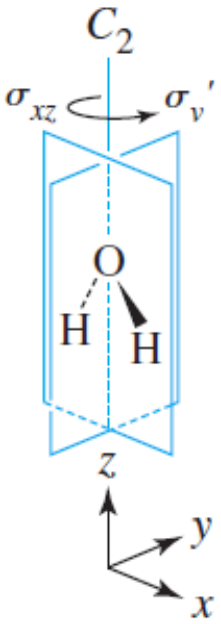

C_2
σ_{xz}
σ_v'
O
H
H
z
y
x

C_{2v} Character Table

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	R_z	xy
B_1	1	−1	1	−1	x, R_y	xz
B_2	1	−1	−1	1	y, R_x	yz

Determine symmetry properties for Hydrogen group orbitals of H_2O

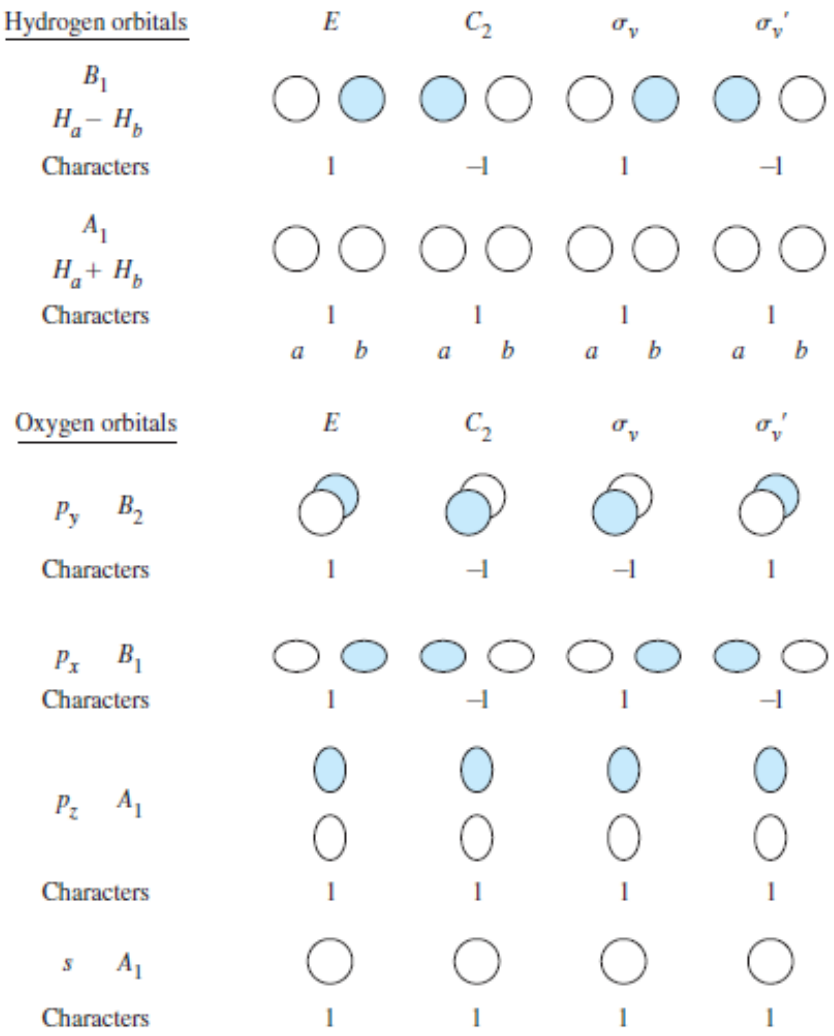
The reducible representation $\Gamma = A_1 + B_1$:

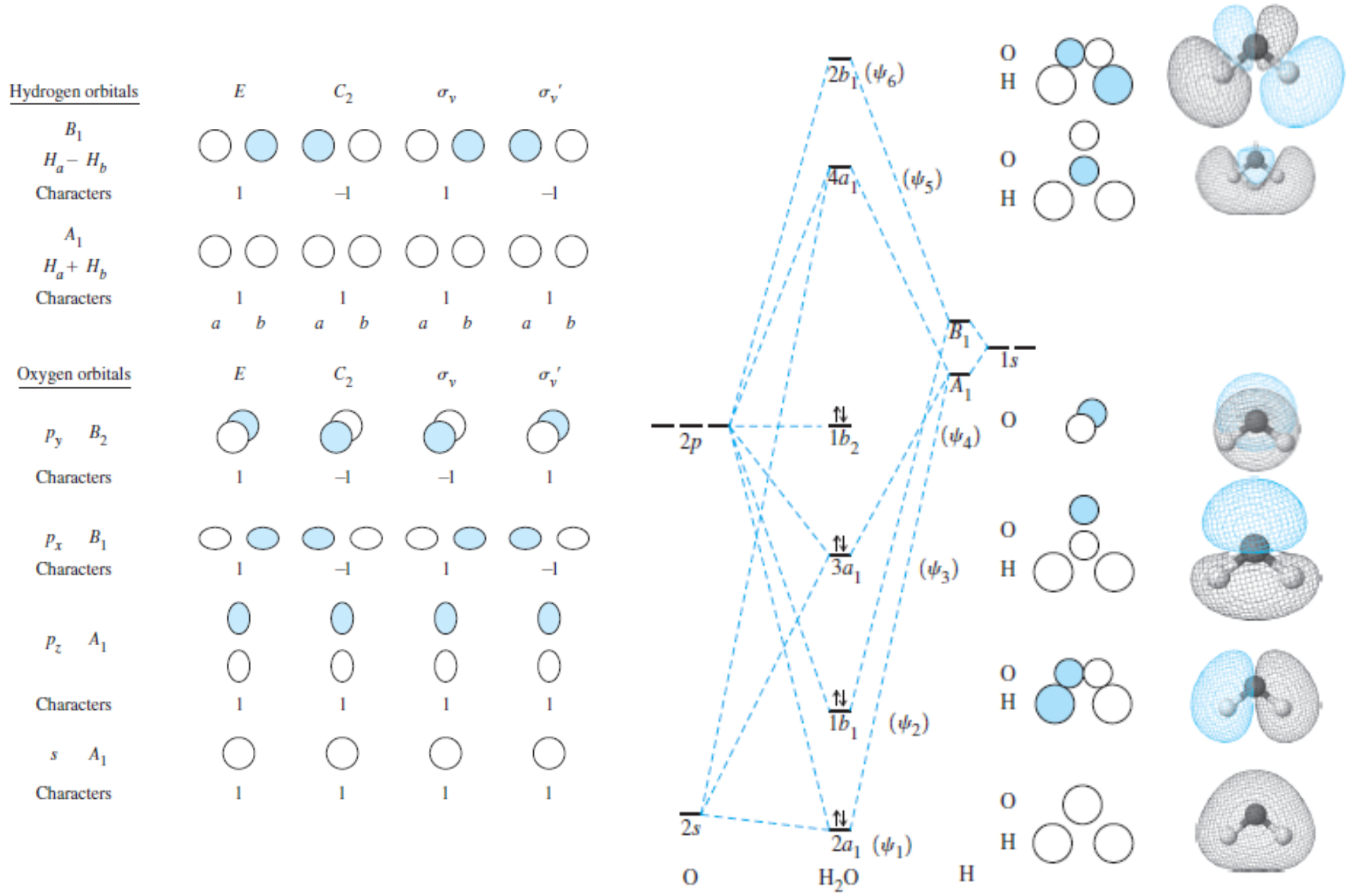
C_{2v}	E	C_2	$\sigma_v(xz)$	$\sigma_v'(yz)$	
Γ	2	0	2	0	
A_1	1	1	1	1	z
B_1	1	−1	1	−1	x

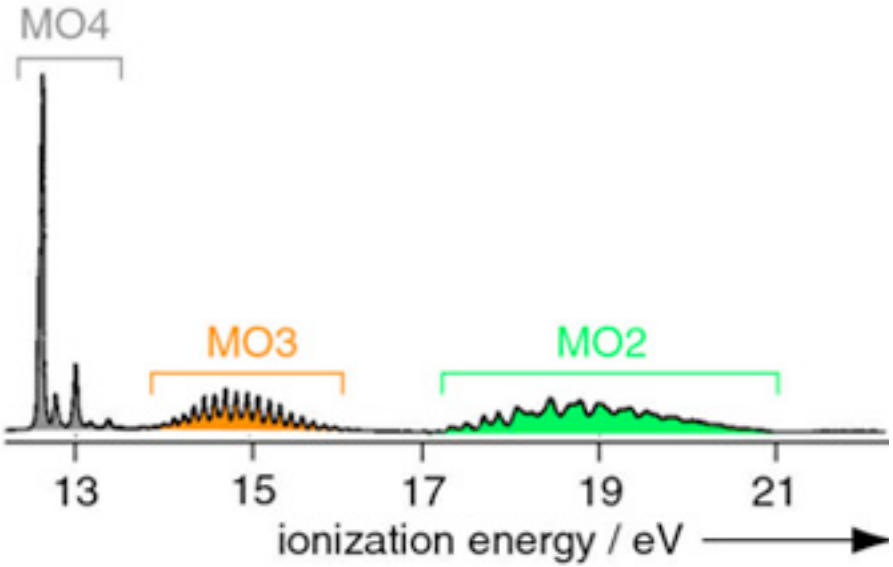
C_{2v} Character Table

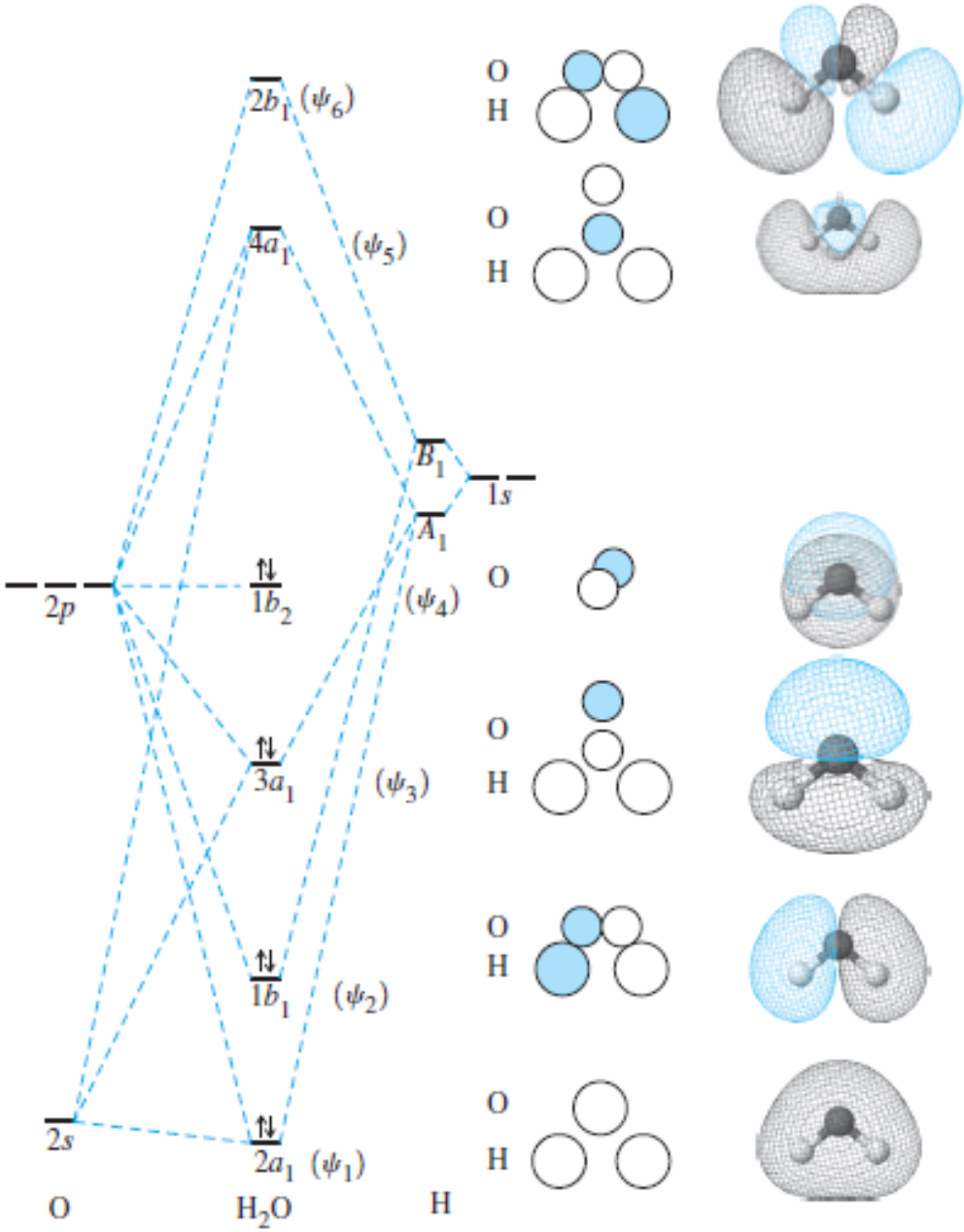
C_{2v}	E	C_2	$\sigma_v(xz)$	$\sigma_v'(yz)$		
A_1	1	1	1	1	z	x^2, y^2, z^2
A_2	1	1	−1	−1	R_z	xy
B_1	1	−1	1	−1	x, R_y	xz
B_2	1	−1	−1	1	y, R_x	yz

Determine irreducible representations for Hydrogen SALCS and AOs on Oxygen


Hydrogen orbitals
E
C2
σv
σv′
B1
Ha − Hb
Characters
1
–1
1
–1
A1
Ha + Hb
Characters
1
1
1
1
a b
a b
a b
a b
Oxygen orbitals
E
C2
σv
σv′
py B2
Characters
1
–1
–1
1
px B1
Characters
1
–1
1
–1
pz A1
Characters
1
1
1
1
s A1
Characters
1
1
1
1


Hydrogen orbitals
E
C2
σv
σv′
B1
Ha − Hb
Characters
1
−1
1
−1
A1
Ha + Hb
Characters
1
1
1
1
a b a b a b a b
Oxygen orbitals
E
C2
σv
σv′
py B2
Characters
1
−1
−1
1
px B1
Characters
1
−1
1
−1
pz A1
Characters
1
1
1
1
s A1
Characters
1
1
1
1
2b1 (ψ6)
4a1 (ψ5)
B1
A1
1s
2p
1b2 (ψ4)
3a1 (ψ3)
1b1 (ψ2)
2s
2a1 (ψ1)
O
H2O
H
O
H
O
H
O
H
O
H


MO4
MO3
MO2
13
15
17
19
21
ionization energy / eV


$2b_1$ (ψ_6)
$4a_1$ (ψ_5)
B_1
A_1
$1s$
$2p$
$1b_2$ (ψ_4)
$3a_1$ (ψ_3)
$1b_1$ (ψ_2)
$2s$
$2a_1$ (ψ_1)
O
H_2O
H
O
H