**TDO Structure Investigation in Aqueous Solution by TOF-MS, UV, Raman and Quantum Chemistry Calculations**

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Table S1 The standard orientation of the I, II, I2-line, II2-line, II2-cyc, I3-cyc and I4-cyc models(in Figure 1) for TDO aqueous solution in B3LYP/cc-PVDZ calculations

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Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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I

1 6 0 1.114271 0.016112 -0.121688

2 16 0 -1.044204 -0.238171 -0.391530

3 7 0 2.070998 -0.896377 -0.195647

4 8 0 -1.282238 1.241278 -0.090583

5 8 0 -1.307821 -1.167561 0.760449

6 1 0 3.018985 -0.759627 0.156433

7 1 0 1.821490 -1.840519 -0.467411

8 7 0 1.273870 1.233473 0.319002

9 1 0 0.362548 1.746638 0.358410

10 1 0 2.125016 1.618172 0.724760

II

1 6 0 1.052778 0.141228 -0.063050

2 16 0 -0.800610 -0.097544 -0.470151

3 7 0 1.607270 -1.085528 0.126133

4 7 0 1.642226 1.265372 -0.047362

5 8 0 -1.317707 1.270340 0.396034

6 8 0 -1.146322 -1.374756 0.268634

7 1 0 2.540987 -1.100965 0.525646

8 1 0 0.952496 -1.799983 0.444382

9 1 0 0.992527 2.029470 -0.261766

10 1 0 -1.027146 1.161230 1.323721

I2-line

1 6 0 -2.336850 0.999091 -0.061932

2 16 0 -1.967982 -0.900396 -0.424195

3 7 0 -1.418854 1.919145 -0.195546

4 7 0 -3.581182 1.119477 0.333420

5 8 0 -3.398593 -1.384941 -0.162700

6 8 0 -1.029028 -1.169891 0.783723

7 1 0 -1.614086 2.887377 0.054254

8 1 0 -0.412504 1.644621 -0.450939

9 1 0 -4.055354 0.187852 0.365208

10 1 0 -4.003773 1.973769 0.680684

11 6 0 2.336850 -0.999091 0.061932

12 16 0 1.967982 0.900396 0.424195

13 7 0 3.581182 -1.119477 -0.333420

14 7 0 1.418854 -1.919145 0.195546

15 8 0 1.029028 1.169891 -0.783723

16 8 0 3.398593 1.384941 0.162700

17 1 0 4.003773 -1.973769 -0.680684

18 1 0 4.055354 -0.187852 -0.365208

19 1 0 0.412504 -1.644621 0.450939

20 1 0 1.614086 -2.887377 -0.054254

II2-cyc

1 6 0 -0.954023 -0.937962 0.878673

2 7 0 -0.401929 -0.322791 1.902756

3 7 0 -0.411158 -1.918943 0.189928

4 16 0 -2.564740 -0.100370 0.107627

5 8 0 -2.210004 -0.415984 -1.367018

6 8 0 -2.197057 1.346948 0.520862

7 1 0 0.640777 -0.272743 1.972773

8 1 0 -0.895068 0.538519 2.152957

9 1 0 0.631343 -1.989684 0.128573

10 1 0 -0.911031 -2.105822 -0.683550

11 6 0 0.954023 0.937962 -0.878673

12 7 0 0.411158 1.918943 -0.189928

13 7 0 0.401929 0.322791 -1.902756

14 16 0 2.564740 0.100370 -0.107627

15 8 0 2.197057 -1.346948 -0.520862

16 8 0 2.210004 0.415984 1.367018

17 1 0 -0.631343 1.989684 -0.128573

18 1 0 0.911031 2.105822 0.683550

19 1 0 -0.640777 0.272743 -1.972773

20 1 0 0.895068 -0.538519 -2.152957

II3-cyc

1 6 0 -2.054215 1.154784 0.000000

2 7 0 -2.192816 0.584258 1.172576

3 7 0 -2.192816 0.584258 -1.172576

4 16 0 -1.575890 3.014721 0.000000

5 8 0 -0.726642 3.009306 -1.301881

6 8 0 -0.726642 3.009306 1.301881

7 1 0 -2.299702 -0.459876 1.280723

8 1 0 -1.914330 1.169203 1.961369

9 1 0 -2.299702 -0.459876 -1.280723

10 1 0 -1.914330 1.169203 -1.961369

11 6 0 2.027180 1.201611 0.000000

12 7 0 1.602390 1.606905 1.172576

13 7 0 1.602390 1.606905 -1.172576

14 16 0 3.398770 -0.142600 0.000000

15 8 0 2.969456 -0.875363 -1.301881

16 8 0 2.969456 -0.875363 1.301881

17 1 0 0.751587 2.221539 1.280723

18 1 0 1.969724 1.073258 1.961369

19 1 0 0.751587 2.221539 -1.280723

20 1 0 1.969724 1.073258 -1.961369

21 6 0 0.027035 -2.356395 0.000000

22 7 0 0.590426 -2.191163 1.172576

23 7 0 0.590426 -2.191163 -1.172576

24 16 0 -1.822880 -2.872121 0.000000

25 8 0 -2.242814 -2.133943 -1.301881

26 8 0 -2.242814 -2.133943 1.301881

27 1 0 1.548115 -1.761663 1.280723

28 1 0 -0.055394 -2.242460 1.961369

29 1 0 1.548115 -1.761663 -1.280723

30 1 0 -0.055394 -2.242460 -1.961369

II4-cyc

1 6 0 -2.697971 -1.876993 0.007575

2 7 0 -2.235423 -2.249159 1.175803

3 7 0 -2.251335 -2.240779 -1.169410

4 1 0 -1.395841 -2.876057 1.278679

5 1 0 -2.655509 -1.772693 1.973922

6 1 0 -1.408531 -2.860038 -1.288735

7 1 0 -2.681608 -1.755705 -1.957009

8 16 0 -4.222733 -0.723452 0.020707

9 8 0 -3.919069 0.059933 -1.286233

10 8 0 -3.896520 0.061491 1.321025

11 6 0 2.694450 1.874891 0.008425

12 7 0 2.231930 2.245485 1.177128

13 7 0 2.246738 2.239102 -1.168036

14 1 0 1.392215 2.872039 1.280473

15 1 0 2.650541 1.766109 1.974227

16 1 0 1.405986 2.861232 -1.287027

17 1 0 2.679367 1.758061 -1.956788

18 16 0 4.221346 0.724126 0.020181

19 8 0 3.919747 -0.057409 -1.288188

20 8 0 3.896245 -0.063888 1.318986

21 6 0 1.894036 -2.677965 -0.007125

22 7 0 2.266093 -2.238384 1.169804

23 7 0 2.269132 -2.218244 -1.175668

24 16 0 0.721802 -4.188282 -0.021792

25 8 0 -0.059707 -3.849785 -1.321246

26 8 0 -0.056651 -3.876308 1.286243

27 1 0 2.896482 -1.403631 1.288701

28 1 0 1.778591 -2.664293 1.958134

29 1 0 2.905774 -1.385916 -1.279757

30 1 0 1.782397 -2.629246 -1.972384

31 6 0 -1.890354 2.676576 -0.007963

32 7 0 -2.257720 2.231941 1.168483

33 7 0 -2.266081 2.218107 -1.176638

34 16 0 -0.722432 4.189578 -0.019523

35 8 0 0.060693 3.857760 -1.319765

36 8 0 0.057021 3.878163 1.287866

37 1 0 -2.890296 1.399162 1.287708

38 1 0 -1.770808 2.658509 1.956780

39 1 0 -2.905802 1.388367 -1.280728

40 1 0 -1.789074 2.637387 -1.974624

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Table S2 The frequencies of the I, II, I2-line, II2-line, II2-cyc, I3-cyc and I4-cyc models(in Figure 1) for TDO aqueous solution in B3LYP/cc-PVDZ calculations

|  |  |  |
| --- | --- | --- |
| Number | Model | Frequencies |
| 1 | I | 68.6571,88.2862,181.4617,276.2997,375.2622,418.4748,426.1832,509.9976,536.5852,550.5230,675.8411,867.5791,,1007.0610,1073.1018,1146.5197,1164.8591,1337.9286,1505.2572,1617.3619,1704.2348, 3108.2616, 3470.3706,3531.8109,3637.8911 |
| 2 | II | 68.7659,216.6568,248.7720,319.2002,352.4572,405.5758,435.7222,496.8159,567.5432,603.9236,656.6092,704.9020,804.6019,1070.9762,1111.5060,1134.8587,1146.8998,1327.0031,1574.2385,1768.2523,3468.8926,3492.7616,3632.4305,3662.4362 |
| 3 | I2-line | 37.2715,47.2674,56.6560,96.1857,116.3008,126.1622,152.8477,175.0452,212.4439,279.3910,288.7709,297.8911,315.4088,315.4875,431.7606,435.4590,439.7778,462.7257,499.2707,505.9706,545.6104,572.9879,591.1805,612.8216,676.5894,678.3874,836.7396,837.2027,930.8975,960.7189,1028.7844,1038.1084,1073.2606,1078.0701,1100.5896,1101.3776,1156.2142,1156.2693,1353.9939,1357.2380,1505.9706,1509.9321,1629.9005,1639.8833,1751.1767,1753.8526,2538.9965,2640.1705,3126.7796,3127.2005,3532.2822, 3532.7525,3601.6931,3601.7197 |
| 4 | II2-cyc | 82.8754,87.8818,126.2233,128.6522,140.4760,180.7623,197.7454,203.0284,240.8926,265.6960,267.5557,309.4463,369.9422,381.8670,390.8667,394.8749,445.3152,451.1147,590.6187,593.8047,644.6617,652.6046,656.4365,658.4314,730.3196,735.7032,741.6843,779.8077,861.8848,862.7168,959.4277,963.6308,1017.9442,1023.5269,1158.4754,1159.9340,1189.7367,1190.8307,1449.1868,1449.4472,1588.7853,1593.9373,1659.8359,1671.2298,1710.1081,1733.3548,3051.8697,3054.2752,3097.6265,3150.5180,3487.7286,3489.0858, 3493.0860,3497.2778 |
| 5 | I3-cyc | 59.0750,59.0750,61.2731,61.2731,86.4641,91.8293,91.8293,95.4969,113.5855,157.2448,157.2448,177.5463,182.7864,182.7864,208.0494,244.7587,269.6002,269.6002,281.7024,321.3931,321.3931,397.5830,397.5830,407.3818,410.5970,425.7366,425.7366,450.8477,458.8690,458.8690,616.7154,617.8026,617.8026,621.3170,621.3170,633.2197,669.8327,669.8327,670.8450,709.4912,709.4912,736.7299,916.3770,916.8876,916.8876,919.6793,944.4266,944.4266,964.3374,964.3374,968.7311,998.7658,1000.4426,1000.4426,1159.6046,1160.9676,1160.9676,1177.5120,1177.5120,1181.6363,1455.9520,1455.9520,1461.1234,1571.1089,1571.1089,1576.6152,1642.5229,1642.5229,1650.5306,1745.9638,1745.9638,1762.3339,2832.7350,2833.0418,2833.0418,2887.0211,2982.2953,2982.2953,3522.4576,3523.2728,3523.2728,3528.1927,3531.4186,3531.4186 |
| 6 | I4-cyc | 21.4480,24.9020,47.8465,71.7766,73.8745,74.0842,74.7158,76.0724,76.3675,81.4917,95.1991,109.0688,109.3133,117.4085, 151.2310,160.4869,167.2622,169.1391,176.5683,177.4760,195.4652,198.3260,252.8635,256.5034,257.9556,262.8518,297.3088,311.9090,312.1866,313.5182,392.4599,399.2423,399.6700,404.9998,406.3302,424.2415,424.7092,440.9139,456.4441,460.9214,461.1190,465.1047,598.3985,603.6007,604.5945,612.1973,613.1523,618.0620,618.2165,621.3076,661.0241,661.7757,662.4793,662.7435,699.9435,707.8727,708.3197,722.9844,908.2264,910.3167,911.1992,914.1288,931.1129,939.8401,940.2007,940.7168, 951.8116,956.6412,956.6755,965.3223,1000.5998,1000.9177, 1001.3958,1002.6982,1157.2748,1166.2709,1169.1377,1169.2612,1172.2263,1455.5932,1457.6719,1457.7663,1460.4159,1563.0750,1567.2889,1567.3751,1571.8880,1631.9860,1635.4691,1635.6298,1641.2913,1754.0874,1757.4746,1757.7669,1765.7583,2864.9915,2867.4587,2868.3333,2868.4226,2919.5399,2996.9241,2998.8578,3028.5821,3532.3386,3532.6920,3533.1594,3534.3832,3538.2591, 3540.5498,3541.1194, 3542.7011 |