

1. MOLECULE

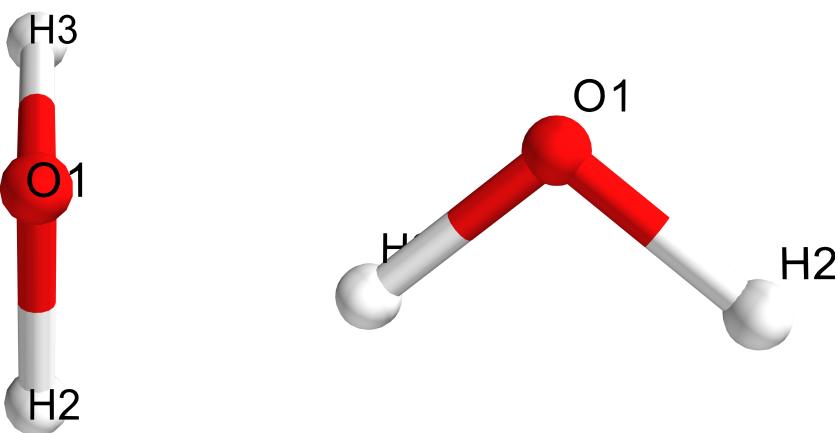


Figure 1: Chemical structure diagram with atomic numbering from two points of view.

Directory name	QuChem
Formula	H2O
Charge	0
Spin multiplicity	1
Monoisotopic mass	18.01056 Da
InChI	1S/H2O/h1H2
SMILES	O

2. COMPUTATIONAL DETAILS

Software	Gaussian	(2009+D.01)
Computational method	DFT	
Functional	B3LYP	
Basis set name	6-31G(d)	
Number of basis set functions	19	
Closed shell calculation	True	
Requested SCF convergence on RMS and Max density matrix	1e-08	1e-06
Requested SCF convergence on energy	1e-06	
Job type: Time-dependent calculation		
Number of calculated excited states and spin state	5	['Singlet-A1' 'Singlet-A2' 'Singlet-B1' 'Singlet-B2']
Job type: Geometry optimization		
Max Force value and threshold	0.000156	0.000450
RMS Force value and threshold	0.000101	0.000300
Max Displacement value and threshold	0.000578	0.001800
RMS Displacement value and threshold	0.000550	0.001200

3. RESULTS

Total molecular energy	-76.40895 hartrees	
HOMO number	5	
LUMO+1 energies	4.03 eV	
LUMO energies	1.70 eV	
HOMO energies	-7.92 eV	
HOMO-1 energies	-10.13 eV	
Geometry optimization specific results		
Converged nuclear repulsion energy	9.08784 Hartrees	
Mean Mulliken atomic charge and standard deviation	0.0000 e-	0.5475 e-
Atoms with negatives charges under the standard deviation	NÅ°	Mulliken charge
O 1		-0.774
Atoms with positives charges over the standard deviation	NÅ°	Mulliken charge

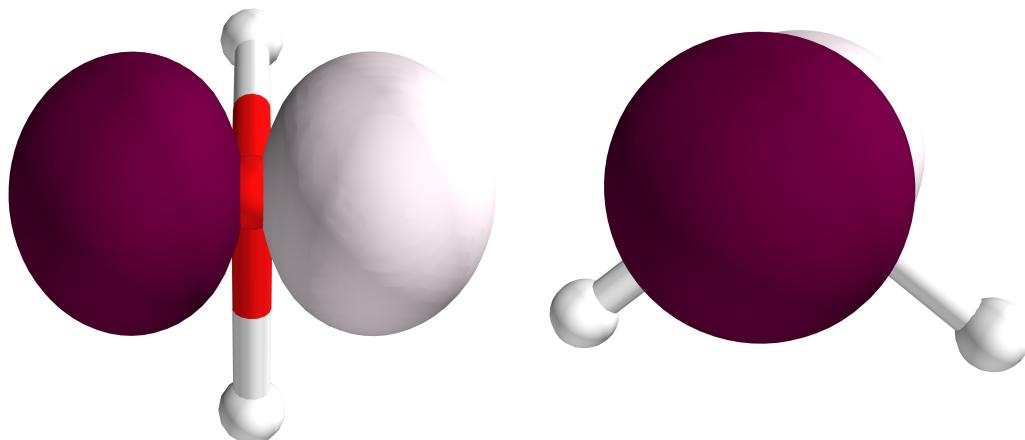


Figure 2: Representation of the HOMO from two points of view.

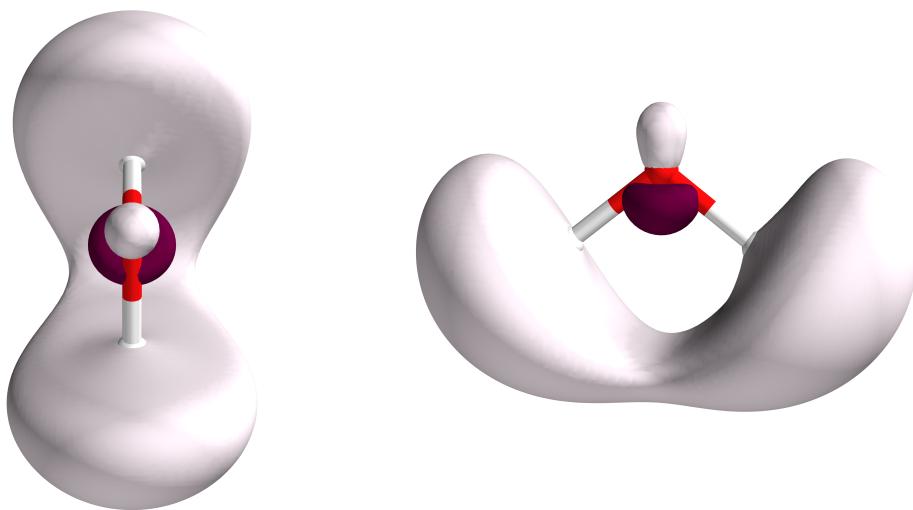


Figure 3: Representation of the LUMO from two points of view.

Table. Results concerning the calculated mono-electronic excitations.

E.S.	Symmetry	nm	cm ⁻¹	f	R	Λ	d _{CT}	q _{CT}	Excitation description : initial OM - ending OM (% if > 5%)
1	Singlet-B1	156	63850	0.014	0.0	0.41	88.49	0.82	5-6(100);
2	Singlet-A2	124	80171	0.000	0.0	0.38	80.85	0.82	5-7(99);
3	Singlet-A1	118	84705	0.095	0.0	0.53	111.71	0.72	4-6(98);
4	Singlet-B2	97	102261	0.072	0.0	0.53	104.36	0.72	4-7(95);
5	Singlet-B2	85	117079	0.398	0.0	0.59	76.69	0.68	3-6(95);

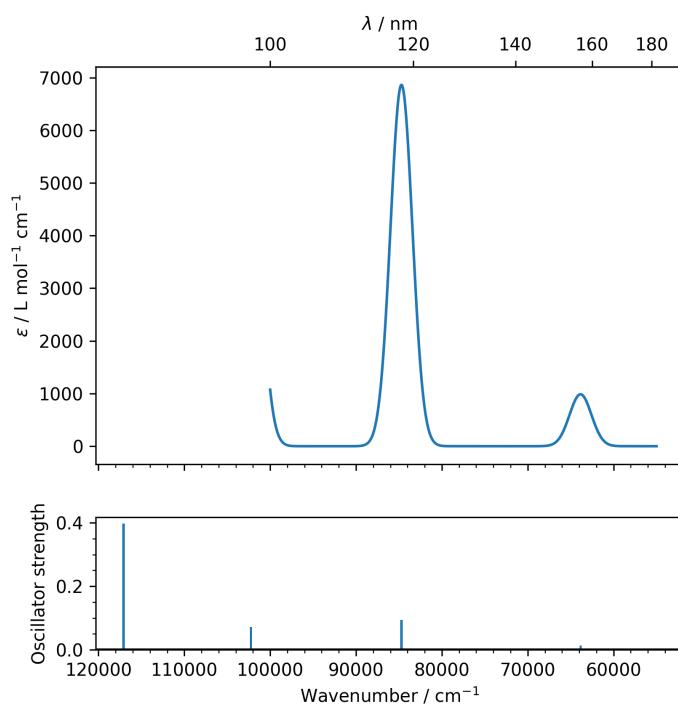


Figure 4: Calculated UV visible Absorption spectrum with a gaussian broadening (FWHM = 3000 cm⁻¹)

Table. Converged cartesian atomic coordinates in Angstroms

Atom	X	Y	Z
O	0.0000	0.0000	0.1198
H	0.0000	0.7613	-0.4792
H	0.0000	-0.7613	-0.4792

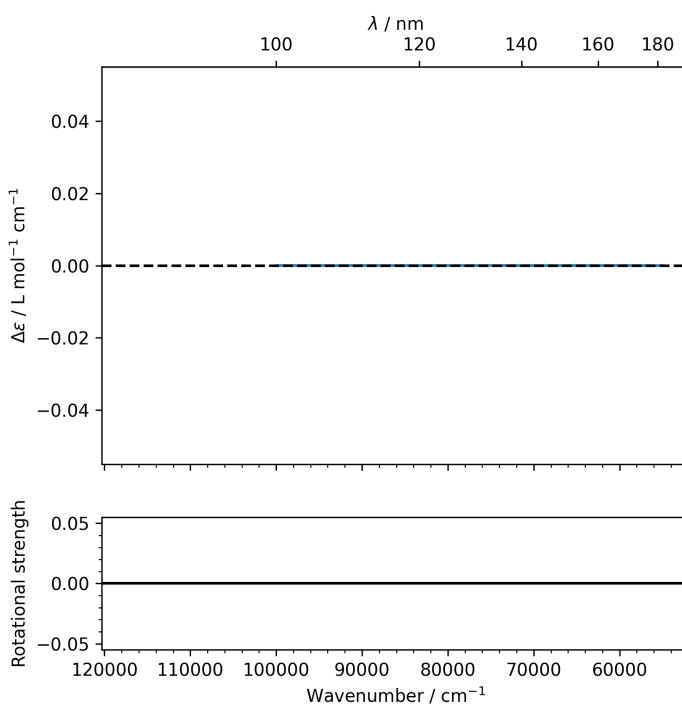


Figure 5: Calculated Circular Dichroism spectrum with a gaussian broadening (FWHM = 3000 cm⁻¹)

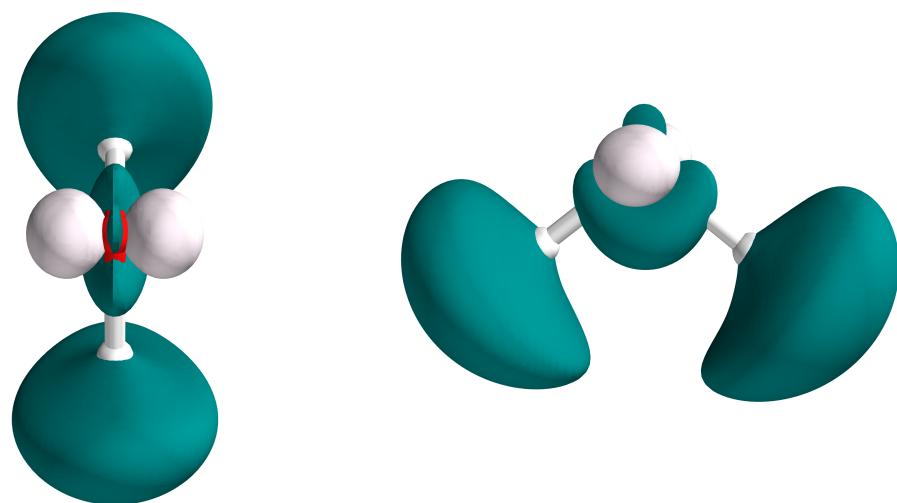


Figure 6: Representation of the Electron Density Difference (S1-S0) from two points of view.

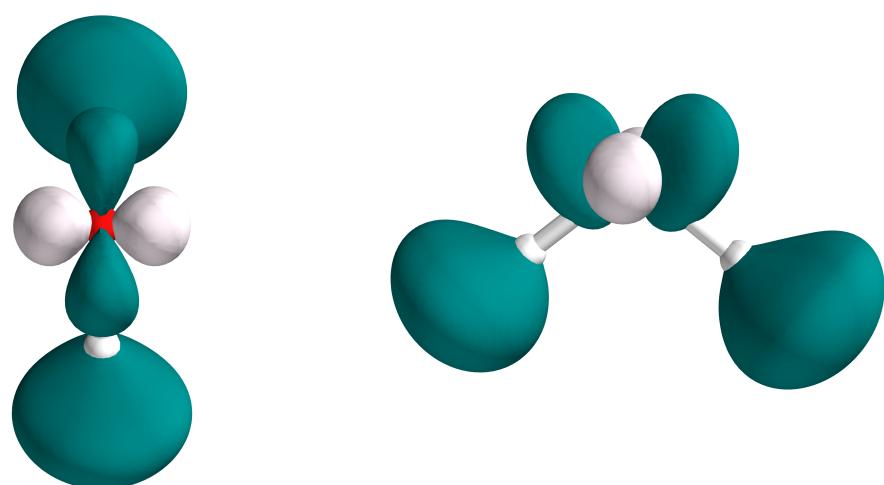


Figure 7: Representation of the Electron Density Difference (S2-S0) from two points of view.