**S1 Table**. Geometric parameters by X-ray for TABA and theoretical calculations at B3LYP/6-311++G(2d,p) and B97D/6-311++G(2d,p) level of theory for the monomer and dimer, respectively. The bond lengths are given in angstroms and the bond angles and dihedral angles are given in degrees. All the calculations were carried out at gas phase.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Bond length** | **Exp.** | **Calculated** | | **Bond angle** | **Exp.** | **Calculated** | |
|  |  | **Monomer**  **B3LYP** | **Dimer**  **B97D** |  |  | **Monomer**  **B3LYP** | **Dimer**  **B97D** |
| C(1)−C(2) | 1.487 | 1.486 | 1.491 | C(2)−C(1)−O(1) | 116.76 | 113.08 | 114.53 |
| C(1)−O(1) | 1.276 | 1.355 | 1.325 | C(2)−C(1)−O(2) | 119.15 | 124.67 | 121.61 |
| C(1)−O(2) | 1.251 | 1.207 | 1.238 | C(2)−C(3)−C(4) | 120.33 | 119.57 | 119.66 |
| C(2)−C(3) | 1.382 | 1.395 | 1.404 | C(3)−C(4)−C(5) | 120.40 | 120.59 | 120.66 |
| C(2)−C(7) | 1.392 | 1.394 | 1.403 | C(4)−C(5)−C(6) | 118.76 | 119.46 | 119.29 |
| C(3)−C(4) | 1.372 | 1.380 | 1.387 | C(5)−C(6)−C(7) | 121.53 | 120.57 | 120.76 |
| C(4)−C(5) | 1.386 | 1.392 | 1.400 | C(6)−C(7)−C(2) | 118.67 | 119.39 | 119.49 |
| C(4)−O(3) | 1.396 | 1.389 | 1.393 | C(7)−C(2)−C(3) | 120.24 | 120.41 | 120.14 |
| C(5)−C(6) | 1.388 | 1.392 | 1.398 | C(4)−O(3)−C(8) | 117.79 | 117.61 | 117.38 |
| C(5)−O(5) | 1.384 | 1.380 | 1.384 | O(3)−C(8)−O(4) | 122.36 | 123.26 | 123.73 |
| C(6)−C(7) | 1.377 | 1.385 | 1.390 | O(3)−C(8)−C(9) | 110.25 | 109.98 | 109.19 |
| C(6)−O(7) | 1.394 | 1.386 | 1.392 | C(5)−O(5)−C(10) | 116.74 | 117.54 | 117.03 |
| C(8)−O(3) | 1.363 | 1.379 | 1.393 | O(5)−C(10)−O(6) | 122.05 | 123.18 | 123.61 |
| C(8)−O(4) | 1.197 | 1.196 | 1.202 | O(5)−C(10)−C(11) | 109.96 | 109.90 | 109.14 |
| C(8)−C(9) | 1.493 | 1.502 | 1.510 | C(6)−O(7)−C(12) | 117.10 | 119.15 | 117.87 |
| C(10)−O(5) | 1.381 | 1.382 | 1.395 | O(7)−C(12)−O(8) | 122.31 | 123.64 | 123.88 |
| C(10)−O(6) | 1.192 | 1.195 | 1.202 | O(7)−C(12)−C(13) | 110.25 | 109.75 | 109.07 |
| C(10)−C(11) | 1.478 | 1.501 | 1.509 | C(3)−C(2)−C(1) −O(2) | 4.25 | 0.20 | -0.53 |
| C(12)−O(7) | 1.365 | 1.380 | 1.394 | C(3)−C(2)−C(1) −O(1) | -175.92 | -179.69 | 179.39 |
| C(12)−O(8) | 1.192 | 1.196 | 1.202 | C(4)−C(3)−C(2) −C(1) | -179.85 | 179.70 | -179.94 |
| C(12)−C(13) | 1.483 | 1.502 | 1.510 | C(5)−C(4)−C(3) −C(2) | 1.23 | 0.22 | -0.68 |
| O(1)−H | 0.820 | 0.980 | 1.016 | C(2)−C(3)−C(4) −O(3) | -176.16 | -176.10 | 175.81 |
| C(3)−H | 0.930 | 1.081 | 1.086 | C(3)−C(4)−O(3) −C(8) | -109.23 | -100.26 | 107.38 |
| C(7)−H | 0.930 | 1.079 | 1.084 | C(4)−O(3)−C(8) −O(4) | -11.47 | -0.17 | -2.91 |
|  |  |  |  | C(4)−O(3)−C(8) −C(9) | 169.53 | 179.26 | 177.42 |
|  |  |  |  | C(4)−C(5)−O(5) −C(10) | 118.38 | 98.49 | -96.69 |
|  |  |  |  | C(5)−O(5)−C(10) −O(6) | -14.27 | -1.98 | 2.227 |
|  |  |  |  | C(5)−O(5)−C(10) −C(11) | 165.64 | 178.08 | -177.65 |
|  |  |  |  | C(4)−C(5)−C(6) −O(7) | 179.91 | -176.44 | 175.56 |
|  |  |  |  | C(5)−C(6)−O(7) −C(12) | 112.99 | -122.11 | 112.02 |
|  |  |  |  | C(6)−O(7)−C(12) −O(8) | 4.07 | 0.25 | 0.10 |
|  |  |  |  | C(6)−O(7)−C(12) −C(13) | -175.75 | -179.80 | -179.85 |