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

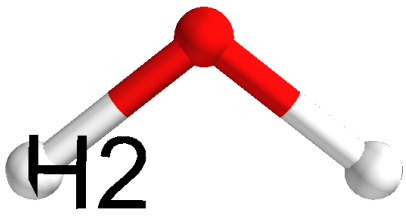

Figure 1: *
Chemical structure diagram with atomic numbering.

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
Temperature	298.15 K

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

This calculation is the result of a geometry optimization process.

Geometry optimization convergence criteria

	Value	Threshold
Maximum Force	0.000156	0.000450
RMS Force	0.000101	0.000300
Maximum Displacement	0.000531	0.001800
RMS Displacement	0.000512	0.001200

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

Sum of electronic and zero-point energy in Hartrees	-76.387786
Sum of electronic and thermal at 298.150000 K	-76.384952
energies in atomic units	
Entropy at 298.150000 K in atomic units	7.193e-05
Enthalpy at 298.150000 K in atomic units	-76.384008
Gibbs free energy at 298.150000 K in atomic units	-76.405454

Table of the most intense molecular vibrations (> 20 km/mol) (1)

Frequencies	Intensity	Symmetry
1713.5448	75.7070	A1