**MOLECULAR CALCULATION REPORT**

**1. MOLECULE**

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

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

**2. COMPUTATIONAL DETAILS**

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
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| |  |  |  | | --- | --- | --- | | 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 | |  |  |  | | |  | | --- | | test | | test | | test | | test | |

Job type: Geometry optimization