Calculated energies for the frontier molecular orbitals (in eV)

HOMO-1	HOMO	LUMO	LUMO+1
-10.13	-7.92	1.70	4.03

1. MOLECULE

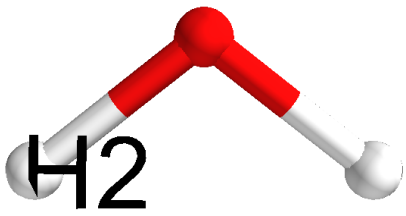

Figure 1: *
Chemical structure diagram with atomic numbering.

InChI	I
SMILES	O
Monoisotopic mass	18.01056 Da
Formula	H2O
Charge	0
Spin multiplicity	1

2. COMPUTATIONAL DETAILS

Software	Gaussian (09revisionD.01)
Computational method	DFT
Functional	B3LYP
Basis set name	6-31G(d)
Number of basis set functions	19
Closed shell calculation	True
Integration grid	Default
Solvent	Gas
Requested SCF convergence on RMS density matrix	1e-08
Requested SCF convergence on MAX density matrix	1e-06
Requested SCF convergence on energy	1e-06
Number of excited states	5

3. RESULTS

3.1 Wavefunction

Total molecular energy	-76.40895 Hartrees
HOMO number	5

Most intense Mulliken atomic charges
mean = 0.000 e, std = 0.547

Atom	number	Mulliken charges
O	1	-0.774

3.2 Geometry

Warning : this calculation does not include a geometry optimization process. This geometry may not be a stationary point for those computational parameters. In this case, results must be used with caution.

Nuclear repulsion energy 9.08784 Hartrees

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

3.3 Thermochemistry and normal modes

Warning : force constants and the resulting vibrational frequencies were not computed.

3.4 Excited states

Calculated mono-electronic excitations

Number	Energy	Symmetry	Oscillator strength	Rotatory strength	Transitions
1	57614.60	Triplet-B1	0.000000	0.0	1
2	74780.50	Triplet-A1	0.000000	0.0	1
3	75555.60	Triplet-A2	0.000000	0.0	1
4	90839.81	Triplet-B2	0.000000	0.0	2
5	105274.71	Triplet-B2	0.000000	0.0	2