Stereoelectronic effects of the glycosidic linkage on the conformational preference of D-Sucrose

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1 Electronic Supplementary Information

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Table S1. Optimized conformations of D-Sucrose (energy with ZPE correction) at M06-2X/6-31++G(d,p) level in vacuum

Entr.	Conformer	Dihedral Angle					Dipole Moment (D)	ΔE (kcal.mol^{-1})
		O5-C1-O1-C8	C1-O1-C8-O8	O5-C5-C6-O6	O8-C8-C7-O7	O8-C11-C12-O12		
1	S1-gg-tg-gg	111.9	-52.5	-66.3	-176.6	-62.1	2.042	0.38
2	S1-gt-tg-gg	111.5	-46.0	88.4	-179.4	-59.2	3.135	0.58
3	S1-tg-tg-gg	111.4	-52.7	-173.4	-177.0	-61.7	3.016	0.00
4	S1-gt-tg-gg^{ccw}	107.9	-36.8	78.0	171.4	-66.2	4.085	2.27
5	S2-gg-gt-tg	86.0	-168.4	-64.6	53.2	171.5	1.781	10.09
6	S2-gg-gt-gg	100.0	-162.5	-65.3	66.2	-59.4	2.715	5.67
7	S2-gg-tg-gg	97.2	-170.0	-65.6	176.8	-60.4	2.496	7.51
8	S2-gt-gt-gg	95.0	-161.4	59.7	61.6	-59.3	3.974	7.16
9	S2-tg-gt-gg	85.5	-169.1	-179.5	53.0	171.5	1.999	9.74
10	S2-tg-gt-gg	99.9	-162.0	-175.3	66.7	-59.6	3.937	5.73
11	S3-gt-tg-gt	104.9	-41.3	-62.8	173.7	172.4	4.122	7.73
12	S3-tg-tg-tg	104.8	-40.4	-178.6	173.2	172.1	4.520	8.21
13	S4-gg-gt-tg	65.9	-78.1	-63.3	47.9	173.4	3.168	10.92
14	S4-gg-gt-tg	68.7	-83.4	-64.1	52.6	172.8	1.655	9.55
15	S4-gg-gt-gt	63.2	-79.8	-63.2	50.4	69.7	3.417	10.38
16	S4-gt-gg-gt	67.3	-80.1	66.8	-74.8	74.2	2.837	9.20
17	S4-gt-gt-tg	68.3	-72.8	66.6	45.8	174.3	3.461	11.21
18	S4-tg-gt-tg	65.6	-79.0	-178.0	48.9	173.2	3.766	11.46
19	S4-tg-gt-gt	64.5	-73.7	175.0	47.8	63.4	5.747	7.84
20	S5-gg-tg-gg	111.4	60.8	-65.4	-176.2	-53.9	2.687	7.90
21	S6-gg-tg-tg	112.5	-48.6	-63.5	-178.4	176.0	2.440	7.72
22	S7-gg-tg-gg	78.5	-179.3	-66.4	-167.4	-74.5	3.400	8.19

Table S2. Optimized conformations of D-Sucrose (energy with ZPE correction) at M06-2X/6-31++G(d,p) level in water (IEF-PCM/bondi)

Entr.	Conformer	Dihedral Angle					Dipole Moment (D)	ΔE (kcal.mol^{-1})
		O5-C1-O1-C8	C1-O1-C8-O8	O5-C5-C6-O6	O8-C8-C7-O7	O8-C11-C12-O12		
1	S1-gg-tg-gg	112.0	-52.5	-61.5	-176.9	-63.6	2.816	0.08
2	S1-gt-tg-gg	110.8	-44.9	83.6	179.3	-58.8	4.984	0.00
3	S1-tg-tg-gg	111.6	-53.3	179.6	-177.1	-62.9	4.315	1.01
4	S1-gt-tg-gg^{ccw}	107.9	-40.3	81.7	171.5	-60.7	7.113	0.75
5	S2-gg-gt-tg	92.5	-171.5	-61.6	52.4	172.7	1.808	6.95
6	S2-gg-gt-gg	97.2	-159.3	-62.9	62.0	-61.0	4.415	2.07
7	S2-gg-tg-gg	90.7	-165.4	-61.7	-178.0	-60.3	3.200	5.11
8	S2-gt-gt-gg	93.8	-160.1	61.9	57.1	-61.1	6.501	1.79
9	S2-tg-gt-gg	93.2	-171.0	-178.8	51.7	-78.1	2.564	7.58
10	S2-tg-gt-gg	97.1	-158.5	179.6	61.6	-61.0	6.103	3.10
11	S3-gt-tg-gt	95.5	-61.9	53.4	173.9	68.7	7.217	3.21
12	S3-tg-tg-tg	103.1	-44.6	-178.4	173.4	174.9	6.496	4.49
13	S4-gg-gt-tg	69.2	-78.9	-62.0	44.9	176.6	4.226	7.67
14	S4-gg-gt-tg	70.5	-78.4	-61.5	46.2	172.3	2.626	8.34
15	S4-gg-gt-gt	68.8	-78.3	-62.0	44.7	67.8	4.805	6.95
16	S4-gt-gg-gt	64.2	-73.0	63.9	-53.1	67.9	3.900	5.74
17	S4-gt-gt-tg	66.1	-75.6	65.1	43.8	175.8	4.730	7.57
18	S4-tg-gt-tg	68.8	-77.0	179.9	44.0	175.7	4.973	8.50
19	S4-tg-gt-gt	67.5	-73.8	172.5	43.4	63.6	7.714	5.39
20	S5-gg-tg-gg	107.1	64.7	-62.7	-150.1	-56.3	3.407	4.15
21	S6-gg-tg-tg	90.4	45.4	-61.2	-175.1	175.0	3.076	8.13
22	S7-gg-tg-gg	74.3	-168.1	-62.1	-167.9	-63.3	4.786	4.89

Table S3. Orbital interactions (kcal mol^{-1}) for the conformations of D-Sucrose calculated at M06-2X/6-31++G(d,p) level

Entry	Orbital Interactions	S1-gt-tg-gg	S2-gt-gt-gg	S3-gt-tg-gt	S1-gg-tg-gg	S1-tg-tg-gg	S1-gt-tg-gg^{ccw}
1	$\eta_{O5} \rightarrow \sigma^*_{O7-HO7}$	-	1.53	-	-	-	-
2	$\eta_{O5} \rightarrow \sigma^*_{O7-HO7}$	-	3.57	-	-	-	-
3	$\eta_{O5} \rightarrow \sigma^*_{O12-HO12}$	3.96	-	-	3.12	2.82	4.69
4	$\eta_{O5} \rightarrow \sigma^*_{O12-HO12}$	4.46	-	-	5.58	5.53	4.48
5	$\eta_{O5} \rightarrow \sigma^*_{O6-HO6}$	-	-	0.51	-	-	-
6	$\eta_{O1} \rightarrow \sigma^*_{O2-HO2}$	-	-	-	-	-	1.21
7	$\eta_{O1} \rightarrow \sigma^*_{O9-HO9}$	-	-	3.84	-	-	-
8	$\eta_{O1} \rightarrow \sigma^*_{O12-HO12}$	-	3.07	-	-	-	-
9	$\eta_{O2} \rightarrow \sigma^*_{O7-HO7}$	3.32	-	4.74	2.83	2.60	-
10	$\eta_{O2} \rightarrow \sigma^*_{O7-HO7}$	7.04	-	7.75	9.64	10.25	-
11	$\eta_{O2} \rightarrow \sigma^*_{O9-HO9}$	-	3.17	-	-	-	-
12	$\eta_{O2} \rightarrow \sigma^*_{O9-HO9}$	-	9.57	-	-	-	-
13	$\eta_{O3} \rightarrow \sigma^*_{O2-HO2}$	-	-	-	0.51	0.75	-
14	$\eta_{O3} \rightarrow \sigma^*_{O4-HO4}$	-	-	-	-	-	0.70
15	$\eta_{O4} \rightarrow \sigma^*_{O3-HO3}$	0.63	0.71	0.70	0.52	-	-
16	$\eta_{O6} \rightarrow \sigma^*_{O4-HO4}$	-	-	-	-	2.19	-
17	$\eta_{O6} \rightarrow \sigma^*_{O4-HO4}$	-	-	-	-	6.97	-
18	$\eta_{O6} \rightarrow \sigma^*_{O7-HO7}$	-	0.91	-	-	-	-
19	$\eta_{O6} \rightarrow \sigma^*_{O7-HO7}$	-	3.89	-	-	-	-
20	$\eta_{O6} \rightarrow \sigma^*_{O12-HO12}$	-	-	2.96	-	-	-
21	$\eta_{O6} \rightarrow \sigma^*_{O12-HO12}$	-	-	13.54	-	-	-
22	$\eta_{O8} \rightarrow \sigma^*_{O12-HO12}$	1.08	0.87	-	0.69	0.75	0.93

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Entry	Orbital Interactions	S1-gt-tg-gg	S2-gt-gt-gg	S3-gt-tg-gt	S1-gg-tg-gg	S1-tg-tg-gg	S1-gt-tg-gg^{ccw}
23	$\eta_{O7} \rightarrow \sigma^*_{O2-HO2}$	-	-	-	-	-	2.40
24	$\eta_{O7} \rightarrow \sigma^*_{O2-HO2}$	-	-	-	-	-	7.68
25	$\eta_{O20} \rightarrow \sigma^*_{O9-HO9}$	-	-	-	2.38	2.29	-
26	$\eta_{O12} \rightarrow \sigma^*_{O6-HO6}$	4.71	-	-	-	-	4.43
27	$\eta_{O12} \rightarrow \sigma^*_{O6-HO6}$	12.36	-	-	-	-	12.21
28	$\sigma_{C1-O1} \rightarrow \sigma^*_{C2-H2}$	0.82	0.85	0.95	0.85	0.87	0.83
29	$\sigma_{C1-O1} \rightarrow \sigma^*_{C8-C9}$	1.11	-	1.18	1.18	1.16	1.17
30	$\sigma_{C1-O1} \rightarrow \sigma^*_{C8-O8}$	-	1.41	-	-	-	-
31	$\sigma_{C2-H2} \rightarrow \sigma^*_{C1-O1}$	4.58	4.54	-	4.52	4.51	4.66
32	$\sigma_{C8-C9} \rightarrow \sigma^*_{C1-O1}$	3.18	0.56	4.22	3.22	3.26	2.89
33	$\sigma_{C8-O8} \rightarrow \sigma^*_{C1-O1}$	-	1.67	-	-	-	-
34	$\eta_{O5} \rightarrow \sigma^*_{C1-O1}$	2.99	2.21	1.54	2.80	2.97	3.14
35	$\eta_{O5} \rightarrow \sigma^*_{C1-O1}$	11.61	13.91	15.54	12.15	11.92	11.98
36	$\eta_{O8} \rightarrow \sigma^*_{C1-O1}$	-	0.63	-	-	-	-
37	$\sigma_{C8-O1} \rightarrow \sigma^*_{C1-C2}$	0.72	0.97	0.72	0.66	0.66	0.61
38	$\sigma_{C8-O1} \rightarrow \sigma^*_{C1-O5}$	-	-	-	0.50	-	-
39	$\sigma_{C8-O1} \rightarrow \sigma^*_{C7-H7a}$	-	0.64	-	-	-	-
40	$\sigma_{C8-O1} \rightarrow \sigma^*_{C7-H7b}$	0.80	-	0.58	0.74	0.74	0.81
41	$\sigma_{C8-O1} \rightarrow \sigma^*_{C8-O8}$	-	0.54	-	-	-	-
42	$\sigma_{C8-O1} \rightarrow \sigma^*_{C9-H9}$	0.88	0.86	-	0.83	0.84	1.00
43	$\sigma_{C1-C2} \rightarrow \sigma^*_{C8-O1}$	1.84	2.49	2.50	1.74	1.78	2.17
44	$\sigma_{C1-O5} \rightarrow \sigma^*_{C8-O1}$	0.57	-	-	0.56	0.56	0.56
45	$\sigma_{C7-H7a} \rightarrow \sigma^*_{C8-O1}$	-	6.88	-	-	-	-

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Entry	Orbital Interactions	S1-gt-tg-gg	S2-gt-gt-gg	S3-gt-tg-gt	S1-gg-tg-gg	S1-tg-tg-gg	S1-gt-tg-gg^{ccw}
46	$\sigma_{C7-H7b} \rightarrow \sigma^*_{C8-O1}$	5.60	-	6.09	5.85	5.85	5.32
47	$\sigma_{C9-H9} \rightarrow \sigma^*_{C8-O1}$	4.49	4.97	-	4.65	4.60	4.34
48	$\sigma_{C9-C10} \rightarrow \sigma^*_{C8-O1}$	-	-	2.24	-	-	-
49	$\sigma_{C11-O8} \rightarrow \sigma^*_{C8-O1}$	0.60	-	1.00	-	-	0.64
50	$\eta_{O8} \rightarrow \sigma^*_{C8-O1}$	19.08	19.94	17.32	19.66	19.65	18.90
51	$\eta_{O1} \rightarrow \sigma^*_{C1-C2}$	0.67	1.73	1.17	0.66	0.70	0.68
52	$\eta_{O1} \rightarrow \sigma^*_{C1-O5}$	0.77	-	-	0.72	0.72	0.71
53	$\eta_{O1} \rightarrow \sigma^*_{C1-H1}$	4.59	3.38	4.26	4.55	4.59	4.45
54	$\eta_{O1} \rightarrow \sigma^*_{C2-H2}$	-	-	-	-	-	-
55	$\eta_{O1} \rightarrow \sigma^*_{C7-C8}$	0.68	3.91	2.03	1.09	1.14	0.57
56	$\eta_{O1} \rightarrow \sigma^*_{C7-H7b}$	-	-	-	-	-	-
57	$\eta_{O1} \rightarrow \sigma^*_{C8-C9}$	1.73	-	2.10	1.81	1.84	1.80
58	$\eta_{O1} \rightarrow \sigma^*_{C8-O8}$	4.71	4.04	2.04	3.66	3.59	5.17
59	$\eta_{O1} \rightarrow \sigma^*_{C9-H9}$	-	-	-	-	-	-
60	$\eta_{O1} \rightarrow \sigma^*_{C1-C2}$	4.60	1.72	2.22	4.59	4.50	3.72
61	$\eta_{O1} \rightarrow \sigma^*_{C1-O5}$	14.76	17.19	16.32	14.57	14.76	14.66
62	$\eta_{O1} \rightarrow \sigma^*_{C1-H1}$	-	2.34	1.13	-	-	-
63	$\eta_{O1} \rightarrow \sigma^*_{C2-H2}$	0.57	-	-	0.62	0.61	0.59
64	$\eta_{O1} \rightarrow \sigma^*_{C7-C8}$	7.44	2.53	5.78	7.18	7.14	7.93
65	$\eta_{O1} \rightarrow \sigma^*_{C7-H7b}$	0.68	-	-	0.58	0.57	0.68
66	$\eta_{O1} \rightarrow \sigma^*_{C8-C9}$	0.56	7.51	-	-	-	0.89
67	$\eta_{O1} \rightarrow \sigma^*_{C8-O8}$	8.87	2.60	13.97	10.77	11.03	7.84
68	$\sigma_{C1-H1} \rightarrow \sigma^*_{C7-H7a}$	-	-	0.89	-	-	-

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Entry	Orbital Interactions	S1-gt-tg-gg	S2-gt-gt-gg	S3-gt-tg-gt	S1-gg-tg-gg	S1-tg-tg-gg	S1-gt-tg-gg^{ccw}
69	$\sigma_{C12-H12a} \rightarrow \sigma^*_{C5-H5}$	-	-	0.52	-	-	-
70	$\eta_{O9} \rightarrow \sigma^*_{C1-H1}$	-	0.60	-	-	-	-
71	$\eta_{O9} \rightarrow \sigma^*_{C12-H12a}$	-	-	0.99	-	-	-
72	$\eta_{O12} \rightarrow \sigma^*_{C10-H10}$	-	0.66	-	0.64	0.62	-
73	$\sigma_{C6-O6} \rightarrow \sigma^*_{C5-O5}$	-	-	-	-	2.12	-
74	$\sigma_{C6-O6} \rightarrow \sigma^*_{C4-C5}$	1.26	1.59	1.36	-	-	1.28
75	$\sigma_{C6-O6} \rightarrow \sigma^*_{C5-H5}$	-	-	-	1.01	-	-
76	$\sigma_{C5-O5} \rightarrow \sigma^*_{C6-O6}$	-	-	-	-	2.14	-
77	$\sigma_{C4-C5} \rightarrow \sigma^*_{C6-O6}$	2.27	2.42	2.60	-	-	2.27
78	$\sigma_{C5-H5} \rightarrow \sigma^*_{C6-O6}$	1.33	0.79	-	4.67	-	1.24
79	$\sigma_{C6-H6a} \rightarrow \sigma^*_{C4-C5}$	-	-	-	3.30	-	-
80	$\sigma_{C6-H6a} \rightarrow \sigma^*_{C5-O5}$	4.54	4.37	4.32	0.72	0.57	4.80
81	$\sigma_{C6-H6a} \rightarrow \sigma^*_{C5-H5}$	-	-	-	-	2.52	-
82	$\sigma_{C6-H6a} \rightarrow \sigma^*_{O6-HO6}$	2.35	-	2.29	-	-	2.48
83	$\sigma_{C6-H6b} \rightarrow \sigma^*_{C4-C5}$	-	-	-	-	2.83	-
84	$\sigma_{C6-H6b} \rightarrow \sigma^*_{C5-O5}$	1.64	1.08	-	4.95	0.57	1.57
85	$\sigma_{C6-H6b} \rightarrow \sigma^*_{C5-H5}$	2.49	2.79	2.73	-	-	2.61
86	$\sigma_{C6-H6b} \rightarrow \sigma^*_{O6-HO6}$	-	2.29	-	2.60	-	-
87	$\sigma_{C5-O1} \rightarrow \sigma^*_{C6-H6a}$	0.74	1.03	0.91	-	-	0.69
88	$\sigma_{C4-C5} \rightarrow \sigma^*_{C6-H6a}$	-	-	-	1.10	-	-
89	$\sigma_{C5-H5} \rightarrow \sigma^*_{C6-H6a}$	-	-	-	-	2.14	-
90	$\sigma_{C5-O5} \rightarrow \sigma^*_{C6-H6b}$	-	-	-	0.95	-	-
91	$\sigma_{C4-C5} \rightarrow \sigma^*_{C6-H6b}$	-	-	-	-	1.07	-

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Table S3 – continuation of the previous page

Entry	Orbital Interactions	S1-gt-tg-gg	S2-gt-gt-gg	S3-gt-tg-gt	S1-gg-tg-gg	S1-tg-tg-gg	S1-gt-tg-gg^{ccw}
92	$\sigma_{C5-H5} \rightarrow \sigma^*_{C6-H6b}$	2.03	2.31	2.27	-	-	2.06
93	$\eta_{O5} \rightarrow \sigma^*_{O6-HO6}$	-	-	0.51	-	-	-
94	$\eta_{O4} \rightarrow \sigma^*_{O6-HO6}$	-	-	-	-	-	-
95	$\eta_{O4} \rightarrow \sigma^*_{O6-HO6}$	-	-	-	-	-	-
96	Σ	165.71	157.24	158.33	155.92	159.29	166.44

Table S4. Cartesian coordinates of S1-gt-tg-gg optimized at M06-2X/6-31++G(d,p) level in water (IEF-PCM/bondi)

Energy (Hartree) = -1297.5808111 ZPE (Hartree) = 0.3740493			
C	0.72648600	-0.44289200	-1.04824300
C	2.07293000	-1.15356000	-0.92097400
C	2.84756900	-0.63389200	0.27740700
C	2.95929000	0.88449900	0.22080500
C	1.54985400	1.47833300	0.11949500
C	1.53132700	2.99428400	0.02349400
C	1.32898600	-2.70473700	-0.72558300
C	1.39826300	-1.26311800	-0.24361400
C	2.21453400	-1.05071000	1.04108000
C	2.62344200	0.40898400	0.88523000
C	2.96185900	0.45448200	-0.60237900
C	2.84362600	1.79420800	-1.29814600
O	0.91911500	0.95517000	-1.06622200
O	0.08844300	-0.79190700	0.04005600
O	1.81416600	-2.54321300	-0.81490100
O	4.11938300	-1.25768300	0.25137700
O	3.60480900	1.29258100	1.41695800
O	0.30727100	3.56172800	0.45996600
O	2.03995200	-0.47208400	-1.21700500
O	0.67031100	-3.49565300	0.24720200
O	1.51837100	-1.27918900	2.23904900
O	3.75585800	0.79027400	1.63437600
O	1.53247700	2.32933600	-1.23396900
H	0.25036000	-0.69307200	-1.99945600
H	2.64892600	-0.94379600	-1.83211500
H	2.31259200	-0.90720300	1.19931100
H	3.54960400	1.17629500	-0.65827500
H	0.97210100	1.17553600	1.00381900
H	2.30581500	3.39977800	0.67859600
H	1.76259300	3.28756400	-1.00971000
H	2.66121200	-3.00762800	-0.75138500
H	4.59910600	-0.99350700	1.04905100
H	4.18664000	2.04072600	1.23424000
H	0.42291900	3.21776800	-0.08716600
H	0.81412900	-2.74956500	-1.69374700
H	2.34367100	-3.09022900	-0.84940400
H	3.11871300	-1.67436800	0.98301700
H	1.76342200	1.05508800	1.11111700
H	3.98517900	0.08033500	-0.73887900
H	3.51532800	2.50789100	-0.81388900
H	3.15392000	1.67836700	-2.34329200
H	0.27506600	-3.26916300	0.18738700
H	1.21419400	-2.19945300	2.23523400
H	3.48462500	0.95188300	2.54756400
H	0.88304600	1.64658800	-1.47853600

Table S5. Cartesian coordinates of S2-gt-gt-gg optimized at M06-2X/6-31++G(d,p) level in water (IEF-PCM/bondi)

Energy (Hartree) = -1297.5779288 ZPE (Hartree) = 0.3740220			
C	0.63314300	-0.03904600	-1.21862700
C	1.07367400	-1.50175600	-1.23359400
C	1.86056800	-1.84200500	0.02189400
C	3.00048300	-0.84678700	0.21341400
C	2.43618400	0.57593700	0.21728900
C	3.49440100	1.65789000	0.30085300
C	0.99409200	2.33888400	-1.03285200
C	1.41171500	1.02890900	-0.37498900
C	2.57010100	0.27751500	-1.05691900
C	3.13168100	-0.54320300	0.10685400
C	2.90561600	0.36613700	1.31423300
C	2.43792000	-0.33824400	2.57506200
O	1.73431400	0.81112400	-1.01178800
O	0.31958100	0.11502400	-0.19460600
O	0.10049100	-2.28865200	-1.35616900
O	2.34662000	-3.16354000	-0.12398600
O	3.61469800	-1.16197600	1.45365000
O	2.89092000	2.94554900	0.34468600
O	1.88308100	1.30530500	0.91466400
O	0.01859100	3.03245600	-0.28295800
O	2.20503700	-0.48036500	-2.18285800
O	4.50801800	-0.84608900	-0.00156400
O	1.23645500	-1.06293200	2.36252300
H	0.22161300	0.23069000	-2.19266800
H	1.72112800	-1.64305900	-2.10797000
H	1.19437900	-1.78016000	0.89536600
H	3.71679900	-0.95614000	-0.61236400
H	1.73861600	0.68335200	1.06191500
H	4.13019300	1.49049200	1.17561900
H	4.11450600	1.62853500	-0.60001600
H	0.13594200	-3.16181800	-1.69660400
H	2.82737700	-3.39357000	0.68391100
H	4.55912500	-0.96559400	1.40979200
H	2.58684100	3.11605900	1.24665200
H	1.88594800	2.96909300	-1.07440500
H	0.66219800	2.15918200	-2.06188500
H	3.32427500	1.00326800	-1.38127900
H	2.54494700	-1.46597300	0.20745800
H	3.82333900	0.92702500	1.52393800
H	3.20075700	-1.05508600	2.89237800
H	2.30639200	0.40709300	3.36913800
H	0.85754500	2.64050400	-0.44089400
H	1.61806000	-1.20840900	-1.90289500
H	4.61635000	-1.57970800	-0.62141900
H	0.62816000	-0.49838500	1.85776400

Table S6. Cartesian coordinates of S3-gt-tg-gt optimized at M06-2X/6-31++G(d,p) level in water (IEF-PCM/bondi)

Energy (Hartree) = -1297.5750817 ZPE (Hartree) = 0.3734382			
C	0.82706900	-0.70047000	-1.04796800
C	2.01014800	-1.58420700	-0.65799000
C	2.69133500	-1.01887100	0.57967400
C	3.07065100	0.43765600	0.33909900
C	1.84434800	1.24018300	-0.10727300
C	2.21013100	2.64782600	-0.54637200
C	1.86150500	-1.96271500	-1.21827500
C	1.49390700	-0.80004500	-0.29390100
C	2.23305500	-0.88713200	1.06973100
C	3.36719500	0.12180100	0.90014600
C	2.74968600	1.16656000	-0.03276100
C	1.97656600	2.26010300	0.69168600
O	1.24680000	0.62167600	-1.24991500
O	0.11180200	-0.80051100	0.00036700
O	1.50274900	-2.88927500	-0.43648300
O	3.83659700	-1.80960500	0.84037100
O	3.59618100	0.93788400	1.55910400
O	1.08908600	3.32415400	-1.10288300
O	1.90090600	0.40240500	-0.91145800
O	1.36258700	-3.19087800	-0.73209300
O	1.43479600	-0.48068000	2.16057400
O	4.44640900	-0.55942100	0.28006300
O	1.56249000	3.27075500	-0.21197300
H	0.40107500	-1.02611000	-1.99942500
H	2.72139000	-1.58584900	-1.49268300
H	1.99536400	-1.06779800	1.43042200
H	3.83314300	0.47194400	-0.45146600
H	1.11195400	1.27980500	0.71168200
H	2.54159800	3.22960000	0.31564500
H	3.02259200	2.60496900	-1.28176400
H	2.21686900	-3.53370200	-0.52922000
H	4.26658700	-1.45665900	1.63229800
H	4.25857100	1.61595600	1.37408400
H	0.89344500	2.91334400	-1.95765100
H	1.51363800	-1.75223600	-2.23685300
H	2.95125100	-2.03369600	-1.24473400
H	2.62232800	-1.89914600	1.22569700
H	3.66352500	0.54115100	1.86718600
H	3.51334300	1.63472500	-0.66298900
H	1.11912500	1.83005300	1.21994000
H	2.64292200	2.71518900	1.43349800
H	0.39082300	-3.14585200	-0.67254600
H	0.51460800	-0.71703100	1.96718300
H	5.16907600	0.06637300	0.13602300
H	0.61194300	3.17881000	-0.40449100

Table S7. Cartesian coordinates of S1-gg-tg-gg optimized at M06-2X/6-31++G(d,p) level in water (IEF-PCM/bondi)

Energy (Hartree) = -1297.5804696 ZPE (Hartree) = 0.3738323			
C	0.62147000	-0.42136900	-1.01628100
C	1.78077900	-1.40311900	-0.85208800
C	2.49017300	-1.16349400	0.46874500
C	2.94975700	0.28365700	0.53530200
C	1.75691700	1.22242200	0.32378000
C	2.16793200	2.68150700	0.22056400
C	1.81912300	-2.19935300	-1.17149000
C	1.67865400	-0.87121300	-0.43962900
C	2.55415800	-0.78233300	0.82022500
C	2.74280600	0.72081000	0.95097800
C	2.89133600	1.13992000	-0.51076200
C	2.40829400	2.53586900	-0.84609300
O	1.09576200	0.90399200	-0.91447000
O	0.33621100	-0.67267900	-0.01676200
O	1.25543100	-2.71629300	-0.93459800
O	3.58156600	-2.06639900	0.52161900
O	3.52461100	0.48678000	1.81660200
O	3.07384900	2.90623500	-0.84942400
O	2.11656200	0.17987900	-1.26467200
O	1.44161700	-3.25200500	-0.30124400
O	1.99760200	-1.34868900	1.97897600
O	3.89625200	1.11216200	1.66590800
O	1.06464600	2.75121100	-0.45698900
H	0.18645000	-0.50080600	-2.01511600
H	2.48852100	-1.22901300	-1.67365900
H	1.79615100	-1.36100000	1.29885500
H	3.69339200	0.45548700	-0.25302200
H	1.05106500	1.10747500	1.15850200
H	1.27213200	3.30211100	0.11017800
H	2.67898900	2.97465200	1.14067400
H	1.97871000	-3.34144500	-0.78005200
H	4.00811000	-1.97551000	1.38518900
H	4.22676600	1.14682500	1.75373900
H	2.62184100	2.68974200	-1.67673700
H	1.21947800	-2.20479800	-2.08968500
H	2.86852700	-2.33965400	-1.44068300
H	3.52796100	-1.23684800	0.58651100
H	1.84013900	1.16339300	1.39155900
H	3.94494000	1.04360300	-0.80286400
H	3.02428400	3.25999200	-0.30509400
H	2.53790500	2.70734100	-1.92198000
H	0.46824500	-3.23524000	-0.26014600
H	1.82373400	-2.28401400	1.79073900
H	3.71217400	1.04880600	2.61230700
H	0.49730300	2.07551500	-0.86828200

Table S8. Cartesian coordinates of S1-tg-tg-gg optimized at M06-2X/6-31++G(d,p) level in water (IEF-PCM/bondi)

Energy (Hartree) = -1297.5791994 ZPE (Hartree) = 0.3740464			
C	0.54656000	-0.59927700	-1.10758900
C	1.69534000	-1.57943900	-0.88205400
C	2.46376800	-1.19461300	0.36902200
C	2.95498000	0.23950700	0.24932400
C	1.78756000	1.18256000	-0.07858000
C	2.26691100	2.57266500	-0.47561900
C	1.94476800	-2.29124800	-0.87965900
C	1.71919700	-0.89201900	-0.32257400
C	2.49098700	-0.62615600	0.97996900
C	2.62806100	0.88785900	0.94260800
C	2.88632100	1.13497800	-0.54297600
C	2.40071000	2.46417200	-1.08256100
O	1.05728400	0.71167400	-1.22004200
O	0.34536900	-0.68664300	-0.02445800
O	1.14565700	-2.88081400	-0.77545900
O	3.53841400	-2.11215000	0.49229300
O	3.55812000	0.56951400	1.48854100
O	2.99773900	3.10901200	0.62315100
O	2.19579900	0.06814800	-1.23298800
O	1.52126300	-3.24749900	0.07622800
O	1.86059500	-1.07120900	2.15365600
O	3.70720700	1.40289100	1.69365300
O	1.02192900	2.67256200	-0.83951100
H	0.04475500	-0.79891200	-2.05694400
H	2.36470200	-1.52283400	-1.75079400
H	1.79927700	-1.27238600	1.24110200
H	3.69336500	0.29205200	-0.56619200
H	1.11835000	1.24503600	0.79145000
H	2.90695000	2.48583800	-1.36176400
H	1.40515100	3.20390800	-0.71470700
H	1.86198900	-3.49216100	-0.54821800
H	3.94551700	-1.99602400	1.36163100
H	3.78613600	1.51318800	1.46120600
H	3.42420100	3.93007500	0.34624800
H	1.42106500	-2.41991300	-1.83475200
H	3.01502300	-2.43001400	-1.04949600
H	3.49181200	-1.06988100	0.87603800
H	1.67994900	1.34598700	1.25280600
H	3.96218800	1.03759300	-0.73729600
H	2.94619000	3.26829100	-0.58038600
H	2.62164800	2.51422200	-2.15604600
H	0.54720700	-3.25374300	0.04399800
H	1.73244100	-2.02875600	2.07034400
H	3.44748600	1.44348400	2.62337200
H	0.51625300	1.92711800	-1.20797200

Table S9. Cartesian coordinates of S1-gt-tg-gg^{ccw} optimized at M06-2X/6-31++G(d,p) level in water (IEF-PCM/bondi)

Energy (Hartree) = -1297.5792451 ZPE (Hartree) = 0.3736817			
C	0.73869600	-0.43781600	-1.06563800
C	2.10581100	-1.11464700	-0.94913000
C	2.86208300	-0.57604400	0.26103400
C	2.91701200	0.94465300	0.22143400
C	1.49320300	1.49133800	0.13264300
C	1.43476400	3.00708800	0.05560400
C	1.31930900	-2.75727200	-0.68277100
C	1.36375800	-1.30471100	-0.22078000
C	2.15499600	-1.04381000	1.06668200
C	2.53963500	0.41872200	0.87991200
C	2.93379200	0.40352500	-0.59888300
C	2.86745200	1.71172500	-1.35678500
O	0.87536200	0.96677700	-1.05653900
O	0.04394900	-0.84453500	0.02983800
O	1.97099100	-2.51950700	-0.89897500
O	4.20065700	-1.04573800	0.28619300
O	3.51296500	1.45460400	1.40111500
O	0.18056300	3.52885700	0.46296000
O	2.01249200	-0.53514400	-1.20353800
O	0.50616300	-3.54055900	0.17770900
O	1.38648500	-1.35353600	2.20383100
O	3.59932900	0.76714000	1.74217300
O	1.57870500	2.30166200	-1.32825600
H	0.25943800	-0.69036500	-2.01440100
H	2.67989300	-0.88130200	-1.85240300
H	2.34111500	-0.88008800	1.18126100
H	3.48582700	1.26372900	-0.66598100
H	0.92690300	1.16155900	1.01456000
H	2.18113300	3.41993100	0.73718800
H	1.68514300	3.32038400	-0.96727300
H	1.26777300	-2.75537500	-0.26345700
H	4.18838200	-2.00151100	0.43327200
H	4.36201300	1.00483900	1.51911200
H	0.51963300	3.18217500	-0.12070000
H	0.86783400	-2.80716500	-1.67820300
H	2.34112300	-3.14752700	-0.73922000
H	3.07371300	-1.64680700	1.04117300
H	1.66156600	1.05702200	1.04810000
H	3.95282300	0.00400900	-0.68453700
H	3.56345400	2.42104900	-0.90019400
H	3.18180500	1.53722800	-2.39267400
H	0.81730700	-3.43805600	1.09003400
H	1.97283200	-1.38367100	2.97197900
H	3.66533700	1.73012400	1.79015700
H	0.90326000	1.63314600	-1.53981100