Calculated energies for the frontier molecular orbitals (in eV)

HOMO-1	HOMO	LUMO	LUMO+1
-26.83	-22.96	-16.74	-7.39

1. MOLECULE

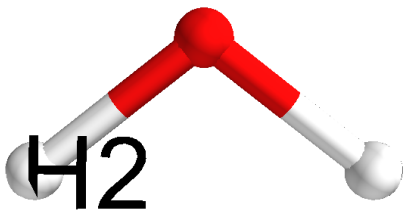

Figure 1: *
Chemical structure diagram with atomic numbering.

InChI	I
SMILES	O
Monoisotopic mass	18.01056 Da
Formula	H2O+
Charge	1
Spin multiplicity	2

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	False
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

3. RESULTS

3.1 Wavefunction

Total molecular energy	-75.95457 Hartrees
HOMO number	5, 4

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.