**Supplementary**



**Figure 1S.** Optimized structure of the iodinated pyruvic ester.

**Table 1S:** Structural parameters of the iodinated pyruvic ester in water solution. Bond lengths are in angstroms, bond angles and dihedral angles are in degrees.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Bond lengths | | Bond angles | | Dihedral angles | |
| C17-I | 2.25 | I-C17-C1 | 111.34 | O6-C1-C17-I | -62.67 |
| C18-O25 | 1.21 | I-C17-C18 | 103.94 | O6-C1-C17-C18 | 179.65 |
| C17-C1 | 1.52 | C17-C18-O25 | 123.64 | I-C17-C1-C2 | 177.41 |
| C1-O6 | 1.43 | C17-C1-O6 | 107.16 | C2-C1-C17-C18 | 59.73 |
| C17-C18 | 1.51 | O6-C1-C2 | 109.43 | O7-C4-O6-C1 | -76.00 |
| C1-C2 | 1.54 | O6-C4-C5 | 111.40 | O13-C2-C1-C17 | 39.90 |
| C4-O6 | 1.41 | C3-C5-O8 | 108.72 | O25-C18-C17-I | -100.24 |
| C9-O8 | 1.43 | O8-C9-O7 | 104.89 | O21-C19-C18-C17 | -167.27 |

**Table 2S:** Structural parameters of hydrogen sulfite in water solution. Bond lengths are in angstroms, bond angles and dihedral angles are in degrees.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Bond lengths | | Bond angles | | Dihedral angles | |
| S-O2 | 1.513 | O2-S-O3 | 111.58 | O2-S-O4-H | -36.07 |
| S-O3 | 1.509 | O2-S-O4 | 100.46 | O3-S-O4-H | 79.26 |
| S-O4 | 1.750 | O2-S-O4 | 103.32 | ------ | ----- |
| O4-H | 0.978 | S2-O4-H | 103.80 | ------ | ------ |