**Supplementary Material**

**Theoretical and experimental investigation on the electrochemical properties, structural and spectroscopic parameters of 6,7-dihydroxy-9-thia-1,4a-diaza fluoren-2-one (DTDFO)**

Hassan Goodarzia[[1]](#footnote-1), Alireza Asgharia[[2]](#footnote-2), Davood Nematollahib[[3]](#footnote-3), Maryam Rajabia[[4]](#footnote-4)

*a Department of Chemistry, Semnan University, Semnan 35195-363, Iran*

*b Faculty of Chemistry, Bu-Ali Sina University, Hamedan, Zip Code 65178-38683, Iran*

**Corresponding author:**

Alireza Asghari

Address: Department of Chemistry, Semnan University, Semnan, Iran

Zip code: 35195-363

Tel.: +98 023135195 363

Fax. +98 023133654110

E-mail: aasghari@semnan.ac.ir

**Table 1S-7S** show the geometrical parameters, charge transfers, IR frequencies, atomic charges, 13C chemical shifts, Gibbs free energies, and energy gaps for the given molecules.

**Table 1S.** Calculated bond lengths (Å) and bond angles (°) of DTDFO at the B3LYP and MPW1PW91 levels of theory.

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Bond length | B3LYP | | MPW1PW91 | | bond angles | B3LYP | | MPW1PW91 | |
| Gas | Sol | Gas | Sol | Gas | Sol | Gas | Sol |
| C1-C2 | 1.3972 | 1.39535 | 1.4004 | 1.39857 | C1-C2-C3 | 120.6307 | 121.00343 | 120.74188 | 121.10421 |
| C1-C6 | 1.39168 | 1.39263 | 1.3943 | 1.39512 | C2-C3-C4 | 118.3764 | 118.13086 | 118.23439 | 117.98856 |
| C1-S13 | 1.76771 | 1.7688 | 1.7688 | 1.77011 | C3-C4-O16 | 124.2755 | 124.5535 | 124.30386 | 124.59957 |
| C2-C3 | 1.39524 | 1.39486 | 1.39784 | 1.39751 | C3-C2-N10 | 127.1365 | 126.93835 | 127.02241 | 126.81893 |
| C2-N10 | 1.40527 | 1.4098 | 1.40621 | 1.41067 | C5-C4-O16 | 114.497 | 114.39646 | 114.40862 | 114.28171 |
| C3-C4 | 1.38814 | 1.38771 | 1.39034 | 1.38998 | C4-C5-O15 | 120.3823 | 120.05199 | 120.287 | 119.95725 |
| C4-C5 | 1.40884 | 1.4128 | 1.41118 | 1.41495 | C6-C5-O15 | 119.712 | 119.65169 | 119.70804 | 119.65857 |
| C4-O16 | 1.37277 | 1.36484 | 1.37407 | 1.36647 | C6-C1-C2 | 120.8152 | 120.8908 | 120.8148 | 120.8925 |
| C5-C6 | 1.38885 | 1.38804 | 1.39162 | 1.39086 | C2-C1-S13 | 111.7896 | 111.6923 | 111.7675 | 111.6694 |
| C5-O15 | 1.35802 | 1.35915 | 1.3599 | 1.36084 | C1-S13-C11 | 90.7486 | 90.64244 | 90.78345 | 90.68341 |
| C9-N10 | 1.38503 | 1.38166 | 1.38598 | 1.38275 | C2-N10-C11 | 115.0698 | 114.8525 | 115.0626 | 114.8811 |
| C9-C8 | 1.34465 | 1.3475 | 1.34798 | 1.35079 | S13-C11-N10 | 110.1591 | 110.7544 | 110.1506 | 110.6891 |
| C8-C7 | 1.47445 | 1.4636 | 1.475 | 1.46487 | S13-C11-N12 | 123.2428 | 123.1245 | 123.2493 | 123.1241 |
| C7-O14 | 1.21406 | 1.22854 | 1.22063 | 1.23372 | N10-C11-N12 | 126.598 | 126.1209 | 126.6 | 126.1867 |
| C7-N12 | 1.41327 | 1.40147 | 1.41476 | 1.40425 | C11-N12-C7 | 119.4359 | 119.1665 | 119.2477 | 118.9735 |
| C11-N12 | 1.27847 | 1.29015 | 1.28279 | 1.29346 | N12-C7-O14 | 121.697 | 120.7982 | 121.5314 | 120.6392 |
| C11-S13 | 1.77782 | 1.76765 | 1.77992 | 1.77101 | C7-C8-C9 | 121.4942 | 121.1996 | 121.3814 | 121.1107 |

**Table 2S.** Delocalization stability energies (charge transfers) calculated at the B3LYP/6-311++G(d,p) level.

|  |  |  |  |
| --- | --- | --- | --- |
| Donor NBO (i) | Acceptor NBO (j) | E(2) E(j)-E(i) F(i,j)  kcal/mol | |
| GAS | SOL |
| BD(C1-C6) | BD\* (C5-O15) | 3.27 | 3.34 |
| BD(C5-C6) | BD\* (C5-O15) | 0.94 | 0.89 |
| LP O 15 | BD\* (C4-C5) | 6.57 | 6.50 |
| LP O 15 | BD\* (C5-C6) | 29.03 | 28.93 |
| BD(C2-C3) | BD\* (C4-O16) | 4.21 | 4.18 |
| BD(C5-C6) | BD\* (C4-O16) | 2.55 | 2.36 |
| BD(C7-O14) | BD\* (C11-N12) | 5.14 | 4.65 |
| BD(C7-O14) | BD\* (C8-C9) | 6.41 | 5.56 |
| LPO14 | BD\*(N12-C7) | 1.47 | 1.36 |
| BD(C11-N12) | BD\* (C7-O14) | 1.63 | 1.79 |
| BD(C2-C3) | BD\* (C1-S13) | 2.87 | 2.98 |

**Table 3S.** The experimental and calculated IR frequencies (cm-1) for the DTDFO compound at B3LYP and MPW1PW91 levels, and errors evaluated by RMSE and MAE methods.

|  |  |  |
| --- | --- | --- |
| Exp. | at B3LYP/ 6-311++G(d, p), scaled by 0.967 | at MPW1PW91/ 6-311++G(d, p), scaled by 0.957 |
|  | 791.006 | 788.568 |
| 831 | 804.544 | 798.138 |
|  | 860.63 | 853.644 |
| 949 | 922.518 | 925.419 |
|  | 1022.119 | 1013.463 |
| 1062.5 | 1047.261 | 1028.775 |
| 1095.7 | 1073.37 | 1058.442 |
|  | 1115.918 | 1106.292 |
| 1208.9 | 1166.202 | 1158.927 |
|  | 1195.212 | 1183.809 |
| 1265.6 | 1216.486 | 1187.637 |
| 1322 | 1274.506 | 1285.251 |
|  | 1308.158 | 1294.821 |
|  | 1401.183 | 1385.736 |
| 1510.6 | 1439.863 | 1448.898 |
|  | 1487.246 | 1475.694 |
|  | 1523.025 | 1511.103 |
| 1623.3 | 1586.847 | 1537.899 |
|  | 1629.395 | 1616.373 |
| 3036.4 | 3072.159 | 3068.142 |
| 3409.9 | 3116.641 | 3095.895 |
|  | 3662.029 | 3676.794 |
|  |  |  |
| Error item | B3LYP/6-311++G(d. p) | MPW1PW91/6-311++G(d, P) |
| RMSE | 96.40 | 106.59 |
| MAE | 60.6 | 71.59 |

**Table 4S.** Natural atomic charges of DTDFO at the given levels of theory.

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Atoms | Atomic charges | | | | Atoms | Atomic charges | | | |
| B3LYP | | MPW1PW91 | | B3LYP | | MPW1PW91 | |
| Gas | Sol | Gas | Sol | Gas | Sol | Gas | Sol |
| C1 | -0.18164 | -0.18228 | -0.22978 | -0.23006 | N10 | -0.4213 | -0.40466 | -0.33237 | -0.38874 |
| C2 | 0.13759 | 0.13561 | 0.13562 | 0.13324 | S13 | 0.37528 | 0.38305 | 0.43364 | 0.43759 |
| C3 | -0.29751 | -0.28577 | -0.31893 | -0.30801 | O14 | -0.66191 | -0.67686 | -0.56772 | -0.69553 |
| C4 | 0.28307 | 0.29187 | 0.27034 | 0.27999 | O15 | -0.6972 | -0.69934 | -0.68117 | -0.71291 |
| C5 | 0.30123 | 0.30161 | 0.29297 | 0.29238 | O16 | -0.56712 | -0.65679 | -0.71033 | -0.65205 |
| C6 | -0.25155 | -0.2614 | -0.27225 | -0.28086 | H17 | 0.21072 | 0.23601 | 0.23875 | 0.26466 |
| C11 | 0.33623 | 0.34063 | 0.28648 | 0.29067 | H18 | 0.23143 | 0.23827 | 0.26442 | 0.27049 |
| N12 | -0.5449 | -0.5883 | -0.53 | -0.57213 | H19 | 0.22531 | 0.23178 | 0.26076 | 0.26703 |
| C7 | 0.61912 | 0.61983 | 0.61419 | 0.61288 | H20 | 0.20303 | 0.22744 | 0.23709 | 0.26259 |
| C8 | -0.29686 | -0.31085 | -0.40423 | -0.34476 | H21 | 0.48025 | 0.49141 | 0.50539 | 0.51623 |
| C9 | 0.03874 | 0.06874 | 0.02868 | 0.03227 | H22 | 0.478 | 0.49999 | 0.50254 | 0.52503 |

Table 5S. The experimental and calculated 13C chemical shifts for DTDFO at the given levels of theory, and errors evaluated by RMSE and MAE methods.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Atoms | δexp | | Calculated chemical shifts | | δexp - δcal(B3LYP) | | δexp - δcal(MPW1PW91) |
| B3LYP | MPW1PW91 |
| C3 | 101.07 | | 114 | 96 | -12.93 | | 5.07 |
| C6 | 109.94 | | 115 | 107 | -5.06 | | 2.94 |
| C10 | 112.94 | | 118 | 110.8 | -5.06 | | 2.14 |
| C1 | 128.27 | | 127.7 | 118 | 0.57 | | 10.27 |
| C2 | 135.72 | | 136.5 | 125 | -0.78 | | 10.72 |
| C11 | 145.95 | | 142 | 133 | 3.95 | | 12.95 |
| C4 | 147.07 | | 147.9 | 141 | -0.83 | | 6.07 |
| C5 | 164.60 | | 152 | 142.5 | 12.6 | | 22.1 |
| C7 | 167.52 | | 177 | 162 | -9.48 | | 5.52 |
| C9 | 168 | | 177 | 163.5 | -9 | | 4.5 |
| Error item | | B3LYP/6-311++G(d. p) | | | | MPW1PW91/6-311++G(d, P) | |
| RMSE | | 5.87 | | | | 5.73 | |
| MAE | | 4.84 | | | | 4.27 | |

**Table 6S.** The change of Gibbs free energy of the given molecules for both oxidized (Ox.) and reduced (Red.) forms in the gas and solution phase, along with the change of the total Gibbs free energy (∆Gtot).

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Mol.1** | ∆G(gas)2 | |  | ∆G(sol)2 | |  | ∆Gtot (kJ/mol) |
| Red | Ox |  | Red | Ox |  |
| **a3** | -382.72090 | -381.17699 |  | -382.72710 | -381.18511 |  | 0 |
| **b3** | -1117.96680 | -1116.39878 |  | -1117.98927 | -1116.46511 |  | -16.52 |
| **a4** | -382.60349 | -381.385159 |  | -382.61165 | -381.39668 |  | 0 |
| **b4** | -1117.47310 | -1116.23029 |  | -1117.98718 | -1116.78990 |  | -17.83 |

1. a: Red=H2Q, ox=Q , b:Red= DTDFO, ox= DTDFOO
2. These energies are in atomic units, Hartree (1 Hartree =2625.49975 kJ mol-1).
3. These energies have been calculated at MPW1PW91level using 6-311++G (d, p) basis set.
4. These energies have been calculated at B3LYP level using 6-311++G (d) basis set.

**Table 7S.** The calculated values of HOMO and LUMO energies (eV), and energy gaps calculated with the 6-311++G(d, p) basis set at the B3LYP and MPW1PW91 levels of theory.

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| DTDFO | MPW1PW91 | |  | B3LYP | |  | ELUMO- EHOMO (eV) | |
| EHOMO | ELUMO |  | EHOMO | ELUMO |  | MPW1PW91 | B3LYP |
| -2.87348 | -0.63342 |  | -2.94084 | -0.72239 |  | 2.240055 | 2.218455 |

Table 8S. Calculated Mulliken charges, and Fukui functions for all the atoms of DTDFO.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| No. | Atom | qN | qN+1 | qN-1 | f+ | f- |
| 1 | C | -0.34149 | -0.32466 | -0.33237 | 0.01683 | -0.00912 |
| 2 | C | 0.362075 | 0.391097 | 0.349004 | 0.029022 | 0.013071 |
| 3 | C | -0.05117 | -0.00782 | -0.15408 | 0.043345 | 0.102915 |
| 4 | C | 0.106247 | 0.149017 | 0.083782 | 0.04277 | 0.022465 |
| 5 | C | 0.174997 | 0.209803 | 0.135954 | 0.034806 | 0.039043 |
| 6 | C | -0.05729 | -0.02562 | -0.12924 | 0.031669 | 0.071942 |
| 7 | C | 0.24833 | 0.255377 | 0.238355 | 0.007047 | 0.009975 |
| 8 | N | -0.35533 | -0.28826 | -0.382 | 0.06707 | 0.026676 |
| 9 | C | 0.318981 | 0.345869 | 0.260164 | 0.026888 | 0.058817 |
| 10 | C | -0.28375 | -0.24139 | -0.33349 | 0.042355 | 0.049749 |
| 11 | C | 0.179359 | 0.196655 | 0.09012 | 0.017296 | 0.089239 |
| 12 | N | -0.4997 | -0.48774 | -0.47309 | 0.011955 | -0.02661 |
| 13 | S | 0.282513 | 0.43886 | 0.16214 | **0.156347** | **0.120373** |
| 14 | O | -0.32609 | -0.21042 | -0.41937 | **0.11567** | 0.093281 |
| 15 | O | -0.40101 | -0.3522 | -0.4317 | 0.048807 | 0.030696 |
| 16 | O | -0.35135 | -0.27659 | -0.39452 | 0.074761 | 0.043169 |
| 17 | H | 0.1015 | 0.142796 | 0.055754 | 0.041296 | 0.045746 |
| 18 | H | 0.115904 | 0.162516 | 0.058794 | 0.046612 | 0.05711 |
| 19 | H | 0.123667 | 0.174702 | 0.058886 | 0.051035 | 0.064781 |
| 20 | H | 0.122412 | 0.157673 | 0.073459 | 0.035261 | 0.048953 |
| 21 | H | 0.262623 | 0.291093 | 0.237442 | 0.02847 | 0.025181 |
| 22 | H | 0.268558 | 0.299248 | 0.246006 | 0.03069 | 0.022552 |

The following materials involve the Cartesian coordinates of optimized structures and the needed information for repeating the related calculation by means of Gaussian software package.

1. The Cartesian coordinates of the optimized structure of the oxidized form of DTDFO in gas phase at MPW1PW91/6-311++g(d,p) level with the following keywords:

-------------------------------------# MPW1PW91/6-311++g(d,p) opt-------------------------------------------------

0 1

N -2.82657000 -0.85352900 -0.00042200

C -3.65420800 0.29343500 0.00017300

C -2.95716100 1.58695400 -0.00045900

C -1.62066300 1.65663400 -0.00030400

N -0.87239600 0.49130800 -0.00017900

C -1.56808300 -0.70807100 -0.00089200

C 0.51218200 0.39750800 -0.00019200

C 0.92895100 -1.01213700 -0.00005800

S -0.45413000 -2.08072500 -0.00019300

C 1.39381200 1.41495100 -0.00009900

C 2.82719200 1.13247800 0.00014000

C 3.27110700 -0.35563000 0.00032400

C 2.22163500 -1.37811700 0.00020400

O 4.44523300 -0.63040000 0.00046900

O 3.66112000 2.00482100 -0.00007200

O -4.85499100 0.19431500 0.00134000

H -3.55845900 2.48444100 -0.00024000

H -1.06225300 2.58143700 0.00045200

H 1.10309000 2.45687400 -0.00027800

H 2.53699000 -2.41351500 0.00045700

1. The Cartesian coordinates of the optimized structure of the oxidized form of DTDFO in solution phase at MPW1PW91/6-311++g(d,p) level with the following keywords:

------------------# MPW1PW91/6-311++g(d,p) opt scrf=(cpcm,solvent=water)-----------------------------

0 1

N 2.82315500 -0.84910500 -0.00002000

C 3.64073500 0.29462300 -0.00015500

C 2.95753300 1.58510500 0.00047700

C 1.61961400 1.65779700 0.00056400

N 0.87316600 0.49395000 0.00019600

C 1.55777500 -0.70395500 0.00006800

C -0.51189200 0.39965300 0.00005300

C -0.92808600 -1.01002600 0.00010800

S 0.45244400 -2.07604900 0.00011000

C -1.39006700 1.41986500 -0.00022000

C -2.81427100 1.12806000 -0.00016100

C -3.25793600 -0.36068500 -0.00001200

C -2.21974500 -1.38294100 0.00010300

O -4.44097200 -0.62000800 -0.00007800

O -3.66446500 1.99151500 -0.00029000

O 4.85113500 0.18186200 -0.00079200

H 3.55367500 2.48569300 0.00077300

H 1.06743800 2.58539600 0.00092000

H -1.09453200 2.45969800 -0.00044500

H -2.52748800 -2.41984500 0.00008600

1. The Cartesian coordinates of the optimized structure of the oxidized form of DTDFO in GAS phase at B3LYP/6-311++g(d,p) level with the following keywords:

------------------------------------# B3LYP/6-311++g(d,p) opt--------------------------------------------------------

0 1

N -2.82657000 -0.85352900 -0.00042200

C -3.65420800 0.29343500 0.00017300

C -2.95716100 1.58695400 -0.00045900

C -1.62066300 1.65663400 -0.00030400

N -0.87239600 0.49130800 -0.00017900

C -1.56808300 -0.70807100 -0.00089200

C 0.51218200 0.39750800 -0.00019200

C 0.92895100 -1.01213700 -0.00005800

S -0.45413000 -2.08072500 -0.00019300

C 1.39381200 1.41495100 -0.00009900

C 2.82719200 1.13247800 0.00014000

C 3.27110700 -0.35563000 0.00032400

C 2.22163500 -1.37811700 0.00020400

O 4.44523300 -0.63040000 0.00046900

O 3.66112000 2.00482100 -0.00007200

O -4.85499100 0.19431500 0.00134000

H -3.55845900 2.48444100 -0.00024000

H -1.06225300 2.58143700 0.00045200

H 1.10309000 2.45687400 -0.00027800

H 2.53699000 -2.41351500 0.00045700

1. The Cartesian coordinates of the optimized structure of the oxidized form of DTDFO in solution phase at B3LYP/6-311++g(d,p) level with the following keywords:

------------------# B3LYP/6-311++g(d,p) opt scrf=(cpcm,solvent=water)-----------------------------

0 1

N -2.82657000 -0.85352900 -0.00042200

C -3.65420800 0.29343500 0.00017300

C -2.95716100 1.58695400 -0.00045900

C -1.62066300 1.65663400 -0.00030400

N -0.87239600 0.49130800 -0.00017900

C -1.56808300 -0.70807100 -0.00089200

C 0.51218200 0.39750800 -0.00019200

C 0.92895100 -1.01213700 -0.00005800

S -0.45413000 -2.08072500 -0.00019300

C 1.39381200 1.41495100 -0.00009900

C 2.82719200 1.13247800 0.00014000

C 3.27110700 -0.35563000 0.00032400

C 2.22163500 -1.37811700 0.00020400

O 4.44523300 -0.63040000 0.00046900

O 3.66112000 2.00482100 -0.00007200

O -4.85499100 0.19431500 0.00134000

H -3.55845900 2.48444100 -0.00024000

H -1.06225300 2.58143700 0.00045200

H 1.10309000 2.45687400 -0.00027800

H 2.53699000 -2.41351500 0.00045700

1. The Cartesian coordinates of the optimized structure of the oxidized form of catechol in gas phase at the B3LYP/6-311++g(d,p) level with the following keywords:

---------------------------------------------- # RB3LYP/6-311++G(d,p) Opt-----------------------------------------

0 1

C -1.77906100 0.73156900 0.00006700

C -1.77905800 -0.73157300 0.00003400

C -0.63816100 -1.45339900 -0.00008000

C 0.67375500 -0.78057600 -0.00044400

C 0.67375200 0.78057700 -0.00024000

C -0.63816500 1.45339700 0.00005900

O 1.72962300 1.38809100 0.00006000

O 1.72962800 -1.38808700 0.00030700

H -2.74288500 1.23477400 0.00021100

H -2.74288000 -1.23478200 0.00021000

H -0.63330500 -2.53937900 0.00004400

H -0.63331200 2.53937700 0.00021800

1. The Cartesian coordinates of the optimized structure of the oxidized form of catechol in solution phase at the B3LYP/6-311++g(d,p) level with the following keywords:

---------------------- # RB3LYP/6-311++G(d,p) Opt scrf=(cpcm, solvent=water)------------------------------

0 1

C 1.77708400 -0.73201700 0.00012300

C 1.77708500 0.73201600 -0.00009100

C 0.63687100 1.45686300 -0.00013500

C -0.66552800 0.78136500 0.00010600

C -0.66552800 -0.78136400 -0.00032100

C 0.63686900 -1.45686300 0.00012700

O -1.73364600 -1.37652800 -0.00008000

O -1.73364600 1.37652800 0.00019500

H 2.74100000 -1.23284100 0.00026700

H 2.74100100 1.23284000 -0.00013200

H 0.63760900 2.54246700 -0.00021500

H 0.63760700 -2.54246700 0.00029900

1. The Cartesian coordinates of the optimized structure of the reduced form of DTDFO in gas phase at MPW1PW91/6-311++g(d,p) level with the following keywords:

-------------------------------------# MPW1PW91/6-311++g(d,p) opt--------------------------------------------------------

0 1

C 0.81565100 -1.01544100 -0.00020400

C 0.43607500 0.32504100 -0.00005700

C 1.39214100 1.33448000 0.00022300

C 2.72850200 0.97172800 0.00022900

C 3.11712100 -0.37699000 0.00008500

C 2.15631900 -1.37445700 -0.00010800

C -3.73829600 0.33014000 0.00024500

C -3.01652400 1.60930200 -0.00097700

C -1.67532900 1.65145000 -0.00086700

N -0.95340200 0.47770400 0.00000200

C -1.66999200 -0.70397600 -0.00010800

N -2.94235600 -0.82333900 -0.00014600

S -0.57497900 -2.08412800 -0.00024100

O -4.94928500 0.26778500 0.00149500

O 4.42538000 -0.71061200 0.00015000

O 3.76350900 1.85956500 0.00048200

H 1.11369700 2.38171000 0.00037800

H 2.47231700 -2.40929400 -0.00020300

H -3.59728100 2.52080000 -0.00168000

H -1.10267900 2.56853400 -0.00144600

H 4.94740500 0.09843200 -0.00008400

H 3.44566700 2.76373000 0.00011400

1. The Cartesian coordinates of the optimized structure of the reduced form of DTDFO in solution phase at the MPW1PW91/6-311++g(d,p) level with the following keywords:

------------------------# opt mpw1pw91/6-311++g(d, p) scrf=(cpcm,solvent=water)-----------------------

0 1

C -0.82355900 -1.02290700 0.00009800

C -0.43936600 0.32376500 -0.00002600

C -1.39865500 1.34048700 -0.00018300

C -2.74098200 0.97828000 -0.00013300

C -3.13437600 -0.37696100 0.00003300

C -2.17103000 -1.38123800 0.00012500

C 3.76175800 0.33866000 -0.00004400

C 3.03096500 1.61989800 0.00048200

C 1.68356400 1.65946000 0.00039300

N 0.95831300 0.47838500 -0.00016300

C 1.68352900 -0.71085800 -0.00015400

N 2.96098900 -0.82767000 -0.00008700

S 0.57613500 -2.10434300 0.00005600

O 4.98077800 0.27603300 -0.00039100

O -4.45330000 -0.70825800 0.00011300

O -3.78434400 1.87240300 -0.00025400

H -1.11715700 2.38965500 -0.00045900

H -2.49049800 -2.41761100 0.00025200

H 3.61120700 2.53481500 0.00092000

H 1.10472200 2.57547800 0.00069300

H -4.96757100 0.11748200 0.00027700

H -3.45014200 2.78173600 -0.00012900

1. The Cartesian coordinates of the optimized structure of the reduced form of DTDFO in gas phase at the B3LYP/6-311++g(d,p) level with the following keywords:

------------------------------------# B3LYP/6-311++g(d,p) opt--------------------------------------------------------

0 1

C 0.82233700 -1.01952400 -0.00010300

C 0.43877600 0.32412900 -0.00010000

C 1.39798400 1.33723800 -0.00020900

C 2.73856500 0.97664200 -0.00007300

C 3.13074200 -0.37648000 -0.00000900

C 2.16725000 -1.37683800 -0.00007600

C -1.68193800 -0.70917100 -0.00000800

N -2.95509700 -0.82550500 0.00005800

C -3.75899300 0.33681500 0.00008200

C -3.02745800 1.61711000 -0.00016600

C -1.68342900 1.65816200 -0.00023200

N -0.95800700 0.47830600 -0.00009100

S -0.57602700 -2.10102600 0.00000000

O 4.44709700 -0.71034500 0.00012000

O 3.77961900 1.87134400 -0.00052700

O -4.97142000 0.27394200 0.00035700

H 1.11817300 2.38443800 -0.00060500

H 2.48613100 -2.41108300 0.00009300

H -3.60853500 2.52892600 -0.00028100

H -1.10923300 2.57448300 -0.00042300

H 4.96348800 0.10606300 0.00125100

H 3.45275400 2.77595800 0.00594600

1. The Cartesian coordinates of the optimized structure of the reduced form of DTDFO in solution phase at B3LYP/6-311++g(d,p) level with the following keywords:

------------------# B3LYP/6-311++g(d,p) opt scrf=(cpcm,solvent=water)-----------------------------

0 1

C 0.82211900 -1.01970700 -0.00030200

C 0.44216500 0.32291400 -0.00034700

C 1.39692700 1.33979700 -0.00038800

C 2.73694400 0.97912300 -0.00012100

C 3.12602200 -0.37904800 -0.00004100

C 2.16673300 -1.38225000 -0.00017100

C -1.67286600 -0.70598900 -0.00001700

N -2.95808200 -0.81869000 0.00021700

C -3.74538300 0.34074300 0.00017100

C -3.02561600 1.61512800 -0.00026400

C -1.67874300 1.65609300 -0.00048500

N -0.95923500 0.47656600 -0.00028900

S -0.58128900 -2.09632900 -0.00002400

O 4.44441800 -0.70938600 0.00025900

O 3.77660200 1.86337800 -0.00031000

O -4.97179000 0.26831400 0.00072900

H 1.11786900 2.38592800 -0.00047000

H 2.48077700 -2.41778600 0.00014300

H -3.59805100 2.53225100 -0.00040900

H -1.10640500 2.57228400 -0.00083100

H 4.96078000 0.10895600 0.00219200

H 3.46322700 2.77523500 0.00664500

1. The Cartesian coordinates of the optimized structure of the reduced form of catechol in gas phase at the B3LYP/6-311++g(d,p) level with the following keywords:

---------------------------------------------- # RB3LYP/6-311++G(d,p) Opt-----------------------------------------

0 1

C -1.91218700 -0.66013400 0.00012000

C -1.88212100 0.73363500 -0.00007300

C -0.65353100 1.40337400 -0.00012200

C 0.53064300 0.67461100 0.00000700

C 0.50374400 -0.73085700 -0.00009500

C -0.72136100 -1.39227100 0.00006100

O 1.66804900 -1.44265500 -0.00009900

O 1.79362800 1.23033000 0.00014300

H -2.86280400 -1.18544400 0.00045600

H -2.80507600 1.30564100 -0.00025600

H -0.61632300 2.49153400 -0.00020900

H -0.72265700 -2.47789200 0.00003200

H 2.39955300 -0.80180600 -0.00009700

H 1.72276500 2.19641700 0.00033900

1. The Cartesian coordinates of the optimized structure of the reduced form of catechol in solution phase at the B3LYP/6-311++g(d,p) level with the following keywords:

---------------------- # RB3LYP/6-311++G(d,p) Opt scrf=(cpcm, solvent=water)------------------------------

0 1

C -1.91524200 -0.65999300 0.00000400

C -1.88170400 0.73447600 -0.00002500

C -0.65281600 1.40593900 -0.00000200

C 0.53355800 0.67753500 0.00002200

C 0.50168100 -0.72947600 -0.00000700

C -0.72291800 -1.39258100 0.00004200

O 1.66839900 -1.44389500 -0.00007700

O 1.79383400 1.22609000 0.00004900

H -2.86601300 -1.18502200 0.00008300

H -2.80398900 1.30773800 -0.00009700

H -0.61579200 2.49294500 -0.00006500

H -0.72795000 -2.47867900 0.00006500

H 2.40301700 -0.80488300 0.00017800

H 1.73750200 2.19493700 -0.00014100

1. E-mail address: Hassan.goodarzi49@gmail.com [↑](#footnote-ref-1)
2. Corresponding author. Tel.: +98 023135195 363.

   E-mail address: aasghari@semnan.ac.ir (A. Asghari), [↑](#footnote-ref-2)
3. E-mail address: nemat@basu.ac.ir [↑](#footnote-ref-3)
4. E-mail address: mrajabi@semnan.ac.ir [↑](#footnote-ref-4)