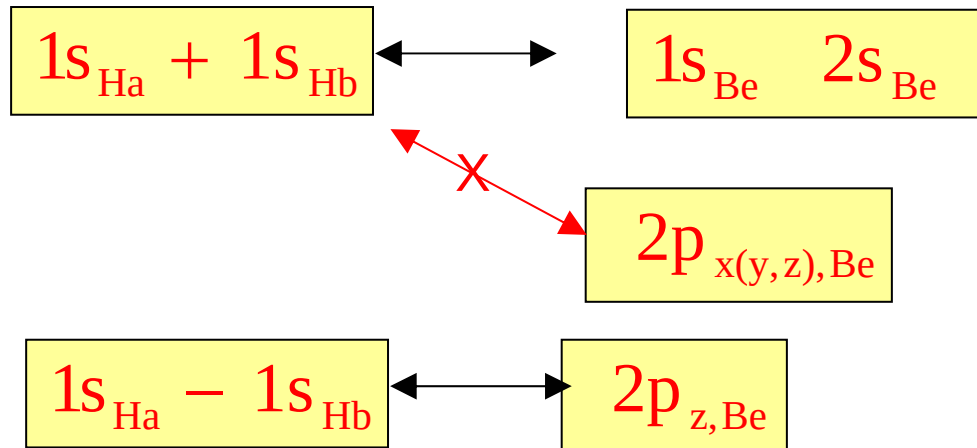


Molécules polyatomiques

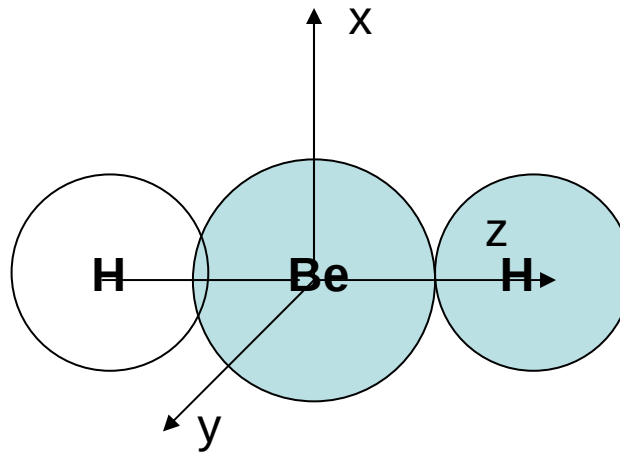
BeH₂



Orbitales de symétrie:

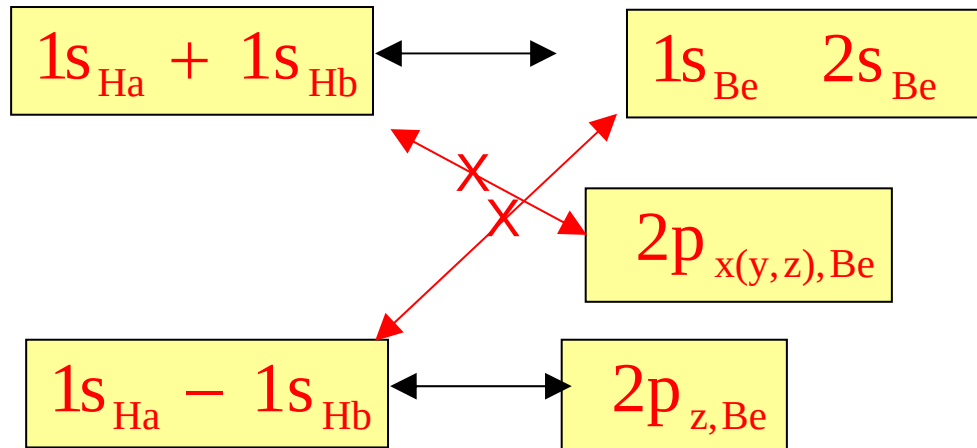


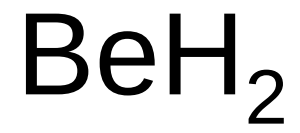
Molécules polyatomiques



$$S_{AB}=0$$

Orbitales de symétrie:





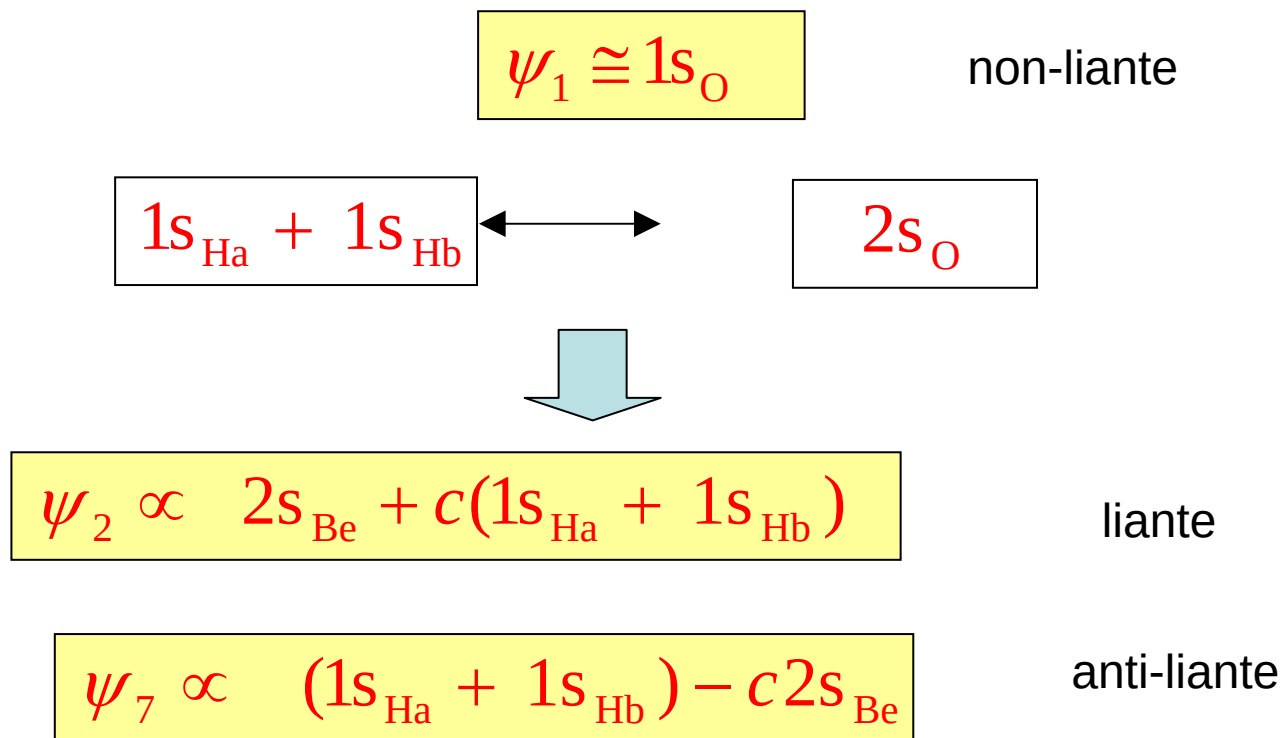
Orbitales moléculaires :

$$\psi_1 \cong 1s_{\text{Be}}$$

non-liante

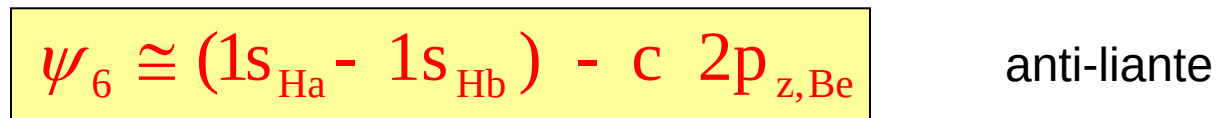
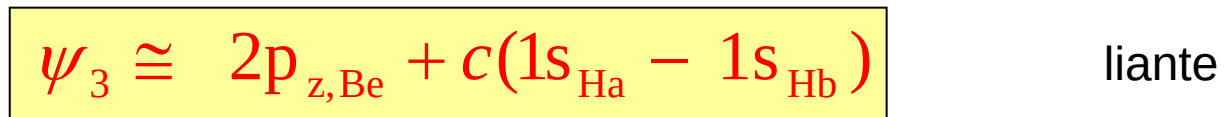
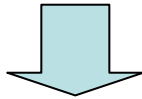
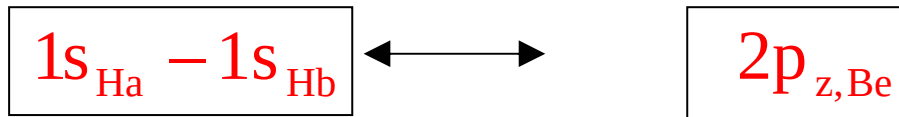


Orbitales moléculaires :

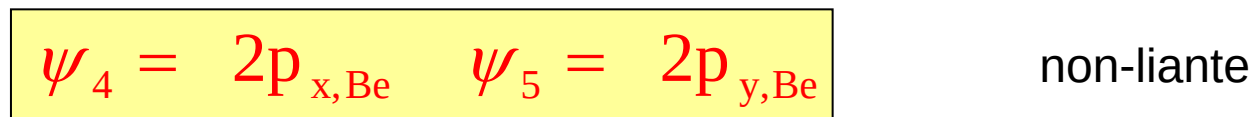




Orbitales moléculaires :

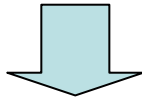
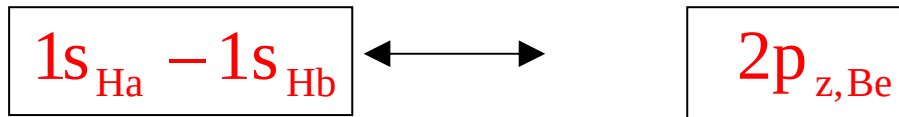


Il reste





Orbitales moléculaires :



$$\boxed{\psi_3 \cong 2p_{z,\text{Be}} + c(1s_{\text{Ha}} - 1s_{\text{Hb}})}$$

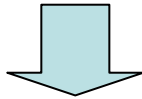
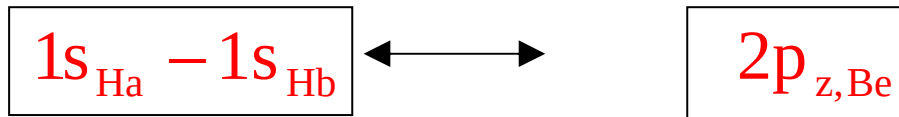
liante p.r. à Be-H_a **et** Be-H_b

$$\boxed{\psi_6 \cong (1s_{\text{Ha}} - 1s_{\text{Hb}}) - c 2p_{z,\text{Be}}}$$

anti-liante p.r. à Be-H_a **et** Be-H_b



Orbitales moléculaires :



$$\psi_3 \cong 2p_{z,\text{Be}} + c(1s_{\text{Ha}} - 1s_{\text{Hb}})$$

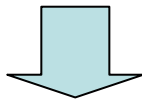
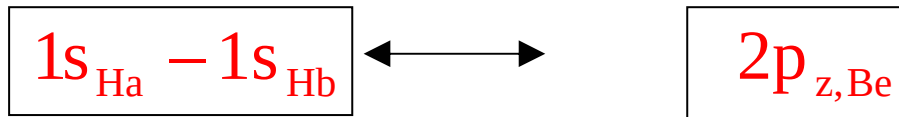
liante p.r. à Be-H_a **et** Be-H_b

$$\psi_2 \propto 2s_{\text{Be}} + c(1s_{\text{Ha}} + 1s_{\text{Hb}})$$

liante p.r. à Be-H_a **et** Be-H_b



Orbitales moléculaires :



$$\boxed{\psi_3 \cong 2p_{z,\text{Be}} + c(1s_{\text{Ha}} - 1s_{\text{Hb}})}$$

liante p.r. à Be-H_a **et** Be-H_b

$$\boxed{\psi_2 \propto 2s_{\text{Be}} + c(1s_{\text{Ha}} + 1s_{\text{Hb}})}$$

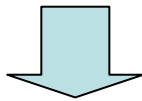
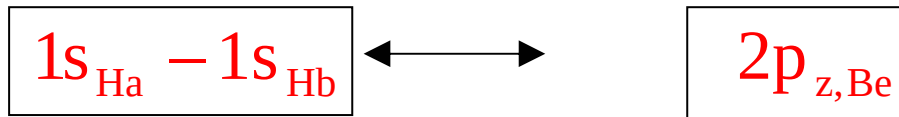
liante p.r. à Be-H_a **et** Be-H_b

$$\boxed{\psi_3 + \psi_2 \propto (2s_{\text{Be}} + 2p_{z,\text{Be}}) + 2c1s_{\text{Ha}}}$$

liante p.r. à Be-H_a



Orbitales moléculaires :



$$\psi_3 \cong 2p_{z,\text{Be}} + c(1s_{\text{Ha}} - 1s_{\text{Hb}})$$

liante p.r. à Be-H_a **et** Be-H_b

$$\psi_2 \propto 2s_{\text{Be}} + c(1s_{\text{Ha}} + 1s_{\text{Hb}})$$

liante p.r. à Be-H_a **et** Be-H_b

$$\psi_3 + \psi_2 \propto (2s_{\text{Be}} + 2p_{z,\text{Be}}) + 2c1s_{\text{Ha}}$$

liante p.r. à Be-H_a

$$\psi_2 - \psi_3 \propto (2s_{\text{Be}} - 2p_{z,\text{Be}}) + 2c1s_{\text{Hb}}$$

liante p.r. à Be-H_b



Orbitales moléculaires :

$$\psi_3 + \psi_2 \propto (2s_{\text{Be}} + 2p_{z,\text{Be}}) + 2c1s_{\text{Ha}}$$

liante p.r. à Be-H_a

$$\psi_2 - \psi_3 \propto (2s_{\text{Be}} - 2p_{z,\text{Be}}) + 2c1s_{\text{Hb}}$$

liante p.r. à Be-H_b

$$2sp_{\pm,\text{Be}} = (2s_{\text{Be}} \pm 2p_{z,\text{Be}})$$

Orbitales hybrides sp



Orbitales moléculaires :

$$\psi_3 + \psi_2 \propto (2s_{\text{Be}} + 2p_{z,\text{Be}}) + 2c1s_{\text{Ha}}$$

liante p.r. à Be-H_a

$$\psi_2 - \psi_3 \propto (2s_{\text{Be}} - 2p_{z,\text{Be}}) + 2c1s_{\text{Hb}}$$

liante p.r. à Be-H_b

$$2sp_{\pm,\text{Be}} = (2s_{\text{Be}} \pm 2p_{z,\text{Be}})$$

Orbitales hybrides sp

Orbitales hybrides

Permettent de décrire des OM de liaisons localisées

Orbitales hybrides

Permettent de décrire des OM de liaisons localisées

Ce sont des OA adaptées à une symétrie locale

Orbitales hybrides

Permettent de décrire des OM de liaisons localisées

Ce sont des OA adaptées à une symétrie locale

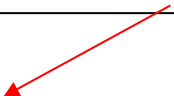
trois types d'OA hybrides: sp , sp^2 , sp^3

Orbitales hybrides

Permettent de décrire des OM de liaisons localisées

Ce sont des OA adaptées à une symétrie locale

trois types d'OA hybrides: sp , sp^2 , sp^3



linéaire

Orbitales hybrides

Permettent de décrire des OM de liaisons localisées

Ce sont des OA adaptées à une symétrie locale

trois types d'OA hybrides: sp , sp^2 , sp^3

↓
trigonal

Orbitales hybrides

Permettent de décrire des OM de liaisons localisées

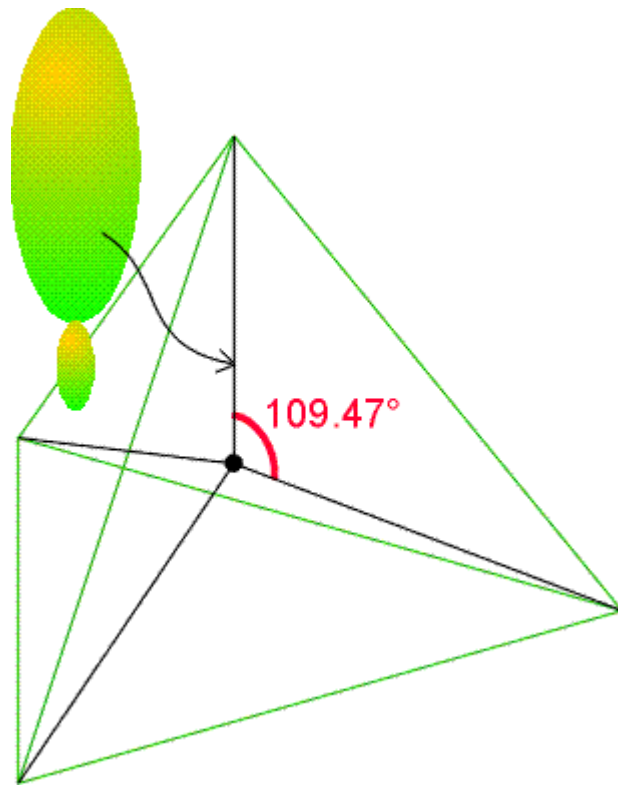
Ce sont des OA adaptées à une symétrie locale

trois types d'OA hybrides: sp , sp^2 , sp^3

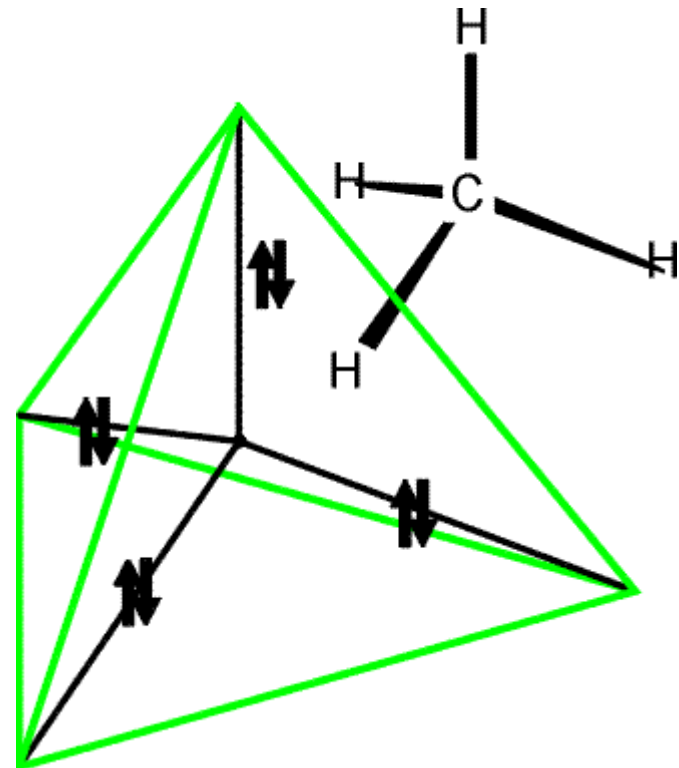


tétraédrique

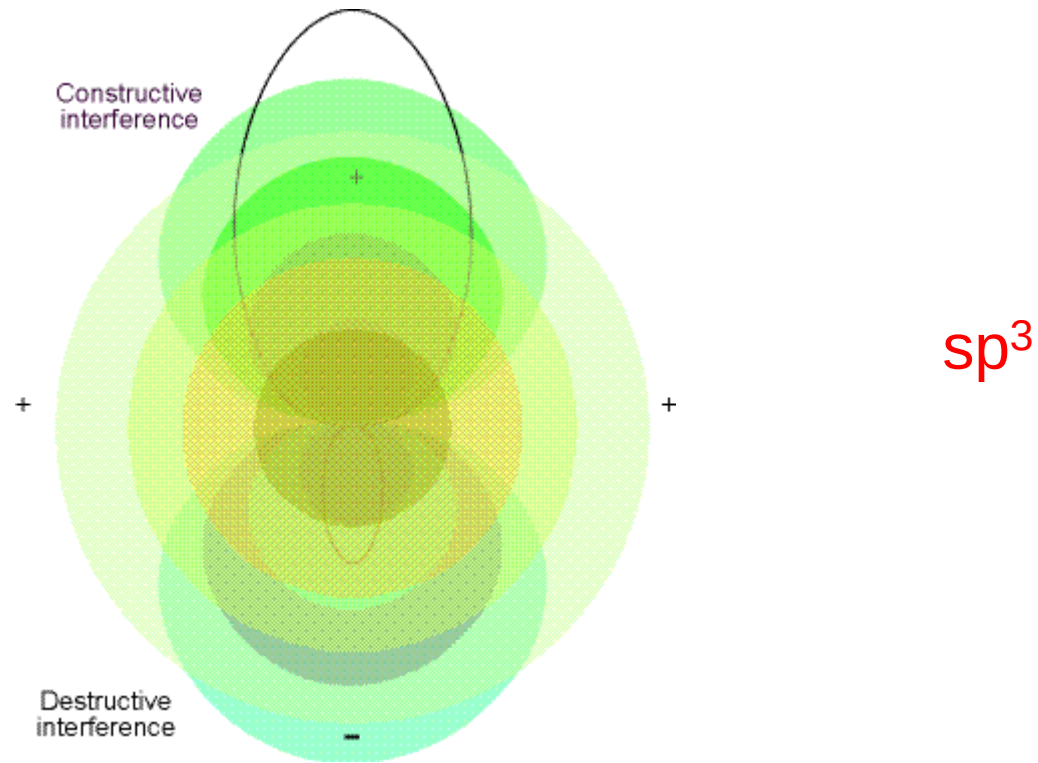
Orbitales hybrides



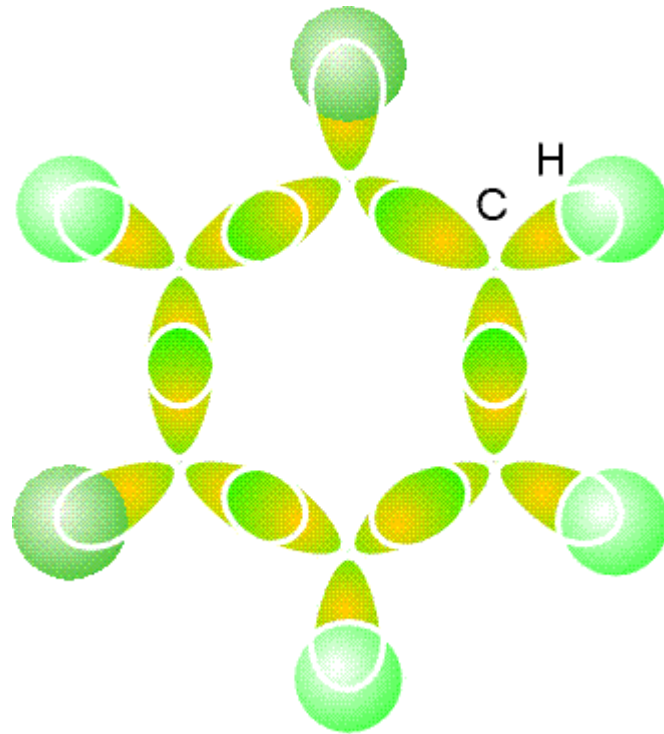
sp^3



Orbitales hybrides



Orbitales hybrides

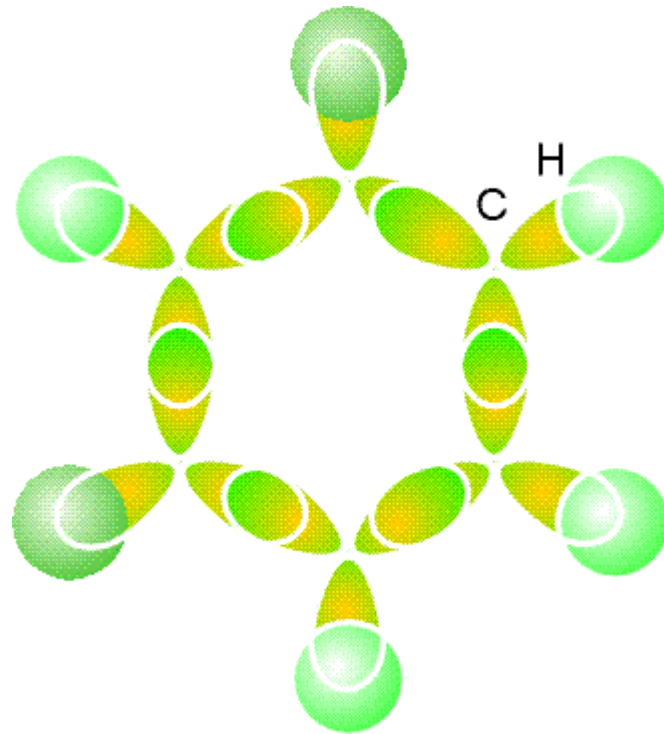


utilisation d'OA hybrides

sp^2

dans la description des
liaisons σ du benzène

Orbitales hybrides



utilisation d'OA hybrides

sp^2

dans la description des
liaisons σ du benzène

$$\sigma_{CH} \cong 2sp_{i,C}^2 + c\,1s$$

$$\sigma_{CH}^* \cong -c\,2sp_{i,C}^2 + 1s$$