

Modeling of Canonical and C2'-O-thiophenylmethyl Modified hexamers of RNA. Insights into the Nature of Structural Changes and Thermal Stability.

Yannick Kokouvi Dzowo, Carly Wolfbrandt, Marino J. E. Resendiz* and Haobin Wang*

Department of Chemistry, University of Colorado Denver, Science Building 1151 Arapahoe St,
Denver, CO 80204

* To whom correspondence should be addressed: Marino.resendiz@ucdenver.edu,

Haobin.wang@ucdenver.edu

Supporting Information Index:

Page	Contents:
3.....	Figure S1. Pseudorotational angles for all models employed
4.....	Figure S2. Measurement of P–P distances.
5.....	Figure S3. Measurements for pseudorotational angles (α , β , γ , δ , ϵ , ζ , χ) for 3:4 .
6.....	Figure S4. Measurements for pseudorotational angles (α , β , γ , δ , ϵ , ζ , χ) for 3:4 . continued.
7.....	Figure S5. Measurements for pseudorotational angles (α , β , γ , δ , ϵ , ζ , χ) for 1:2 .
8.....	Figure S6. Measurements for kappa angle (κ°) for 3:4 .
9.....	Figure S7. Measurements for kappa angle (κ°) for 3:4 .
10.....	Figure S8. Measurements for pseudorotational (α , β , γ , δ , ϵ , ζ , χ) and torsional (ν_0 - ν_4) angles for 1:2 after adjusting orientation of C2'-O-H bond.
11.....	Figure S9. Measurements for kappa angle (κ°) for 1:2 after adjusting orientation of C2'-O-H bond.
12-17.....	Figure S10. X-Y coordinates for 3 at level: B3LYP/3-21G*.
18-24.....	Figure S11. X-Y coordinates for 3 at level: B3LYP-GD3/3-21G*.
25-31.....	Figure S12. X-Y coordinates for 3 at level: B3LYP-GD3/6-31G*.
32-44.....	Figure S13. X-Y coordinates for 3:4 at level: B3LYP /6-31G*.
45-51.....	Figure S14. X-Y coordinates for 4 at level: B3LYP /3-21G*.
52-58.....	Figure S15. X-Y coordinates for 4 at level: B3LYP-GD3/3-21G*.

59-65.....	Figure S16. X-Y coordinates for 4 at level: B3LYP-GD3/6-31G*.
66-78.....	Figure S17. X-Y coordinates for 3:4 at level: B3LYP-GD3/3-21G*.
79-91.....	Figure S18. X-Y coordinates for 3:4 at level: B3LYP-GD3/6-31G*.
92-104.....	Figure S19. X-Y coordinates for 3:4 at level: B97D3/3-21G*.
104-117.....	Figure S20. X-Y coordinates for 3:4 at level: B97D3/6-31G*.
118-123.....	Figure S21. X-Y coordinates for 1 at level: B3LYP/3-21G*.
124-129.....	Figure S22. X-Y coordinates for 1 at level: B3LYP-GD3/3-21G*.
131-135.....	Figure S23. X-Y coordinates for 1 at level: B3LYP-GD3/6-31G*.
136-146.....	Figure S24. X-Y coordinates for 1:2 at level: B3LYP/3-21G*.
147-152.....	Figure S25. X-Y coordinates for 2 at level: B3LYP/3-21G*.
153-158.....	Figure S26. X-Y coordinates for 2 at level: B3LYP-GD3/3-21G*.
159-164.....	Figure S27. X-Y coordinates for 2 at level: B3LYP-GD3/6-31G*.
165-175.....	Figure S28. X-Y coordinates for 1:2 at level: B3LYP-GD3/3-21G*.
176-186.....	Figure S29. X-Y coordinates for 1:2 at level: B3LYP-GD3/6-31G*.
187-197.....	Figure S30. X-Y coordinates for 1:2 at level: B97D3/3-21G*.
198-208.....	Figure S31. X-Y coordinates for 1:2 at level: B97D3/6-31G*.
208-220.....	Figure S32. Images of all the structures and levels of theory.
221-230.....	Figure S33. X-Y coordinates for 1:2 at level: B97D3/3-21G*. Adjustment of all C3'-C2'-O2'-H2' to 180°
231-240.....	Figure S34. X-Y coordinates for 1:2 at level: B97D3/3-21G*. Adjustment of one strand C3'-C2'-O2'-H2' to 180° and another randomized.
241-250.....	Figure S35. X-Y coordinates for 1:2 at level: B3LYP-GD3/6-31G*. Adjustment of all C3'-C2'-O2'-H2' to 180°
251-260.....	Figure S36. X-Y coordinates for 1:2 at level: B3LYP-GD3/6-31G*. Adjustment of one strand C3'-C2'-O2'-H2' to 180° and another randomized.
261-270.....	Figure S37. X-Y coordinates for 1:2 at level: B3LYP-GD3/6-31G*. Adjustment of one strand C3'-C2'-O2'-H2' to 360° and another randomized.

Oligonucleotide 3 & 4				Oligonucleotide 1 & 2					
B3LYP/3-21G*	5.7	5.5		5.7 B3LYP/3-21G*		6.1	6.4		6.1
	5.2	5.7				5.7	6.1		5.7
	5.7	5.6				5.9	5.8		5.9
	5.1	5.6				5.1	6		5.1
B3LYP-GD3/3-21G*	6.2	6.2		6.2 B3LYP-GD3/3-21G*		5	6.1		5
	4.9	5.8				6.2	5.2		6.2
	5.9	5.5				6.6	6		6.6
	4.6	5.1				4.6	6.7		4.6
B3LYP-GD3/6-31G*	5.6	6.3		5.6 B3LYP-GD3/6-31G*		5.2	6.1		5.2
	6	6.1				6.3	5.3		6.3
	5.7	6				6.5	6		6.5
	5	5.7				5	6.6		5
B97D3/3-21G*	6.1	6.2		6.1 B97D3/3-21G*		4.9	6.1		4.9
	4.9	5.8				6.2	4.6		6.2
	5.7	5.6				6.5	6.1		6.5
	4.5	5.3				4.5	6.7		4.5
B97D3/6-31G*	5.5	6.3		5.5 B97D3/6-31G*		5.2	6.1		5.2
	6.1	6.1				6.3	5.3		6.3
	5.7	5.9				6.5	6.1		6.5
	5	5.7				4.9	6.6		4.9
B3LYP-GD3/3-21G*_O	6.2	6.2				5.66	5.995		6.4
	4.9	5.8				0.721402	0.540443		6.1
	5.9	5.5							5.8
	4.6	5.1							6
B3LYP-GD3/6-31G*_O	5.6	6.3							6.1
	6	6.1							5.2
	5.7	6							6
	5	5.7							6.7
	5.464286	5.810714							6.1
	0.525085	0.346773							5.3
									6
									6.6
									6.1
									4.6
Oligonucleotide 3:4				Oligonucleotide 1:2					6.1
B3LYP/3-21G*	5.7	5.5		5.8 B3LYP/3-21G*		6.1	6.4		6.7
	5.2	5.7				5.7	6.1		6.1
	5.7	5.6				5.9	5.8		5.3
	5.1	5.6				5.1	6		6.1
	5.425	5.6				5.7	6.075		6.6
	0.320156	0.08165				0.432049	0.25		5.8275
									0.65162
B3LYP-GD3/3-21G*	6.2	6.2		6.2 B3LYP-GD3/3-21G*		5	6.1		
	4.9	5.8				6.2	5.2		
	5.9	5.5				6.6	6		
	4.6	5.1				4.6	6.7		
	5.4	5.65				5.6	6		
	0.770281	0.465475				0.95219	0.616441		
B3LYP-GD3/6-31G*	5.6	6.3		5.7 B3LYP-GD3/6-31G*		5.2	6.1		
	6	6.1				6.3	5.3		
	5.7	6				6.5	6		
	5	5.7				5	6.6		
	5.575	6.025				5.75	6		
	0.419325	0.25				0.759386	0.535413		
B97D3/3-21G*	6.1	6.2		6 B97D3/3-21G*		4.9	6.1		
	4.9	5.8				6.2	4.6		
	5.7	5.6		5.6375		6.5	6.1		
	4.5	5.3		0.47427		4.5	6.7		
	5.3	5.725				5.525	5.875		
	0.730297	0.377492				0.974252	0.895824		
B97D3/6-31G*	5.5	6.3		B97D3/6-31G*		5.2	6.1		
	6.1	6.1				6.3	5.3		
	5.7	5.9				6.5	6.1		
	5	5.7				4.9	6.6		
	5.575	6				5.725	6.025		
	0.457347	0.258199				0.7932	0.537742		
B3LYP-GD3/3-21G*_O	6.2	6.2							
	4.9	5.8							
	5.9	5.5							
	4.6	5.1							
	5.4	5.65							
	0.770281	0.465475							
B3LYP-GD3/6-31G*_O	5.6	6.3							
	6	6.1							
	5.7	6							
	5	5.7							
	5.575	6.025							
	0.419325	0.25							

Figure S2. Measurement of P–P distances.

										primers:									
										purines									

Figure S4. Measurements for pseudorotational angles ($\alpha, \beta, \gamma, \delta, \epsilon, \zeta, \chi$) for 3:4

			χ		α		β		γ		δ		ε		ζ		
		pyrimidines: purines	O4'-C1'-N1-C2 O4'-C1'-N9-C4		O3'-P-O5'-C5'		P-O5'-C5'-C4'		O5'-C5'-C4'-C3'		C5'-C4'-C3'-O3'		C4'-C3'-O3'-P		C3'-O3'-P-O5'		
			χ	ID	α	ID	β	ID	γ	ID	δ	ID	ε	ID	ζ	ID	
1.2 83LYP/3-210*	Method:	Nucleobase	χ	ID	α <td>ID</td> <td>β</td> <td>ID</td> <td>γ</td> <td>ID</td> <td>δ</td> <td>ID</td> <td>ε<td>ID</td><td>ζ<td>ID</td></td></td>	ID	β	ID	γ	ID	δ	ID	ε <td>ID</td> <td>ζ<td>ID</td></td>	ID	ζ <td>ID</td>	ID	
	3'	C 1	O7-C2-N17-C18								C6-C5-C4-O16						
	G 2	-158.976 O66-C61-N86-C80	-68.931	O16-P91-O60-C65	-176.374	P91-O60-C65-C64	54.447	O60-C65-C64-C63	88.859	C65-C64-C63-O75	-158.793	C64-C63-O75-P155	-69.272	C63-O75-P155-O125			
	A 3	-144.921 O131-C126-N150-C144	-73.176	O75-P155-O125-C130	-162.741	P155-O125-C130-C129	47.057	O125-C130-C129-C128	90.181	C130-C129-C128-O140	-157.975	C129-C128-O140-P219	-66.442	C128-O140-P219-O188			
	G 4	-140.380 O194-C189-N174-C175	-71.086	O140-P219-O188-C193	-171.346	P219-O188-C193-C192	50.661	O188-C193-C192-C191	92.831	C193-C192-C191-O203	-155.599	C192-C191-O203-P281	-65.594	C191-O203-P281-O253			
	C 5	-144.271 O259-C254-N269-C270	-81.152	O203-P281-O253-C258	-147.618	P281-O253-C258-C257	44.01	O253-C258-C257-C256	92.366	C258-C257-C256-O268	-152.016	C257-C256-O268-P345	-68.476	C256-O268-P345-O318			
	U 6	- O324-C319-N334-C335	-	-	-	-	-	-	-	-	C323-C322-C321-O333	-	-	-	-	-	
	avg	147.139	-73.58625	-164.51975	49.04375	91.05925	-156.18075	-67.5285									
	stdev	8.141161219	5.33327544	12.59568798	4.512812233	1.867182972	3.024718651	1.601296454									
	5'	G 7	O35-C30-N55-C49									C34-C33-C32-O44					
	C 8	-156.201 O100-C95-N110-C111	-44.734	O173-P185-O94-C99	-198.447	P185-O94-C99-C98	51.068	O94-C99-C98-C97	93.421	C99-C98-C97-O109	-160.548	C98-C97-O109-P122	-66.989	C97-O109-P122-O29			
	U 9	-158.771 O164-C159-N174-C175	-48.573	O217-P250-O158-C163	-194.087	P250-O158-C163-C162	47.977	O158-C163-C162-C161	88.762	C163-C162-C161-O173	-152.014	C162-C161-O173-P185	-85.894	C161-O173-P185-O94			
	C 10	-164.533 O288-C223-N238-C239	-85.782	O299-P315-O222-C227	-177.862	P315-O222-C227-C226	51.246	O222-C227-C226-C225	86.828	C227-C226-C225-O237	-153.681	C226-C225-O237-P250	-49.66	C225-O237-P250-O158			
	G 11	-145.573 O290-C285-N310-C304	-57.871	O363-P378-O284-C289	-214.323	P378-O284-C289-C288	50.633	O284-C289-C288-C287	88.15	C289-C288-C287-O299	-136.903	C288-C287-O299-P315	-84.061	C287-O299-P315-O222			
	A 12	- O354-C349-N373-C367	-	-	-	-	-	-	-	-	C353-C352-C351-O363	-	-	-	-	-	
	avg	-156.2095	-59.24	-194.9285	50.231	89.29025	-150.7865	-81.651									
	stdev	7.936471487	18.53430018	17.08927399	15.254567042	2.869668317	9.965328912	10.04870595									
1.2 83LYP-GD3/3-210*	Method:	Nucleobase	χ	ID	α <td>ID</td> <td>β</td> <td>ID</td> <td>γ</td> <td>ID</td> <td>δ</td> <td>ID</td> <td>ε<td>ID</td><td>ζ<td>ID</td></td></td>	ID	β	ID	γ	ID	δ	ID	ε <td>ID</td> <td>ζ<td>ID</td></td>	ID	ζ <td>ID</td>	ID	
	3'	C 1	O7-C2-N17-C18								C6-C5-C4-O16						
	G 2	-145.439 O66-C61-N86-C80	-82.464	O16-P91-O60-C65	-148.999	P91-O60-C65-C64	40.529	O60-C65-C64-C63	88.265	C65-C64-C63-O75	-150.135	C64-C63-O75-P155	-63.588	C63-O75-P155-O125			
	A 3	-155.813 O131-C126-N150-C144	-69.678	O75-P155-O125-C130	-183.757	P155-O125-C130-C129	49.141	O125-C130-C129-C128	88.806	C130-C129-C128-O140	-160.795	C129-C128-O140-P219	-71.41	C128-O140-P219-O188			
	G 4	-172.224 O194-C189-N174-C175	-64.515	O140-P219-O188-C193	-190.544	P219-O188-C193-C192	59.858	O188-C193-C192-C191	92.421	C193-C192-C191-O203	-169.238	C192-C191-O203-P281	-61.249	C191-O203-P281-O253			
	C 5	-157.595 O259-C254-N269-C270	-82.137	O203-P281-O253-C258	-140.894	P281-O253-C258-C257	47.623	O253-C258-C257-C256	92.366	C258-C257-C256-O268	-151.518	C257-C256-O268-P345	-69.242	C256-O268-P345-O318			
	U 6	- O324-C319-N334-C335	-	-	-	-	-	-	-	-	C323-C322-C321-O333	-	-	-	-	-	
	avg	-157.76775	-74.6985	-166.0485	49.28775	86.72	-157.9215	-72.29725									
	stdev	11.02772462	9.028535596	24.74573911	7.984126225	6.489110279	8.906075997	14.43469181									
	5'	G 7	O35-C30-N55-C49									C34-C33-C32-O44					
	C 8	-150.39 O100-C95-N110-C111	-35.357	O173-P185-O94-C99	-207.302	P185-O94-C99-C98	40.928	O94-C99-C98-C97	92.016	C99-C98-C97-O109	-155.096	C98-C97-O109-P122	-58.285	C97-O109-P122-O29			
	U 9	-161.288 O164-C159-N174-C175	-76.321	O217-P250-O158-C163	-190.489	P250-O158-C163-C162	45.095	O158-C163-C162-C161	80.418	C163-C162-C161-O173	-154.118	C162-C161-O173-P185	-93.348	C161-O173-P185-O94			
	C 10	-162.887 O288-C223-N238-C239	-53.507	O299-P315-O222-C227	-185.07	P315-O222-C227-C226	55.918	O222-C227-C226-C225	87.531	C227-C226-C225-O237	-155.287	C226-C225-O237-P250	-64.024	C225-O237-P250-O158			
	G 11	-167.119 O290-C285-N310-C304	-57.805	O363-P378-O284-C289	-243.965	P378-O284-C289-C288	64.372	O284-C289-C288-C287	83.469	C289-C288-C287-O299	-158.018	C288-C287-O299-P315	-84.061	C287-O299-P315-O222			
	A 12	- O354-C349-N373-C367	-	-	-	-	-	-	-	-	C353-C352-C351-O363	-	-	-	-	-	
	avg	-160.416	-55.7475	-199.2065	51.7825	85.861	-155.63215	-72.571									
	stdev	7.124666776	16.81561317	35.43889521	10.6140454	5.030310726	1.66946426	15.41700219									
1.2 83LYP-GD3/6-310*	Method:	Nucleobase	χ	ID	α <td>ID</td> <td>β</td> <td>ID</td> <td>γ</td> <td>ID</td> <td>δ</td> <td>ID</td> <td>ε<td>ID</td><td>ζ<td>ID</td></td></td>	ID	β	ID	γ	ID	δ	ID	ε <td>ID</td> <td>ζ<td>ID</td></td>	ID	ζ <td>ID</td>	ID	
	3'	C 1	O7-C2-N17-C18								C6-C5-C4-O16						
	G 2	-155.019 O66-C61-N86-C80	-80.43	O16-P91-O60-C65	-163.912	P91-O60-C65-C64	50.796	O60-C65-C64-C63	83.494	C65-C64-C63-O75	-137.559	C64-C63-O75-P155	-76.126	C63-O75-P155-O125			
	A 3	-162.593 O131-C126-N150-C144	-69.843	O75-P155-O125-C130	-199.893	P155-O125-C130-C129	57.562	O125-C130-C129-C128	83.195	C130-C129-C128-O140	-152.042	C129-C128-O140-P219	-67.605	C128-O140-P219-O188			
	G 4	-174.809 O194-C189-N174-C175	-69.026	O140-P219-O188-C193	-199.532	P219-O188-C193-C192	64.828	O188-C193-C192-C191	84.342	C193-C192-C191-O203	-161.847	C192-C191-O203-P281	-60.573	C191-O203-P281-O253			
	C 5	-161.239 O259-C254-N269-C270	-82.038	O203-P281-O253-C258	-148.215	P281-O253-C258-C257	51.631	O253-C258-C257-C256	79.268	C258-C257-C256-O268	-149.832	C257-C256-O268-P345	-80.595	C256-O268-P345-O318			
	U 6	- O324-C319-N334-C335	-	-	-	-	-	-	-	-	C323-C322-C321-O333	-	-	-	-	-	
	avg	-163.415	-75.33425	-170.388	56.20425	82.5475	-150.32	-71.22475									
	stdev	8.281036811	6.852123193	21.63991887	6.450411717	2.257395162	9.981955019	8.914149889									
	5'	G 7	O35-C30-N55-C49									C34-C33-C32-O44					
	C 8	-156.107 O100-C95-N110-C111	-62.554	O173-P185-O94-C99	-197.281	P185-O94-C99-C98	54.827	O94-C99-C98-C97	84.459	C99-C98-C97-O109	-149.699	C98-C97-O109-P122	-62.471	C97-O109-P122-O29			
	U 9	-160.205 O164-C159-N174-C175	-77.342	O217-P250-O158-C163	-192.035	P250-O158-C163-C162	45.144	O158-C163-C162-C161	80.328	C163-C162-C161-O173	-149.973	C162-C161-O173-P185	-93.348	C161-O173-P185-O94			
	C 10	-162.399 O288-C223-N238-C239	-69.111	O299-P315-O222-C227	-184.137	P315-O222-C227-C226	59.118	O222-C227-C226-C225	83.299	C227-C226-C225-O237	-153.255	C226-C225-O237-P250	-67.852	C225-O237-P250-O158			
	G 11	-158.97 O290-C285-N310-C304	-58.426	O363-P378-O284-C289	-237.333	P378-O284-C289-C288	64.007	O284-C289-C288-C287	81.554	C289-C288-C287-O299	-152.466	C288-C287-O299-P315	-84.061	C287-O299-P315-O222			
	A 12	- O354-C349-N373-C367	-	-	-	-	-	-	-	-	C353-C352-C351-O363	-	-	-	-	-	
	avg	-159.44375	-66.8325	-195.2135	57.274	82.41	-151.34825	-89.39775									
	stdev	2.58707021	8.276103245	31.60865335	5.546072073	1.830863366	1.779175722	6.662123504									
1.2 897D3/3-210*	Method:	Nucleobase	χ	ID	α <td>ID</td> <td>β</td> <td>ID</td> <td>γ</td> <td>ID</td> <td>δ</td> <td>ID</td> <td>ε<td>ID</td><td>ζ<td>ID</td></td></td>	ID	β	ID	γ	ID	δ	ID	ε <td>ID</td> <td>ζ<td>ID</td></td>	ID	ζ <td>ID</td>	ID	
	3'	C 1	O7-C2-N17-C18								C6-C5-C4-O16						
	G 2	-141.818 O66-C61-N86-C80	-82.03	O16-P91-O60-C65	-150.036	P91-O60-C65-C64	40.386	O60-C65-C64-C63	90.202	C65-C64-C63-O75	-142.289	C64-C63-O75-P155	-66.664	C63-O75-P155-O125			
	A 3	-155.261 O131-C126-N150-C144	-71.044	O75-P155-O125-C130	-186.914	P155-O125-C130-C129	44.324	O125-C130-C129-C128	90.561	C130-C129-C128-O140	-159.241	C129-C128-O140-P219	-63.198	C128-O140-P219-O188			
	G 4	-175.663 O194-C189-N174-C175	-69.156	O140-P219-O188-C193	-194.694	P219-O188-C193-C192	60.412	O188-C193-C192-C191	90.519	C193-C192-C191-O203	-167.601	C192-C191-O203-P281	-60.094	C191-O203-P281-O253			
	C 5	-155.791 O259-C254-N269-C270	-80.714	O203-P281-O253-C258	-127.222	P281-O253-C258-C257	47.248	O253-C258-C257-C256	77.619	C258-C257-C256-O268	-150.58	C257-C256-O268-P345	-91.903	C256-O268-P345-O318			
	U 6	- O324-C319-N334-C335	-	-	-	-	-	-	-	-	C323-C322-C321-O333	-	-	-	-	-	
	avg	-157.13325	-75.736	-165.2165	48.0925	87.2525	-154.92775	-70.61475									
	stdev	13.942925	6.575362702	24.19584071	6.680917674	6.406171419	10.92178744	14.40370678									
	5'	G 7	O35-C30-N55-C49									C34-C33-C32-O44					
	C 8	-151.428 O100-C95-N110-C111	-37.053	O173-P185-O94-C99	-207.622	P185-O94-C99-C98	39.05	O94-C99-C98-C97	92.756	C99-C98-C97-O109	-154.39	C98-C97-O109-P122	-58.596	C97-O109-P122-O29			
	U 9	-159.332 O164-C159-N174-C175	-83.687	O217-P250-O158-C163	-142.254	P250-O158-C163-C162	45.229	O158-C163-C162-C161	81.191	C163-C162-C161-O173	-145.894	C162-C161-O173-P185	-93.348				

30/3-21G*	ID	34 - B3LYP/6-31G*	ID	34 - B97D3/3-21G*	ID	34 - B97D3/6-31G*	ID
99	H9-C3-O10-H11	98.778	H9-C3-O10-H11	100.538	H9-C3-O10-H11	98.927	H9-C3-O10-H11
17	H68-C62-O69-C410	-39.623	H68-C62-O69-C410	-37.887	H68-C62-O69-C410	-41.156	H68-C62-O69-C410
22	H131-C125-O132-C399	-50.974	H131-C125-O132-C399	-46.388	H131-C125-O132-C399	-50.772	H131-C125-O132-C399
45	H192-C186-O193-C388	-171.749	H192-C186-O193-C388	-170.794	H192-C186-O193-C388	-169.384	H192-C186-O193-C388
52	H255-C249-O256-C378	-53.254	H255-C249-O256-C378	-56.618	H255-C249-O256-C378	-53.759	H255-C249-O256-C378
3	H318-C312-O319-H320	89.852	H318-C312-O319-H320	97.375	H318-C312-O319-H320	92.87	H318-C312-O319-H320
11	H37-C31-O38-H39	-39.262	H37-C31-O38-H39	-41.148	H37-C31-O38-H39	-39.733	H37-C31-O38-H39
44	H101-C95-O102-C454	-57.6	H101-C95-O102-C454	-52.066	H101-C95-O102-C454	-58.769	H101-C95-O102-C454
52	H163-C157-O164-C443	-52.9	H163-C157-O164-C443	-52.066	H163-C157-O164-C443	-53.028	H163-C157-O164-C443
77	H225-C219-O226-C432	-44.427	H225-C219-O226-C432	-43.379	H225-C219-O226-C432	-46.186	H225-C219-O226-C432
2	H285-C279-O286-C421	32.119	H285-C279-O286-C421	33.546	H285-C279-O286-C421	31.022	H285-C279-O286-C421
8	H348-C342-O349-H350	76.502	H348-C342-O349-H350	86.861	H348-C342-O349-H350	80.158	H348-C342-O349-H350

Figure S6. Measurements for kappa angle (κ°) for 3:4.

2:G*	ID	1:2 - B31P-G03/6-31G*	ID	1:2 - B97D3/3-21G*	ID	1:2 - B97D3/6-31G*	ID
104.327	H9-C3-O10-H11	98.75	H9-C3-O10-H11	105.626	H9-C3-O10-H11	99.198	H9-C3-O10-H11
100.904	H68-C62-O69-H70	88.36	H68-C62-O69-H70	99.508	H68-C62-O69-H70	90.703	H68-C62-O69-H70
97.309	H133-C127-O134-H135	97.571	H133-C127-O134-H135	99.73	H133-C127-O134-H135	97.889	H133-C127-O134-H135
99.147	H196-C190-O197-H198	96.596	H196-C190-O197-H198	98.749	H196-C190-O197-H198	97.28	H196-C190-O197-H198
	H261-C255-O262-H263		H261-C255-O262-H263		H261-C255-O262-H263		H261-C255-O262-H263
	H326-C320-O327-H328	87.178	H326-C320-O327-H328	96.505	H326-C320-O327-H328	89.811	H326-C320-O327-H328
-40.949	H37-C31-O38-H39		-41.492	H37-C31-O38-H39		-38.812	H37-C31-O38-H39
101.826	H102-C96-O103-H104		97.969	H102-C96-O103-H104		98.401	H102-C96-O103-H104
	H166-C160-O167-H168			H166-C160-O167-H168			H166-C160-O167-H168
103.046	H230-C224-O231-H232		99.302	H230-C224-O231-H232		99.877	H230-C224-O231-H232
102.126	H292-C286-O293-H294		99.759	H292-C286-O293-H294		100.054	H292-C286-O293-H294
H356-C350-O357-H358		62.142	H356-C350-O357-H358	56.406	H356-C350-O357-H358	61.49	H356-C350-O357-H358

Figure S7. Measurements for kappa angle (κ°) for 1:2.

Figure S8. Measurements for pseudorotational (α , β , γ , δ , ε , ζ , χ) and torsional (ν_0 - ν_4) angles for **1:2** after adjusting orientation of C2'-O-H bond.

	3'-CGA GCU-5'	Duplex 1:2			
	5'-GCU CGA-3'				
	Measurement of κ°				
	Adjustment of C3'-C2'-O2'-H2'				
	All 180°	one strand 180° one random	All 180°	one strand 180° one random	All 360°
	B3LYP-GD3/3-21G*	B3LYP-GD3/3-21G*	B3LYP-GD3/6-31G*	B3LYP-GD3/6-31G*	B3LYP-GD3/6-31G*
1	142.131	137.957	133.614	134.822	127.198
2	173.36	172.178	144.549	151.353	127.149
3	171.485	165.501	147.105	155.299	127.029
4	146.94	124.958	128.512	129.244	126.953
5		179.89	155.071	160.29	126.571
6	129.055	128.647	126.554	126.774	126.581
7	139.763	139.511	136.8	138.642	120.68
8	145.658	101.265	132.528	98.055	126.623
9	175.682	174.567	158.094	179.317	126.43
10	145.437	103.488	132.078	99.812	127.209
11	176.457	102.752	141.409	99.796	127.536
12					
	154.5968	139.1558182	139.6649091	133.9458182	126.3599091
	17.66973239	30.07404266	10.53010619	26.88376973	1.914617009

Figure S9. Measurements for kappa angle (κ°) for 1:2 after adjusting orientation of C2'-O-H bond.

8	32.251208000	11.438679000	2.181378000
6	33.817559000	8.077191000	0.939803000
6	34.014868000	7.800351000	2.439083000
6	33.190150000	8.912197000	3.114990000
6	31.977388000	9.013814000	2.170688000
6	31.264523000	10.346508000	2.182264000
8	32.539653000	8.761315000	0.805098000
1	33.817929000	7.153862000	0.357337000
1	35.067125000	7.759876000	2.721212000
8	33.280055000	6.593080000	2.827584000
1	33.870154000	5.800053000	2.734437000
1	33.713037000	9.867282000	3.122009000
1	31.274303000	8.210530000	2.406308000
1	30.684562000	10.407071000	3.110231000
1	30.598768000	10.432106000	1.321393000
8	32.816414000	8.541420000	4.458890000
7	38.752098000	8.333204000	-0.176494000
6	38.021357000	7.289847000	0.358046000
7	38.665349000	6.136390000	0.634985000
7	36.715189000	7.387631000	0.606285000
6	36.192490000	8.596800000	0.282418000
6	36.844543000	9.707970000	-0.253875000
6	38.243401000	9.633175000	-0.529200000
8	39.017478000	10.484370000	-0.999357000
7	35.936417000	10.761060000	-0.431393000
6	34.762877000	10.298650000	-0.011895000
7	34.874975000	8.970453000	0.440067000
1	39.748610000	8.214865000	-0.351942000
1	39.656943000	6.005574000	0.479896000
1	38.127593000	5.372451000	1.026656000
1	33.832584000	10.855934000	-0.010388000
8	28.152541000	15.563349000	-0.028482000
6	28.395156000	12.253974000	-1.826853000
6	29.760698000	12.108139000	-1.118761000
6	29.682899000	13.141243000	0.025279000
6	28.193666000	13.175537000	0.393097000
6	27.707353000	14.512205000	0.909488000
8	27.489074000	12.906714000	-0.888746000
1	28.032367000	11.267068000	-2.104471000
1	30.605668000	12.318520000	-1.767002000

8	29.827067000	10.754630000	-0.582159000
1	29.944903000	14.122467000	-0.380827000
1	27.981997000	12.378413000	1.111906000
1	28.146834000	14.706468000	1.892115000
1	26.617248000	14.547873000	0.967149000
8	30.441265000	12.837207000	1.217909000
7	28.455554000	13.059910000	-3.060047000
6	28.726915000	12.346919000	-4.274092000
8	29.056942000	11.137520000	-4.188995000
7	28.583373000	13.033859000	-5.444126000
6	28.284199000	14.340740000	-5.442344000
7	28.044127000	14.934232000	-6.632914000
6	28.185079000	15.098621000	-4.223843000
6	28.239178000	14.408863000	-3.052411000
1	28.131276000	14.358432000	-7.465249000
1	27.720480000	15.907428000	-6.726293000
1	28.036136000	16.166410000	-4.236382000
1	28.117681000	14.871096000	-2.077823000
15	32.096674000	12.681758000	1.121366000
8	32.766161000	13.873456000	1.735179000
8	32.446479000	12.233149000	-0.282793000
8	25.313820000	20.232709000	-0.648850000
6	23.920410000	16.661963000	-1.987630000
6	25.108661000	16.117116000	-1.145598000
6	25.580336000	17.394326000	-0.429020000
6	24.263019000	18.081214000	-0.086023000
6	24.368492000	19.554199000	0.246861000
8	23.470404000	17.885270000	-1.345353000
1	23.106771000	15.942965000	-2.065730000
1	25.877890000	15.657816000	-1.765115000
8	24.618074000	15.177763000	-0.141657000
1	26.125282000	18.025034000	-1.133238000
1	23.767839000	17.549021000	0.730723000
1	24.775728000	19.620624000	1.261654000
1	23.386897000	20.030463000	0.207125000
8	26.376019000	17.185052000	0.756576000
7	24.400821000	16.979291000	-3.361789000
6	24.645718000	15.861454000	-4.167868000
8	24.292066000	14.713442000	-3.846513000
7	25.345558000	16.149555000	-5.324934000
6	25.861481000	17.402147000	-5.722027000

8	26.675559000	17.460400000	-6.676966000
6	25.390943000	18.493216000	-4.912876000
1	25.644185000	19.503644000	-5.191054000
6	24.710919000	18.257882000	-3.761105000
1	25.615800000	15.344918000	-5.889615000
1	24.391459000	19.093493000	-3.130726000
15	28.026499000	17.123030000	0.541302000
8	28.620239000	17.199324000	1.913112000
8	28.414689000	18.009553000	-0.601792000
8	23.125584000	25.481225000	-1.371864000
6	20.118335000	22.298657000	-1.486715000
6	21.463953000	21.518131000	-1.482512000
6	22.514946000	22.627626000	-1.282410000
6	21.763193000	23.604827000	-0.380981000
6	22.363813000	24.995780000	-0.230004000
8	20.444340000	23.679718000	-1.068459000
1	19.445846000	21.831686000	-0.768783000
1	21.662285000	20.936828000	-2.380731000
8	21.479836000	20.677043000	-0.278470000
1	22.676079000	23.126776000	-2.239869000
1	21.633364000	23.156536000	0.610621000
1	23.083857000	24.949271000	0.590414000
1	21.571696000	25.701241000	0.031305000
8	23.753559000	22.202079000	-0.659374000
7	19.389182000	22.341483000	-2.752965000
6	18.273354000	21.441847000	-2.881885000
8	18.120501000	20.548133000	-2.010782000
7	17.429963000	21.641068000	-3.931825000
6	17.678592000	22.587382000	-4.850506000
7	16.735288000	22.788505000	-5.799829000
6	18.892452000	23.357078000	-4.838221000
6	19.707446000	23.224041000	-3.752774000
1	15.891768000	22.226792000	-5.713725000
1	16.654404000	23.679194000	-6.303066000
1	19.161659000	24.027142000	-5.644767000
1	20.637228000	23.792026000	-3.645594000
15	24.845662000	21.440787000	-1.655353000
8	26.046805000	22.305861000	-1.883147000
8	24.053642000	20.890435000	-2.825107000
8	21.557887000	27.075329000	-5.895397000
6	17.943299000	27.720319000	-3.900821000

6	18.694584000	26.771261000	-2.923765000
6	20.143296000	26.792465000	-3.448368000
6	20.247686000	28.172234000	-4.114925000
6	21.382080000	28.309112000	-5.113983000
8	18.943675000	28.281053000	-4.814384000
1	17.436921000	28.484833000	-3.307006000
1	18.258218000	25.770793000	-2.929413000
8	18.581953000	27.387485000	-1.606010000
1	20.261713000	26.045535000	-4.232629000
1	20.334499000	28.944311000	-3.341304000
1	22.310930000	28.394988000	-4.551256000
1	21.200676000	29.157246000	-5.774510000
8	21.127310000	26.602148000	-2.392614000
7	12.987583000	26.784019000	-4.580655000
6	13.595815000	27.536666000	-3.594990000
7	12.818409000	28.134150000	-2.672359000
7	14.921118000	27.689449000	-3.539243000
6	15.585838000	27.023780000	-4.509378000
6	15.064239000	26.193516000	-5.509039000
6	13.651899000	26.064439000	-5.626186000
8	12.960252000	25.471283000	-6.484720000
7	16.111057000	25.680945000	-6.298529000
6	17.221839000	26.214996000	-5.803245000
7	16.949840000	27.038325000	-4.710703000
1	11.970832000	26.726236000	-4.617055000
1	11.809460000	28.050034000	-2.659935000
1	13.269351000	28.692517000	-1.956892000
1	18.226778000	26.077303000	-6.185724000
15	22.568364000	25.904085000	-2.847037000
8	23.511977000	26.950703000	-3.367706000
8	22.262496000	24.670012000	-3.670899000
8	18.496862000	25.401384000	-9.469327000
6	17.426127000	29.182556000	-9.864288000
6	18.353449000	29.413470000	-8.654542000
6	19.030659000	28.053624000	-8.543527000
6	19.301101000	27.697111000	-10.016402000
6	19.427303000	26.192266000	-10.273711000
8	18.111543000	28.232294000	-10.732729000
1	17.210160000	30.117517000	-10.382893000
1	17.801726000	29.703670000	-7.755098000
8	19.346183000	30.395147000	-9.060795000

1	20.174486000	30.130946000	-8.566908000
1	18.355274000	27.322774000	-8.111848000
1	20.193535000	28.228085000	-10.357471000
1	20.465172000	25.916872000	-10.054116000
1	19.208145000	25.997920000	-11.326544000
8	20.262546000	28.153063000	-7.769589000
7	12.444248000	29.901567000	-8.522313000
6	13.389005000	30.781224000	-8.924470000
7	14.675821000	30.522875000	-9.247633000
6	14.960364000	29.205765000	-9.183565000
6	14.063082000	28.185837000	-8.828725000
6	12.766056000	28.578785000	-8.439191000
7	11.853640000	27.700681000	-7.978646000
7	14.681566000	26.934652000	-8.914218000
6	15.927954000	27.188059000	-9.293147000
7	16.157608000	28.564233000	-9.455799000
1	13.079790000	31.818322000	-8.981576000
1	12.144884000	26.766361000	-7.671480000
1	10.952740000	28.062200000	-7.682107000
1	16.718839000	26.462237000	-9.438734000
15	20.939571000	26.698180000	-7.333023000
8	22.028375000	26.321928000	-8.289814000
8	19.777439000	25.710459000	-7.150176000
1	32.720492000	7.543351000	4.378114000
1	18.924778000	25.361047000	-8.535122000
6	18.756139000	26.384371000	-0.543488000
1	19.557577000	25.691461000	-0.797857000
1	19.036313000	26.959754000	0.346060000
6	16.206166000	26.019547000	-0.676100000
6	17.471417000	25.629906000	-0.322130000
16	17.455750000	24.065833000	0.457676000
6	15.722988000	23.967742000	0.334362000
6	15.201925000	25.064565000	-0.299007000
1	16.000077000	26.930938000	-1.218962000
1	15.194315000	23.109552000	0.719576000
1	14.146624000	25.195786000	-0.495787000
6	20.773032000	19.381663000	-0.490941000
1	19.855470000	19.576820000	-1.062005000
1	21.437953000	18.695232000	-1.023290000
6	20.314499000	17.563617000	1.301132000
6	20.451117000	18.859194000	0.874432000

16	20.120233000	19.989973000	2.163598000
6	19.777724000	18.695749000	3.273330000
6	19.922631000	17.469164000	2.680973000
1	20.487715000	16.705577000	0.665678000
1	19.516539000	18.906673000	4.298879000
1	19.770878000	16.531415000	3.197542000
6	24.402041000	13.819324000	-0.719978000
1	24.039082000	13.925355000	-1.748977000
1	25.357110000	13.284630000	-0.742524000
6	23.081030000	11.820928000	0.280884000
6	23.391040000	13.150296000	0.158432000
16	22.371768000	14.138268000	1.173183000
6	21.514895000	12.740288000	1.750613000
6	21.997279000	11.584650000	1.195514000
1	23.596567000	11.036664000	-0.257005000
1	20.722690000	12.842934000	2.476090000
1	21.611758000	10.600992000	1.425904000
6	30.652330000	9.869600000	-1.473872000
1	31.633281000	9.786378000	-1.016038000
1	30.702765000	10.340034000	-2.459308000
6	29.013403000	8.249925000	-2.579874000
6	29.960884000	8.555409000	-1.631621000
16	30.241213000	7.199913000	-0.563458000
6	29.066548000	6.236729000	-1.403324000
6	28.499472000	6.918991000	-2.450505000
1	28.720891000	8.972690000	-3.331644000
1	28.865002000	5.222303000	-1.094304000
1	27.751790000	6.493943000	-3.106005000

Figure S10. X-Y coordinates for **3** at level: B3LYP/3-21G*.

8	32.241564000	11.438407000	2.188237000
6	33.505133000	8.001015000	0.988372000
6	33.591811000	7.638645000	2.477078000
6	32.872832000	8.819317000	3.154056000
6	31.711582000	9.066482000	2.174795000
6	31.139903000	10.460482000	2.191237000
8	32.296874000	8.793252000	0.824851000
1	33.464494000	7.116083000	0.351156000
1	34.615715000	7.457009000	2.804488000
8	32.690485000	6.520831000	2.770443000
1	33.173826000	5.663570000	2.642612000
1	33.499418000	9.709306000	3.193939000
1	30.925393000	8.330367000	2.361033000
1	30.566816000	10.580453000	3.117570000
1	30.494228000	10.609406000	1.324348000
8	32.411024000	8.471829000	4.476690000
7	38.534343000	8.029451000	0.372080000
6	37.705764000	7.012036000	0.805349000
7	38.264739000	5.824382000	1.119601000
7	36.386610000	7.167304000	0.921992000
6	35.956670000	8.406537000	0.575912000
6	36.709853000	9.496926000	0.136257000
6	38.124548000	9.360108000	0.001453000
8	38.980945000	10.181942000	-0.366875000
7	35.872050000	10.596998000	-0.102309000
6	34.642333000	10.182390000	0.187153000
7	34.649969000	8.840858000	0.610382000
1	39.537437000	7.867851000	0.298212000
1	39.259404000	5.648032000	1.055948000
1	37.655887000	5.079162000	1.436211000
1	33.742613000	10.780295000	0.117619000
8	28.236645000	15.699419000	-0.033321000
6	28.474552000	12.459017000	-1.765874000
6	29.840379000	12.290118000	-1.074506000
6	29.791094000	13.320370000	0.068786000
6	28.309453000	13.351862000	0.462647000
6	27.837346000	14.692992000	0.970918000

8	27.578705000	13.086404000	-0.805493000
1	28.104119000	11.482301000	-2.068462000
1	30.678369000	12.481031000	-1.736893000
8	29.877364000	10.940931000	-0.535989000
1	30.049504000	14.301158000	-0.340603000
1	28.114140000	12.554300000	1.184445000
1	28.327080000	14.922855000	1.921724000
1	26.751472000	14.727227000	1.076112000
8	30.558364000	13.012474000	1.254017000
7	28.556395000	13.302104000	-2.970427000
6	28.908579000	12.626797000	-4.183140000
8	29.260205000	11.421557000	-4.109932000
7	28.814828000	13.342159000	-5.340289000
6	28.495136000	14.644432000	-5.317218000
7	28.290978000	15.260408000	-6.504089000
6	28.334725000	15.370756000	-4.086083000
6	28.335936000	14.649547000	-2.932315000
1	28.420447000	14.704938000	-7.344626000
1	27.925239000	16.219348000	-6.587840000
1	28.174976000	16.437243000	-4.075406000
1	28.186260000	15.088385000	-1.950276000
15	32.192084000	12.710304000	1.151748000
8	32.959504000	13.831485000	1.784000000
8	32.508756000	12.253608000	-0.258086000
8	25.261693000	20.045420000	-1.037337000
6	24.029053000	16.423438000	-1.880028000
6	25.241090000	16.002289000	-1.017658000
6	25.649584000	17.357164000	-0.426750000
6	24.313774000	18.009149000	-0.094212000
6	24.361661000	19.519806000	-0.001961000
8	23.438548000	17.583472000	-1.240511000
1	23.285275000	15.637160000	-1.987179000
1	26.024823000	15.519956000	-1.597004000
8	24.781658000	15.125498000	0.054085000
1	26.134834000	17.943771000	-1.208147000
1	23.902423000	17.584224000	0.823236000
1	24.783843000	19.767351000	0.978792000
1	23.363032000	19.947901000	-0.100343000

8	26.488968000	17.322223000	0.747728000
7	24.520961000	16.803629000	-3.230879000
6	24.946348000	15.739693000	-4.031474000
8	24.791156000	14.552344000	-3.696986000
7	25.581800000	16.143325000	-5.191329000
6	25.929598000	17.464298000	-5.565242000
8	26.731427000	17.644098000	-6.515406000
6	25.323324000	18.469173000	-4.737852000
1	25.428031000	19.518550000	-4.955820000
6	24.670716000	18.112023000	-3.605379000
1	25.970841000	15.395223000	-5.763207000
1	24.277068000	18.879616000	-2.957205000
15	28.126554000	17.285038000	0.449467000
8	28.792249000	17.451191000	1.779602000
8	28.439820000	18.095952000	-0.770667000
8	23.265712000	25.352254000	-1.742964000
6	20.222282000	22.253660000	-1.822215000
6	21.561929000	21.470316000	-1.844708000
6	22.613669000	22.569348000	-1.625479000
6	21.864466000	23.545372000	-0.724830000
6	22.477028000	24.930014000	-0.592162000
8	20.559199000	23.636370000	-1.428215000
1	19.578749000	21.793967000	-1.075349000
1	21.754547000	20.907791000	-2.756218000
8	21.574868000	20.614711000	-0.655399000
1	22.786381000	23.065452000	-2.580147000
1	21.723505000	23.093692000	0.264148000
1	23.180844000	24.904019000	0.242356000
1	21.687030000	25.654577000	-0.381218000
8	23.842191000	22.131010000	-0.990201000
7	19.456693000	22.293106000	-3.057895000
6	18.312612000	21.425501000	-3.127932000
8	18.153408000	20.568050000	-2.221278000
7	17.450703000	21.615406000	-4.161468000
6	17.687446000	22.546247000	-5.100569000
7	16.732259000	22.729277000	-6.040845000
6	18.904370000	23.315866000	-5.121900000
6	19.752487000	23.175575000	-4.063895000

1	15.890650000	22.170093000	-5.915604000
1	16.609874000	23.654443000	-6.488848000
1	19.158670000	23.975078000	-5.940582000
1	20.694909000	23.725593000	-3.980808000
15	24.908178000	21.339370000	-1.986706000
8	26.169172000	22.133505000	-2.144231000
8	24.122270000	20.881347000	-3.200632000
8	21.699242000	26.983323000	-6.291397000
6	18.147227000	27.723764000	-4.241864000
6	18.868557000	26.717952000	-3.299665000
6	20.313595000	26.711923000	-3.817316000
6	20.458060000	28.092782000	-4.471262000
6	21.609467000	28.193740000	-5.450091000
8	19.153919000	28.245821000	-5.170204000
1	17.686147000	28.503638000	-3.632348000
1	18.406644000	25.731134000	-3.365444000
8	18.755933000	27.259187000	-1.951803000
1	20.415757000	25.965480000	-4.604923000
1	20.565066000	28.851809000	-3.686944000
1	22.533609000	28.176417000	-4.874160000
1	21.505236000	29.087841000	-6.063507000
8	21.287869000	26.499582000	-2.757270000
7	13.186917000	26.695500000	-4.568580000
6	13.814155000	27.651103000	-3.793810000
7	13.065077000	28.387574000	-2.952285000
7	15.131452000	27.858448000	-3.857687000
6	15.763074000	27.061825000	-4.746957000
6	15.218021000	26.069254000	-5.566561000
6	13.815415000	25.841767000	-5.536402000
8	13.103710000	25.074592000	-6.217973000
7	16.233749000	25.487464000	-6.345456000
6	17.356035000	26.105073000	-5.996916000
7	17.114587000	27.076253000	-5.025565000
1	12.172878000	26.609702000	-4.538307000
1	12.064373000	28.268582000	-2.854899000
1	13.529653000	29.088921000	-2.387247000
1	18.346292000	25.944224000	-6.407612000
15	22.702924000	25.761050000	-3.219530000

8	23.674459000	26.768812000	-3.767617000
8	22.350896000	24.529251000	-4.028880000
8	18.130612000	25.832883000	-9.606499000
6	16.922510000	29.516770000	-8.928750000
6	18.068870000	29.527422000	-7.901523000
6	18.786012000	28.241303000	-8.266539000
6	18.746795000	28.240560000	-9.796452000
6	18.871448000	26.830328000	-10.380940000
8	17.431133000	28.843803000	-10.123606000
1	16.588527000	30.530866000	-9.153419000
1	17.726845000	29.538867000	-6.864602000
8	18.923812000	30.655368000	-8.244935000
1	19.845981000	30.344770000	-8.017761000
1	18.227753000	27.396396000	-7.885207000
1	19.543284000	28.889206000	-10.170603000
1	19.941962000	26.589867000	-10.403871000
1	18.470614000	26.827828000	-11.397265000
8	20.162265000	28.241947000	-7.810693000
7	12.152982000	29.627070000	-6.865813000
6	13.079682000	30.601501000	-7.010263000
7	14.333525000	30.482473000	-7.502858000
6	14.605722000	29.223293000	-7.899749000
6	13.725094000	28.129755000	-7.838982000
6	12.458219000	28.360999000	-7.266723000
7	11.547136000	27.378280000	-7.099690000
7	14.327689000	26.986705000	-8.381537000
6	15.542521000	27.373160000	-8.750767000
7	15.767611000	28.731986000	-8.469726000
1	12.784465000	31.591464000	-6.683864000
1	11.846991000	26.402257000	-7.136731000
1	10.657917000	27.613836000	-6.671464000
1	16.325475000	26.749987000	-9.162116000
15	20.900815000	26.764462000	-7.679464000
8	21.845441000	26.561906000	-8.824241000
8	19.796334000	25.716083000	-7.477193000
1	32.182806000	7.499134000	4.369891000
1	18.714545000	25.625848000	-8.789074000
6	18.766173000	26.161932000	-0.964344000

1	19.614879000	25.500210000	-1.136033000
1	18.866458000	26.660258000	0.005273000
6	16.285107000	25.863014000	-1.538929000
6	17.479799000	25.382216000	-1.066493000
16	17.383337000	23.673374000	-0.733492000
6	15.713280000	23.623432000	-1.212145000
6	15.270479000	24.853538000	-1.627514000
1	16.152352000	26.883781000	-1.863873000
1	15.160695000	22.697117000	-1.174356000
1	14.271662000	25.038417000	-1.999305000
6	20.884610000	19.315593000	-0.906664000
1	19.930104000	19.521300000	-1.406674000
1	21.529296000	18.675414000	-1.512101000
6	21.075301000	17.451447000	0.862633000
6	20.687427000	18.693970000	0.433358000
16	19.895238000	19.589122000	1.707765000
6	20.069984000	18.256074000	2.812512000
6	20.711992000	17.195436000	2.227985000
1	21.628193000	16.770407000	0.233331000
1	19.710377000	18.330721000	3.827397000
1	20.933970000	16.272458000	2.744552000
6	24.585273000	13.733419000	-0.449789000
1	24.238522000	13.774416000	-1.489863000
1	25.544298000	13.210091000	-0.439552000
6	23.245599000	11.798223000	0.642278000
6	23.565445000	13.116104000	0.449700000
16	22.547541000	14.168715000	1.396686000
6	21.673654000	12.811769000	2.043799000
6	22.151621000	11.622312000	1.559180000
1	23.760465000	10.983060000	0.152088000
1	20.875250000	12.959305000	2.755181000
1	21.755733000	10.656495000	1.841272000
6	30.689123000	10.040662000	-1.422322000
1	31.657161000	9.923123000	-0.950698000
1	30.766543000	10.518547000	-2.402293000
6	28.984078000	8.528256000	-2.555711000
6	29.941614000	8.762154000	-1.597457000
16	30.118739000	7.386550000	-0.531018000

6	28.890208000	6.509940000	-1.392028000
6	28.380398000	7.233949000	-2.441046000
1	28.747001000	9.277385000	-3.300931000
1	28.616997000	5.508487000	-1.094433000
1	27.612601000	6.864190000	-3.106721000

Figure S11. X-Y coordinates for **3** at level: B3LYP-GD3/3-21G*.

8	32.093160000	11.033630000	2.241830000
6	31.694833000	7.504587000	1.029685000
6	32.692848000	7.068525000	2.119438000
6	32.777675000	8.323303000	3.002510000
6	31.333934000	8.859443000	2.927409000
6	31.188848000	10.356691000	3.110750000
8	30.851258000	8.473236000	1.619075000
1	31.108125000	6.652433000	0.676775000
1	33.655415000	6.758037000	1.701071000
8	32.120495000	6.056947000	2.943601000
1	32.291779000	5.191034000	2.542409000
1	33.458063000	9.051856000	2.555256000
1	30.724324000	8.353236000	3.687984000
1	31.411916000	10.597570000	4.158524000
1	30.163607000	10.663455000	2.879355000
8	33.227442000	8.068529000	4.314429000
7	33.420653000	6.507433000	-3.619906000
6	32.812059000	5.672020000	-2.712266000
7	32.566525000	4.389497000	-3.110100000
7	32.417527000	6.071137000	-1.517708000
6	32.662463000	7.384452000	-1.295337000
6	33.272113000	8.316497000	-2.135779000
6	33.710352000	7.889885000	-3.431766000
8	34.260563000	8.525863000	-4.328955000
7	33.334898000	9.559793000	-1.527096000
6	32.781947000	9.382961000	-0.348942000
7	32.349311000	8.076917000	-0.150393000
1	33.684823000	6.147611000	-4.531152000
1	33.157650000	3.977086000	-3.820424000
1	32.313057000	3.758463000	-2.360618000
1	32.625093000	10.140293000	0.407967000
8	29.356810000	16.573212000	1.365260000
6	28.932447000	13.527745000	-0.733238000
6	30.057216000	12.812203000	0.051464000
6	30.250544000	13.771792000	1.239858000
6	28.820215000	14.247889000	1.506468000
6	28.665409000	15.608264000	2.158875000

8	28.208836000	14.290718000	0.204906000
1	28.268224000	12.813762000	-1.211454000
1	30.969631000	12.695780000	-0.542736000
8	29.600754000	11.568308000	0.542581000
1	30.866213000	14.610343000	0.897822000
1	28.304096000	13.500385000	2.120870000
1	29.085055000	15.570872000	3.172691000
1	27.600381000	15.850704000	2.211630000
8	30.783383000	13.225443000	2.429919000
7	29.430373000	14.397395000	-1.820009000
6	29.513663000	13.831547000	-3.118898000
8	29.299747000	12.618484000	-3.257645000
7	29.818183000	14.660155000	-4.158722000
6	30.101348000	15.943855000	-3.932946000
7	30.412828000	16.715195000	-5.011026000
6	30.091662000	16.521063000	-2.626697000
6	29.721092000	15.707603000	-1.601381000
1	30.068191000	16.389163000	-5.906917000
1	30.363147000	17.718970000	-4.894762000
1	30.301690000	17.566997000	-2.442570000
1	29.612974000	16.067356000	-0.585766000
15	32.349146000	12.658563000	2.456766000
8	32.847854000	12.898751000	3.854088000
8	33.082154000	13.116245000	1.227769000
8	26.219766000	20.805263000	-1.213484000
6	25.347728000	16.972066000	-1.687363000
6	26.340729000	16.620192000	-0.558302000
6	26.745801000	18.028446000	-0.107054000
6	25.399400000	18.743815000	-0.163981000
6	25.412768000	20.252579000	-0.167614000
8	24.791428000	18.222386000	-1.370757000
1	24.557706000	16.224583000	-1.789488000
1	27.167326000	16.004977000	-0.905800000
8	25.677321000	15.991280000	0.524707000
1	27.427322000	18.458304000	-0.848106000
1	24.796556000	18.425886000	0.696211000
1	25.842450000	20.569083000	0.792040000
1	24.389674000	20.618520000	-0.230068000

8	27.299774000	18.122115000	1.190025000
7	26.031603000	17.046135000	-3.015544000
6	26.476577000	15.840464000	-3.548549000
8	26.357724000	14.766244000	-2.963015000
7	27.066272000	15.947172000	-4.791479000
6	27.275069000	17.110584000	-5.551212000
8	27.867452000	17.040008000	-6.630327000
6	26.745169000	18.297699000	-4.925025000
1	26.828149000	19.245399000	-5.439961000
6	26.156749000	18.227768000	-3.703845000
1	27.504127000	15.096419000	-5.132197000
1	25.740880000	19.106433000	-3.222808000
15	28.950123000	18.181578000	1.397467000
8	29.152338000	18.734612000	2.778471000
8	29.605504000	18.756952000	0.171348000
8	23.553729000	25.729834000	-2.546812000
6	20.813957000	22.399569000	-1.999624000
6	22.190564000	21.677280000	-2.145745000
6	23.194759000	22.851265000	-2.083812000
6	22.420951000	23.889808000	-1.274841000
6	22.933315000	25.323020000	-1.328425000
8	21.094446000	23.787744000	-1.813632000
1	20.297692000	21.992407000	-1.129860000
1	22.275471000	21.127300000	-3.087337000
8	22.401809000	20.810429000	-1.045551000
1	23.317599000	23.240285000	-3.097793000
1	22.406272000	23.585846000	-0.215549000
1	23.716630000	25.415585000	-0.570799000
1	22.119939000	26.006926000	-1.066753000
8	24.444391000	22.590167000	-1.473463000
7	19.901353000	22.259743000	-3.125524000
6	18.776878000	21.392010000	-3.006742000
8	18.627600000	20.734313000	-1.966953000
7	17.905957000	21.331031000	-4.053030000
6	18.148061000	22.012468000	-5.171934000
7	17.272145000	21.885682000	-6.203388000
6	19.306653000	22.838525000	-5.338675000
6	20.151154000	22.943842000	-4.279901000

1	16.357429000	21.513288000	-5.978163000
1	17.250454000	22.647515000	-6.876997000
1	19.496664000	23.373271000	-6.259379000
1	21.035222000	23.580905000	-4.296284000
15	25.603532000	21.800164000	-2.379834000
8	26.713177000	22.753334000	-2.731025000
8	24.894316000	21.020488000	-3.461804000
8	20.675427000	27.440568000	-7.089937000
6	17.980774000	27.347107000	-4.482876000
6	18.953120000	26.615307000	-3.533076000
6	20.297311000	26.812008000	-4.248924000
6	20.130658000	28.204249000	-4.876061000
6	20.960352000	28.460131000	-6.117249000
8	18.730985000	28.289352000	-5.219457000
1	17.193296000	27.838563000	-3.907619000
1	18.681805000	25.561441000	-3.426454000
8	18.911440000	27.282769000	-2.281578000
1	20.385236000	26.063402000	-5.041879000
1	20.372489000	28.962166000	-4.118286000
1	22.019737000	28.412881000	-5.848987000
1	20.729557000	29.453787000	-6.512066000
8	21.405673000	26.731807000	-3.370602000
7	13.902437000	24.453025000	-4.986823000
6	14.084356000	25.559461000	-4.190774000
7	13.079733000	25.848492000	-3.305135000
7	15.177382000	26.292287000	-4.224196000
6	16.065598000	25.872421000	-5.153780000
6	15.918920000	24.857716000	-6.097606000
6	14.759741000	24.021911000	-6.029608000
8	14.455809000	23.036585000	-6.707693000
7	17.030983000	24.796459000	-6.922071000
6	17.839404000	25.730575000	-6.470534000
7	17.303903000	26.423212000	-5.395379000
1	13.068470000	23.889394000	-4.864919000
1	12.134479000	25.719681000	-3.654295000
1	13.205219000	26.745590000	-2.850271000
1	18.803077000	25.988042000	-6.886211000
15	22.815697000	26.071258000	-3.974287000

8	23.653458000	27.137185000	-4.627416000
8	22.477265000	24.814092000	-4.741859000
8	17.571759000	26.859006000	-10.979478000
6	15.388308000	29.042588000	-8.522560000
6	16.655589000	29.110247000	-7.652086000
6	17.694678000	28.534599000	-8.615181000
6	17.238833000	29.090029000	-9.967828000
6	17.679308000	28.260969000	-11.174325000
8	15.798083000	29.135068000	-9.874033000
1	14.697842000	29.851383000	-8.266762000
1	16.548072000	28.520898000	-6.736685000
8	16.921703000	30.473075000	-7.363073000
1	17.865424000	30.505462000	-7.124996000
1	17.611447000	27.446348000	-8.612304000
1	17.615704000	30.115781000	-10.074723000
1	18.713999000	28.545436000	-11.415762000
1	17.052999000	28.528687000	-12.032032000
8	19.014614000	28.947885000	-8.311707000
7	11.522946000	26.571618000	-6.121492000
6	12.009800000	27.819898000	-5.984762000
7	13.034545000	28.392857000	-6.622718000
6	13.584697000	27.556028000	-7.517775000
6	13.174078000	26.245518000	-7.795405000
6	12.094886000	25.755646000	-7.032336000
7	11.609890000	24.493182000	-7.191755000
7	13.963544000	25.676163000	-8.780545000
6	14.827308000	26.618830000	-9.088108000
7	14.652249000	27.783010000	-8.358228000
1	11.508109000	28.433482000	-5.239566000
1	12.260082000	23.795025000	-7.536502000
1	10.956316000	24.171948000	-6.488419000
1	15.613923000	26.544038000	-9.829442000
15	20.285787000	27.908707000	-8.619415000
8	21.382305000	28.736824000	-9.217070000
8	19.747509000	26.661657000	-9.288418000
1	32.848447000	7.202487000	4.553597000
1	18.338578000	26.617089000	-10.403633000
6	19.032585000	26.405320000	-1.155299000

1	19.945075000	25.807979000	-1.231152000
1	19.126611000	27.074167000	-0.293277000
6	16.518815000	25.806046000	-1.266915000
6	17.832158000	25.502795000	-1.015742000
16	18.003521000	23.818898000	-0.584300000
6	16.294014000	23.551887000	-0.723463000
6	15.638330000	24.692858000	-1.100802000
1	16.196027000	26.784633000	-1.600719000
1	15.882562000	22.570143000	-0.528531000
1	14.568740000	24.742129000	-1.274531000
6	21.778492000	19.530237000	-1.196094000
1	20.706633000	19.664232000	-1.403491000
1	22.232518000	18.988484000	-2.037132000
6	22.229911000	17.395028000	0.171367000
6	21.990518000	18.737591000	0.055790000
16	21.935699000	19.495625000	1.631086000
6	22.241506000	17.977659000	2.426276000
6	22.371753000	16.956842000	1.525260000
1	22.327802000	16.742484000	-0.689083000
1	22.325346000	17.937695000	3.504386000
1	22.579950000	15.931242000	1.810530000
6	25.195159000	14.668492000	0.252623000
1	24.134368000	14.735204000	-0.031978000
1	25.743364000	14.217403000	-0.578475000
6	25.831803000	12.522639000	1.516349000
6	25.360984000	13.806520000	1.463988000
16	24.920771000	14.374362000	3.060279000
6	25.383791000	12.857746000	3.779602000
6	25.842514000	11.976970000	2.839213000
1	26.179489000	11.990058000	0.638773000
1	25.302954000	12.719107000	4.849815000
1	26.192064000	10.976865000	3.070405000
6	29.452429000	10.552291000	-0.473166000
1	30.104263000	9.727556000	-0.186274000
1	29.763015000	10.936070000	-1.450351000
6	27.100162000	10.408680000	-1.530647000
6	28.026093000	10.106457000	-0.564545000
16	27.307959000	9.130766000	0.697489000

6	25.760332000	9.155027000	-0.093289000
6	25.804741000	9.863901000	-1.263242000
1	27.350014000	11.010330000	-2.399058000
1	24.915492000	8.643385000	0.348973000
1	24.946009000	9.998419000	-1.912052000

Figure S12. X-Y coordinates for **3** at level: B3LYP-GD3/6-31G*.

8	31.735704000	18.602943000	-14.437787000
6	32.831886000	15.256537000	-13.061726000
6	31.594061000	14.673945000	-13.748979000
6	31.120825000	15.847636000	-14.629591000
6	32.458345000	16.417363000	-15.124781000
6	32.420899000	17.881165000	-15.511725000
8	33.386330000	16.247699000	-13.973285000
1	33.559217000	14.486044000	-12.815653000
1	30.857114000	14.269084000	-13.060419000
8	32.053754000	13.636703000	-14.683796000
1	31.529773000	13.847582000	-15.515385000
1	30.529463000	16.597872000	-14.109450000
1	32.812304000	15.816819000	-15.966410000
1	31.875134000	17.967823000	-16.459130000
1	33.446095000	18.241482000	-15.654453000
8	30.377869000	15.329558000	-15.778951000
7	32.463004000	15.946406000	-11.790356000
6	32.475420000	15.188712000	-10.592802000
8	32.786254000	13.965657000	-10.662878000
7	32.161411000	15.822613000	-9.427320000
6	31.825019000	17.135880000	-9.408143000
7	31.506839000	17.691644000	-8.237901000
6	31.829825000	17.905772000	-10.617604000
6	32.162561000	17.283760000	-11.776709000
1	31.511021000	17.132129000	-7.356915000
1	31.242571000	18.670548000	-8.198847000
1	31.580070000	18.955922000	-10.604337000
1	32.180184000	17.803359000	-12.730569000
8	32.991208000	12.739514000	0.318978000
6	33.730116000	11.305302000	-3.138741000
6	35.198419000	11.357802000	-2.682380000
6	35.119030000	11.538547000	-1.148816000
6	33.846398000	10.735499000	-0.792295000
6	33.090442000	11.266169000	0.409168000
8	32.966945000	10.824309000	-1.992094000
1	33.611773000	10.642940000	-3.998320000
1	35.773468000	12.127871000	-3.199137000

8	35.793584000	10.022575000	-2.802997000
1	36.223369000	9.926568000	-3.692617000
1	34.980070000	12.579890000	-0.863651000
1	34.122228000	9.689040000	-0.632430000
1	33.636249000	11.014842000	1.323176000
1	32.076066000	10.865053000	0.449876000
8	36.301847000	11.018088000	-0.506412000
7	32.453720000	14.382020000	-7.024245000
6	32.997644000	13.110743000	-7.063151000
7	33.237702000	12.581791000	-8.274231000
7	33.296690000	12.414383000	-5.951674000
6	33.006824000	13.074744000	-4.812310000
6	32.439206000	14.346331000	-4.673196000
6	32.122379000	15.083402000	-5.848572000
8	31.616073000	16.238109000	-5.913114000
7	32.280063000	14.668185000	-3.314997000
6	32.747912000	13.621535000	-2.651496000
7	33.214713000	12.619055000	-3.522143000
1	32.294371000	14.897983000	-7.939300000
1	33.040432000	13.082043000	-9.164156000
1	33.647114000	11.654608000	-8.298071000
1	32.776323000	13.479704000	-1.581024000
8	28.576989000	14.239244000	-14.356306000
6	29.102701000	12.384246000	-11.110635000
6	27.646855000	11.873437000	-11.235441000
6	27.298713000	12.288337000	-12.675500000
6	28.602337000	12.011909000	-13.424494000
6	28.825381000	12.822659000	-14.678054000
8	29.656166000	12.425604000	-12.452259000
1	29.702809000	11.741073000	-10.467300000
1	26.996648000	12.338457000	-10.494189000
8	27.613063000	10.419796000	-11.123276000
1	27.100194000	13.360376000	-12.695446000
1	28.687075000	10.940937000	-13.631547000
1	28.154003000	12.497088000	-15.475930000
1	29.868481000	12.697193000	-14.980944000
8	26.186323000	11.579016000	-13.265746000
7	28.834209000	14.520744000	-6.617965000

6	29.220387000	13.240655000	-6.975476000
7	29.460339000	12.356807000	-5.999260000
7	29.344512000	12.862705000	-8.258124000
6	29.095265000	13.854601000	-9.132241000
6	28.724696000	15.176647000	-8.875118000
6	28.539897000	15.561307000	-7.519307000
8	28.125767000	16.678670000	-7.080522000
7	28.519410000	15.861486000	-10.086594000
6	28.737598000	14.965549000	-11.039846000
7	29.102731000	13.715883000	-10.501764000
1	28.728557000	14.747504000	-5.588937000
1	29.304495000	12.562172000	-4.991143000
1	29.743509000	11.426779000	-6.287345000
1	28.665416000	15.104343000	-12.106476000
15	28.702101000	15.327404000	-15.599493000
8	28.167084000	14.726684000	-16.859724000
8	28.293784000	16.647589000	-15.025967000
8	28.418098000	15.565761000	2.039265000
6	28.397208000	13.035131000	-0.781407000
6	29.837194000	12.665542000	-0.367564000
6	29.968791000	13.388407000	0.986737000
6	28.584535000	13.188661000	1.609148000
6	28.175744000	14.231003000	2.619894000
8	27.660548000	13.302927000	0.440221000
1	27.916377000	12.238016000	-1.344999000
1	30.569799000	12.976221000	-1.110265000
8	29.899121000	11.226946000	-0.109116000
1	30.138919000	14.452491000	0.816506000
1	28.517991000	12.182542000	2.030071000
1	28.778374000	14.123938000	3.525650000
1	27.112720000	14.150875000	2.862045000
8	30.986984000	12.863357000	1.868104000
7	28.378643000	14.249287000	-1.640725000
6	28.637070000	14.041067000	-3.010759000
8	28.970098000	12.871366000	-3.371717000
7	28.494699000	15.082140000	-3.867202000
6	28.105147000	16.305008000	-3.423388000
7	27.914999000	17.264184000	-4.330997000

6	27.917119000	16.540146000	-2.016192000
6	28.061776000	15.492794000	-1.161547000
1	28.036128000	17.045490000	-5.340465000
1	27.404245000	18.113778000	-4.089195000
1	27.669558000	17.524674000	-1.649840000
1	27.973579000	15.575993000	-0.084090000
15	32.512318000	13.511041000	1.716813000
8	33.301152000	12.972188000	2.869461000
8	32.402337000	14.962909000	1.366196000
8	24.492130000	11.791473000	-11.383695000
6	23.824471000	11.134440000	-7.643576000
6	22.343337000	10.932621000	-8.017000000
6	22.430223000	10.962512000	-9.553773000
6	23.665879000	10.099078000	-9.818559000
6	24.338787000	10.341267000	-11.149179000
8	24.590939000	10.461337000	-8.691336000
1	24.077192000	10.712034000	-6.671552000
1	21.667632000	11.665792000	-7.574909000
8	21.955782000	9.566123000	-7.656821000
1	22.611791000	11.984123000	-9.885671000
1	23.396559000	9.046140000	-9.719273000
1	23.697875000	9.936404000	-11.937668000
1	25.327268000	9.880228000	-11.193395000
8	21.292516000	10.418133000	-10.256580000
7	24.169618000	15.433709000	-4.805561000
6	23.624263000	14.226854000	-4.516844000
7	23.569676000	13.158117000	-5.329535000
6	24.115607000	13.408777000	-6.541633000
6	24.711146000	14.610370000	-6.957148000
6	24.759435000	15.666602000	-6.018231000
7	25.343220000	16.851338000	-6.236109000
7	25.147280000	14.507094000	-8.282883000
6	24.826071000	13.273045000	-8.657845000
7	24.200163000	12.557130000	-7.628339000
1	23.229775000	14.142256000	-3.512100000
1	26.052446000	16.936007000	-6.966004000
1	25.336368000	17.555296000	-5.480169000
1	24.950333000	12.835779000	-9.636765000

15	24.681359000	12.234704000	-12.981328000
8	23.728068000	11.445728000	-13.824595000
8	24.784607000	13.728598000	-12.982791000
8	25.424863000	19.931017000	2.247056000
6	23.977409000	16.715286000	0.927790000
6	25.262282000	16.069223000	1.497478000
6	25.806116000	17.185215000	2.413557000
6	24.538952000	17.827340000	2.992297000
6	24.667780000	19.303333000	3.334494000
8	23.555295000	17.733981000	1.871763000
1	23.183933000	15.988695000	0.769296000
1	25.960663000	15.795105000	0.708120000
8	24.915948000	14.899252000	2.299215000
1	26.313449000	17.932453000	1.802361000
1	24.177097000	17.251839000	3.848143000
1	25.201367000	19.409231000	4.284647000
1	23.672754000	19.750165000	3.393082000
8	26.695094000	16.748282000	3.466200000
7	24.248926000	17.347387000	-0.382463000
6	24.009620000	16.560562000	-1.518796000
8	23.519314000	15.412107000	-1.434418000
7	24.385259000	17.144451000	-2.704187000
6	24.987893000	18.389493000	-2.869806000
8	25.411891000	18.738444000	-4.012907000
6	25.113528000	19.167956000	-1.664283000
1	25.501015000	20.173909000	-1.663425000
6	24.764625000	18.617904000	-0.476224000
1	24.269778000	16.515973000	-3.572045000
1	24.904587000	19.156519000	0.451349000
15	28.324716000	16.828991000	3.119789000
8	29.026986000	16.453105000	4.386905000
8	28.610803000	18.064155000	2.323162000
8	19.202667000	11.510121000	-9.336485000
6	18.697804000	12.476826000	-5.867315000
6	17.200284000	12.593398000	-6.257824000
6	17.097881000	11.710896000	-7.523763000
6	18.174379000	10.625882000	-7.353129000
6	18.877616000	10.259207000	-8.645692000

8	19.175961000	11.208661000	-6.407623000
1	18.802651000	12.493197000	-4.781053000
1	16.940167000	13.628866000	-6.457270000
8	16.309523000	12.210070000	-5.170722000
1	17.346822000	12.299555000	-8.407418000
1	17.745197000	9.729607000	-6.901650000
1	18.201003000	9.651628000	-9.258070000
1	19.798031000	9.708917000	-8.440222000
8	15.795154000	11.091605000	-7.698513000
7	20.825879000	16.843956000	-4.414674000
6	20.235829000	15.848432000	-3.655011000
7	20.127771000	16.064915000	-2.335509000
7	19.770886000	14.704312000	-4.191061000
6	19.933119000	14.633842000	-5.527042000
6	20.528652000	15.572994000	-6.365951000
6	21.022464000	16.784977000	-5.806793000
8	21.559002000	17.743236000	-6.425755000
7	20.475249000	15.141525000	-7.698853000
6	19.869107000	13.958811000	-7.670493000
7	19.505386000	13.602705000	-6.354960000
1	21.121007000	17.749451000	-3.947006000
1	20.438792000	16.945762000	-1.881498000
1	19.687120000	15.338603000	-1.782388000
1	19.711551000	13.302758000	-8.512018000
15	20.107672000	11.490485000	-10.725015000
8	19.351532000	10.832391000	-11.834795000
8	20.690952000	12.871818000	-10.804691000
8	22.292225000	24.317425000	-0.355886000
6	20.850961000	20.860231000	0.086801000
6	22.015481000	20.426556000	0.993154000
6	22.773577000	21.756631000	1.131852000
6	21.626946000	22.742820000	1.358320000
6	21.934871000	24.191490000	1.060847000
8	20.571867000	22.253122000	0.416956000
1	19.954077000	20.260522000	0.225633000
1	22.595117000	19.609850000	0.574228000
8	21.499414000	20.072623000	2.315827000
1	23.284696000	21.973177000	0.193454000

1	21.272058000	22.638053000	2.386217000
1	22.765828000	24.514678000	1.693353000
1	21.064524000	24.813620000	1.291930000
8	23.725562000	21.824541000	2.217593000
7	21.256706000	20.743842000	-1.339196000
6	21.185222000	19.457922000	-1.921604000
8	20.850155000	18.488562000	-1.173236000
7	21.465941000	19.330652000	-3.245369000
6	21.842824000	20.404838000	-3.990757000
7	22.052923000	20.243729000	-5.296205000
6	22.007290000	21.691921000	-3.371447000
6	21.692868000	21.824955000	-2.058459000
1	21.881974000	19.320738000	-5.746156000
1	22.181145000	21.070283000	-5.887382000
1	22.353164000	22.532809000	-3.950253000
1	21.788658000	22.757855000	-1.511312000
15	25.321967000	21.534374000	1.841713000
8	26.153679000	22.367618000	2.763936000
8	25.477534000	21.557042000	0.343537000
8	14.457730000	13.254623000	-7.833500000
6	14.018614000	16.668349000	-6.193038000
6	12.804344000	16.841199000	-7.123845000
6	12.628567000	15.413745000	-7.665034000
6	12.928736000	14.541278000	-6.441935000
6	13.464451000	13.157079000	-6.746797000
8	14.016342000	15.289022000	-5.745804000
1	13.988037000	17.346645000	-5.342790000
1	12.979815000	17.578430000	-7.907182000
8	11.625573000	17.178170000	-6.324117000
1	13.383832000	15.233978000	-8.427522000
1	12.050604000	14.485543000	-5.793129000
1	12.660545000	12.494470000	-7.072886000
1	13.964450000	12.753276000	-5.862066000
8	11.320201000	15.128800000	-8.216117000
7	15.289195000	16.939406000	-6.911005000
6	15.776609000	18.261583000	-6.875491000
8	15.020294000	19.151420000	-6.375857000
7	17.028870000	18.504487000	-7.342083000

6	17.780342000	17.507503000	-7.879965000
7	19.040323000	17.760818000	-8.231681000
6	17.226889000	16.189860000	-8.037255000
6	16.002213000	15.936659000	-7.514393000
1	19.460566000	18.689789000	-8.033116000
1	19.661491000	16.974498000	-8.449077000
1	17.801407000	15.414021000	-8.515280000
1	15.530110000	14.960481000	-7.553980000
15	14.747626000	11.881387000	-8.729391000
8	13.504460000	11.048241000	-8.765123000
8	15.507530000	12.335807000	-9.936639000
8	22.639146000	27.958035000	-4.544696000
6	19.467077000	25.303943000	-4.454003000
6	19.984123000	25.056752000	-3.015089000
6	21.108898000	26.097338000	-2.890442000
6	20.461821000	27.281385000	-3.614780000
6	21.378557000	28.429498000	-3.963355000
8	19.944214000	26.631954000	-4.851845000
1	18.377552000	25.242628000	-4.443633000
1	20.290331000	24.022967000	-2.848104000
8	18.851995000	25.426997000	-2.169546000
1	21.999223000	25.786567000	-3.438571000
1	19.628151000	27.643958000	-3.004821000
1	21.637450000	28.937300000	-3.031678000
1	20.869240000	29.116445000	-4.639656000
8	21.456217000	26.435614000	-1.525081000
7	18.113945000	21.001090000	-6.685603000
6	17.355336000	21.899325000	-5.954117000
7	16.073526000	21.588410000	-5.719161000
7	17.860406000	23.053022000	-5.482346000
6	19.159293000	23.227729000	-5.782169000
6	20.001447000	22.384743000	-6.504276000
6	19.464960000	21.179010000	-7.028795000
8	20.066451000	20.315965000	-7.736233000
7	21.296292000	22.924062000	-6.560772000
6	21.233667000	24.078620000	-5.901167000
7	19.938266000	24.306006000	-5.401461000
1	17.673297000	20.085033000	-6.998508000

1	15.648361000	20.682060000	-6.005212000
1	15.536008000	22.249571000	-5.169387000
1	22.018998000	24.822592000	-5.837426000
15	22.858573000	25.795752000	-0.883910000
8	23.179539000	26.622318000	0.321986000
8	23.811869000	25.504640000	-2.001828000
8	10.393388000	16.749870000	-9.951946000
6	10.945895000	20.460857000	-9.635345000
6	9.886726000	20.505028000	-10.745995000
6	9.190591000	19.125476000	-10.676155000
6	9.286493000	18.751379000	-9.177923000
6	9.489394000	17.261946000	-8.912587000
8	10.486009000	19.471124000	-8.667005000
1	11.040493000	21.447729000	-9.185609000
1	10.325218000	20.718899000	-11.725723000
8	8.910018000	21.497337000	-10.327166000
1	8.035220000	21.063686000	-10.575649000
1	9.688294000	18.369305000	-11.281051000
1	8.402417000	19.124743000	-8.653635000
1	8.523972000	16.745792000	-8.966541000
1	9.943447000	17.111815000	-7.930713000
8	7.820983000	19.377659000	-11.114346000
7	12.302505000	20.072204000	-10.075886000
6	13.305930000	21.063068000	-10.064144000
8	13.046138000	22.268450000	-9.875928000
7	14.580741000	20.583293000	-10.258984000
6	14.975826000	19.254130000	-10.437555000
8	16.196864000	18.961852000	-10.535044000
6	13.883553000	18.311472000	-10.473737000
1	14.038087000	17.251695000	-10.602828000
6	12.618468000	18.744190000	-10.267959000
1	15.352613000	21.325352000	-10.209223000
1	11.802619000	18.033287000	-10.212803000
15	11.154621000	15.271803000	-9.863973000
8	10.224677000	14.193755000	-10.323720000
8	12.514716000	15.495112000	-10.471482000
8	23.148407000	25.983050000	-9.076268000
6	19.325607000	26.839988000	-9.449861000

6	19.458194000	27.367045000	-8.004825000
6	20.966719000	27.335165000	-7.823395000
6	21.485273000	27.838879000	-9.177769000
6	22.910481000	27.365697000	-9.482685000
8	20.522521000	27.281819000	-10.162829000
1	18.417849000	27.215951000	-9.923556000
1	18.926302000	26.760321000	-7.269511000
8	19.017430000	28.755588000	-8.030140000
1	19.591575000	29.209461000	-7.349575000
1	21.301860000	26.318568000	-7.653700000
1	21.427180000	28.930427000	-9.199169000
1	23.591105000	28.049029000	-8.958070000
1	23.086506000	27.434842000	-10.559206000
8	21.419164000	28.214420000	-6.753874000
7	16.524054000	22.495597000	-10.064276000
6	16.121704000	23.784762000	-9.940610000
7	16.905138000	24.858083000	-9.737312000
6	18.219552000	24.533751000	-9.684008000
6	18.754027000	23.243029000	-9.812948000
6	17.850182000	22.171923000	-9.981084000
7	18.224631000	20.889673000	-10.058130000
7	20.148915000	23.276066000	-9.754035000
6	20.458392000	24.556172000	-9.587088000
7	19.313047000	25.368683000	-9.517575000
1	15.048215000	23.923243000	-9.992028000
1	19.158505000	20.635438000	-9.740229000
1	17.512646000	20.150992000	-10.207703000
1	21.456332000	24.972773000	-9.496653000
15	22.923190000	27.853374000	-6.140598000
8	23.904705000	28.892978000	-6.588395000
8	23.206290000	26.386395000	-6.468183000
1	36.564172000	10.275082000	-1.133832000
1	31.798041000	19.578503000	-14.613233000
1	7.264848000	18.567668000	-10.975890000
1	23.274762000	26.018828000	-8.050506000
1	12.674082000	18.978888000	-5.929704000
6	11.638372000	18.614058000	-5.912050000
1	11.050855000	19.183608000	-6.635392000

6	11.074835000	18.660409000	-4.524921000
16	11.035869000	17.186443000	-3.591486000
6	10.381513000	18.023386000	-2.215595000
1	10.151867000	17.489694000	-1.306245000
6	10.198964000	19.356795000	-2.472043000
1	9.794557000	20.056821000	-1.753830000
1	10.528957000	20.728641000	-4.197472000
6	10.595390000	19.723020000	-3.804505000
6	16.349564000	10.787237000	-4.774751000
6	15.696132000	10.721196000	-3.427791000
16	15.610895000	12.171059000	-2.461225000
6	14.859731000	11.306272000	-1.154575000
1	14.573970000	11.820214000	-0.249770000
6	14.682626000	9.981519000	-1.456217000
1	14.224610000	9.268421000	-0.784818000
1	15.112101000	8.651093000	-3.192040000
6	15.162444000	9.645102000	-2.768452000
1	17.392203000	10.448773000	-4.710968000
1	15.819807000	10.187676000	-5.517523000
6	21.684367000	9.387532000	-6.209297000
6	21.597369000	7.907986000	-5.989535000
16	22.381978000	6.833493000	-7.118737000
6	21.917804000	5.442877000	-6.185035000
1	22.181420000	4.449258000	-6.513114000
6	21.196755000	5.794230000	-5.074474000
1	20.802740000	5.080965000	-4.363812000
1	20.467314000	7.690163000	-4.157551000
6	21.009684000	7.214954000	-4.963808000
1	20.756709000	9.903226000	-5.949286000
1	22.509121000	9.812677000	-5.621383000
6	27.594080000	10.033175000	-9.680907000
6	27.532147000	8.545900000	-9.606402000
16	28.711265000	7.529059000	-10.393653000
6	27.925123000	6.090459000	-9.813221000
1	28.311142000	5.115204000	-10.066639000
6	26.817176000	6.385663000	-9.062111000
1	26.181983000	5.634704000	-8.613425000
1	25.759532000	8.260350000	-8.430083000

6	26.587382000	7.797523000	-8.950275000
1	26.692561000	10.438058000	-9.211660000
1	28.477424000	10.447757000	-9.179453000
6	18.991301000	25.034082000	-0.758719000
1	19.651024000	24.163094000	-0.663057000
1	19.436875000	25.856121000	-0.192290000
6	16.478786000	24.570010000	-1.038041000
6	17.608517000	24.689581000	-0.275238000
16	17.269719000	24.372097000	1.408868000
6	15.587358000	24.074073000	1.064395000
6	15.317531000	24.216334000	-0.269362000
1	16.488858000	24.731845000	-2.104442000
1	14.906573000	23.811740000	1.859136000
1	14.334055000	24.076483000	-0.696585000
6	20.796052000	18.760426000	2.307053000
1	20.701708000	18.414446000	1.269925000
1	21.399144000	18.035382000	2.854296000
6	18.542191000	18.049504000	3.389601000
6	19.447025000	18.971322000	2.930937000
16	18.842026000	20.598545000	3.103748000
6	17.353714000	20.020173000	3.788319000
6	17.334316000	18.653020000	3.880891000
1	18.720197000	16.982537000	3.378360000
1	16.584399000	20.712369000	4.093974000
1	16.503837000	18.089869000	4.284056000
6	24.622876000	13.727628000	1.423491000
1	24.062526000	14.064515000	0.540215000
1	25.566092000	13.288370000	1.084130000
6	23.567759000	11.447624000	2.077017000
6	23.812217000	12.784086000	2.255913000
16	22.973963000	13.404894000	3.654845000
6	22.280946000	11.845545000	3.985776000
6	22.682417000	10.907066000	3.072015000
1	23.994458000	10.866400000	1.270669000
1	21.636161000	11.701419000	4.838978000
1	22.374315000	9.870985000	3.100194000
6	29.909193000	10.441535000	-1.376592000
1	30.943539000	10.187477000	-1.621693000

1	29.518871000	11.067792000	-2.187659000
6	28.110818000	9.085651000	-0.149059000
6	29.034165000	9.243827000	-1.148246000
16	29.078782000	7.843222000	-2.191737000
6	27.828757000	7.054502000	-1.268841000
6	27.417270000	7.829848000	-0.219010000
1	27.948427000	9.839632000	0.605166000
1	27.475656000	6.075738000	-1.553968000
1	26.652369000	7.525858000	0.482271000

Figure S13. X-Y coordinates for **3:4** at level: B3LYP /6-31G*.

8	31.950725000	19.429178000	-13.591787000
6	32.829613000	15.911510000	-14.602815000
6	31.346423000	15.751278000	-14.951642000
6	30.835366000	17.205255000	-14.964586000
6	32.034999000	17.986941000	-15.516443000
6	32.119978000	19.425819000	-15.048014000
8	33.225939000	17.253683000	-15.005367000
1	33.434356000	15.152660000	-15.094750000
1	30.824687000	15.100310000	-14.256421000
8	31.234858000	15.237155000	-16.323532000
1	30.557202000	15.849985000	-16.741128000
1	30.551155000	17.574932000	-13.982272000
1	32.023986000	17.949607000	-16.608873000
1	31.323195000	19.993428000	-15.542151000
1	33.089296000	19.843608000	-15.340872000
8	29.718302000	17.320178000	-15.913620000
7	33.029087000	15.764454000	-13.138730000
6	33.183836000	14.433790000	-12.645968000
8	33.167426000	13.488615000	-13.472396000
7	33.332221000	14.268730000	-11.298127000
6	33.305763000	15.327121000	-10.472030000
7	33.437492000	15.086738000	-9.151611000
6	33.138961000	16.666564000	-10.954776000
6	33.003040000	16.839711000	-12.298483000
1	33.528850000	14.127469000	-8.832678000
1	33.410841000	15.832052000	-8.465322000
1	33.111615000	17.506452000	-10.277389000
1	32.836856000	17.809233000	-12.755056000
8	28.278939000	15.755076000	-14.496579000
6	29.389972000	13.255297000	-12.034108000
6	27.926299000	12.782042000	-11.890743000
6	27.256582000	13.489423000	-13.079930000
6	28.307444000	13.377834000	-14.187103000
6	28.252632000	14.474268000	-15.230138000
8	29.603760000	13.513909000	-13.450871000
1	30.103148000	12.513118000	-11.680764000

1	27.505162000	13.069529000	-10.928430000
8	27.835487000	11.340434000	-12.100782000
1	27.098219000	14.537399000	-12.834979000
1	28.254149000	12.392386000	-14.655722000
1	27.331848000	14.392541000	-15.812838000
1	29.127788000	14.410092000	-15.880611000
8	25.993092000	12.900782000	-13.491815000
7	30.129650000	14.663089000	-7.287726000
6	30.462232000	13.472726000	-7.905526000
7	30.927324000	12.466563000	-7.146497000
7	30.323107000	13.297140000	-9.224768000
6	29.887044000	14.394745000	-9.879303000
6	29.582244000	15.649314000	-9.346274000
6	29.624538000	15.817727000	-7.938027000
8	29.235634000	16.797847000	-7.248347000
7	29.125879000	16.507813000	-10.359724000
6	29.131129000	15.778692000	-11.467044000
7	29.591779000	14.470207000	-11.226265000
1	30.160462000	14.722301000	-6.269997000
1	31.033679000	12.540696000	-6.141431000
1	31.151634000	11.585904000	-7.596608000
1	28.836725000	16.098887000	-12.451921000
15	28.182399000	17.202463000	-15.267046000
8	27.256603000	17.117819000	-16.441959000
8	28.052107000	18.210573000	-14.163363000
8	24.803811000	12.634411000	-11.256102000
6	25.033249000	11.056671000	-7.696137000
6	23.492543000	11.137113000	-7.702219000
6	23.198265000	11.499777000	-9.169326000
6	24.221899000	10.656561000	-9.934376000
6	24.571595000	11.171312000	-11.311100000
8	25.433818000	10.695298000	-9.058990000
1	25.376287000	10.299713000	-6.991508000
1	23.105335000	11.864663000	-6.988925000
8	22.986411000	9.785729000	-7.456682000
1	23.406443000	12.558314000	-9.317069000
1	23.862331000	9.627456000	-9.999009000
1	23.731002000	10.979140000	-11.980682000

1	25.474840000	10.695422000	-11.696813000
8	21.867793000	11.170600000	-9.649227000
7	27.075005000	13.780793000	-3.839827000
6	26.397500000	12.615715000	-3.851810000
7	25.876788000	11.980888000	-4.924945000
6	26.086773000	12.666074000	-6.067914000
6	26.762030000	13.890261000	-6.199165000
6	27.294751000	14.450730000	-5.013220000
7	28.007241000	15.588902000	-4.962471000
7	26.763740000	14.292823000	-7.546301000
6	26.110206000	13.333141000	-8.197463000
7	25.683102000	12.318647000	-7.343195000
1	26.257548000	12.132658000	-2.892230000
1	28.298032000	16.119388000	-5.795360000
1	28.329988000	15.897876000	-4.049384000
1	25.895656000	13.289678000	-9.251475000
15	24.647651000	13.446116000	-12.691489000
8	23.476219000	12.906013000	-13.457925000
8	24.814001000	14.899863000	-12.357285000
8	20.362009000	11.294882000	-7.627100000
6	18.831621000	10.820778000	-4.222842000
6	17.505852000	11.237840000	-4.908199000
6	17.816862000	11.009217000	-6.401164000
6	18.808366000	9.837503000	-6.445021000
6	19.785413000	9.936664000	-7.599037000
8	19.522086000	9.895398000	-5.130464000
1	18.644064000	10.347760000	-3.258431000
1	17.269066000	12.282108000	-4.720797000
8	16.329628000	10.535401000	-4.406137000
1	18.312378000	11.895415000	-6.788154000
1	18.280238000	8.885603000	-6.514500000
1	19.227237000	9.771082000	-8.523668000
1	20.599314000	9.218898000	-7.512162000
8	16.638473000	10.710587000	-7.192937000
7	20.081169000	14.692121000	-1.107221000
6	19.176336000	13.666957000	-0.892837000
7	18.485485000	13.661920000	0.260818000
7	18.966752000	12.697012000	-1.791133000

6	19.738686000	12.800464000	-2.895249000
6	20.709094000	13.770851000	-3.169300000
6	20.892254000	14.848856000	-2.262377000
8	21.619366000	15.868027000	-2.379112000
7	21.299033000	13.526380000	-4.419118000
6	20.678520000	12.457288000	-4.895405000
7	19.717262000	11.972430000	-4.000086000
1	20.171250000	15.432612000	-0.411970000
1	18.592585000	14.381993000	0.965561000
1	17.810665000	12.921487000	0.416920000
1	20.805692000	12.013738000	-5.867313000
15	20.583672000	12.039512000	-9.080245000
8	19.433754000	11.723623000	-9.991172000
8	21.025209000	13.439453000	-8.747035000
8	14.652197000	11.956496000	-8.053348000
6	15.771313000	15.302642000	-5.453111000
6	14.795250000	15.905116000	-6.506296000
6	14.313820000	14.660608000	-7.277909000
6	14.318844000	13.588269000	-6.189353000
6	14.197476000	12.148753000	-6.667329000
8	15.655765000	13.833474000	-5.575873000
1	15.455044000	15.632653000	-4.464821000
1	15.248301000	16.647083000	-7.159352000
8	13.636326000	16.451673000	-5.788999000
1	15.078202000	14.384201000	-8.003864000
1	13.535181000	13.800766000	-5.455280000
1	13.139848000	11.881040000	-6.671086000
1	14.746434000	11.495756000	-5.986364000
8	12.995535000	14.768414000	-7.883289000
7	17.175147000	15.675729000	-5.585799000
6	17.674698000	16.650715000	-4.666419000
8	16.856367000	17.276451000	-3.939414000
7	19.021428000	16.829651000	-4.609732000
6	19.839003000	16.193263000	-5.464859000
7	21.173346000	16.350156000	-5.277546000
6	19.336544000	15.349645000	-6.511173000
6	18.002133000	15.080282000	-6.504115000
1	21.463800000	16.578826000	-4.320104000

1	21.788053000	15.694284000	-5.753383000
1	19.988149000	14.848827000	-7.216135000
1	17.557642000	14.356847000	-7.183723000
15	16.213844000	11.693108000	-8.456670000
8	16.202724000	10.892474000	-9.724788000
8	17.013991000	12.975752000	-8.379956000
8	11.536192000	16.475761000	-9.016083000
6	11.975976000	20.408541000	-8.614820000
6	10.472872000	20.444663000	-8.931590000
6	10.064072000	18.962629000	-8.861704000
6	10.927540000	18.453054000	-7.697089000
6	11.183571000	16.963099000	-7.668109000
8	12.222375000	19.184941000	-7.866228000
1	12.263874000	21.288189000	-8.040082000
1	10.260026000	20.922723000	-9.888765000
8	9.816888000	21.109969000	-7.812499000
1	8.970407000	20.571531000	-7.714608000
1	10.307776000	18.417844000	-9.774164000
1	10.473317000	18.766543000	-6.753951000
1	10.256676000	16.464987000	-7.365015000
1	11.973425000	16.722576000	-6.956490000
8	8.637986000	18.962959000	-8.555194000
7	12.792813000	20.367318000	-9.859155000
6	12.874096000	21.566488000	-10.572761000
8	12.274882000	22.591355000	-10.196404000
7	13.656338000	21.499102000	-11.708066000
6	14.374689000	20.382574000	-12.201408000
8	15.044466000	20.486849000	-13.248388000
6	14.224976000	19.210711000	-11.375120000
1	14.737547000	18.300966000	-11.645114000
6	13.461084000	19.238780000	-10.257534000
1	13.724288000	22.358807000	-12.251168000
1	13.369922000	18.358532000	-9.636460000
15	12.894104000	15.608901000	-9.306316000
8	12.572464000	14.681658000	-10.443388000
8	14.107395000	16.512725000	-9.377812000
1	32.065609000	20.361448000	-13.266597000
1	8.387106000	18.085277000	-8.162574000

1	14.861640000	17.919404000	-4.897088000
6	13.854997000	17.850333000	-5.325020000
1	13.732056000	18.538130000	-6.165736000
6	12.809583000	18.111408000	-4.286941000
16	12.309982000	16.822164000	-3.220272000
6	11.243293000	17.888895000	-2.354126000
1	10.643816000	17.519313000	-1.536543000
6	11.270306000	19.159022000	-2.868716000
1	10.673168000	19.974232000	-2.484418000
1	12.327239000	20.203902000	-4.533457000
6	12.167831000	19.285415000	-3.985220000
6	16.263475000	9.069719000	-4.602416000
6	15.187584000	8.586607000	-3.677729000
16	14.785833000	9.540552000	-2.272392000
6	13.622787000	8.359001000	-1.748204000
1	13.046646000	8.517704000	-0.849790000
6	13.550721000	7.299196000	-2.614420000
1	12.883536000	6.459013000	-2.480880000
1	14.539899000	6.703324000	-4.522321000
6	14.450358000	7.432542000	-3.728789000
1	17.223838000	8.609030000	-4.342806000
1	16.022950000	8.841922000	-5.642730000
6	22.874202000	9.504235000	-5.994907000
6	22.732365000	8.027228000	-5.836564000
16	23.942294000	6.926850000	-6.449066000
6	23.040899000	5.550079000	-5.888491000
1	23.411128000	4.549863000	-6.052267000
6	21.874372000	5.924004000	-5.271930000
1	21.165562000	5.220735000	-4.857910000
1	20.830318000	7.859638000	-4.845921000
6	21.693111000	7.348045000	-5.250122000
1	21.982658000	9.990739000	-5.594414000
1	23.763228000	9.892044000	-5.482395000
6	28.150740000	10.610880000	-10.837748000
6	28.046771000	9.150653000	-11.123769000
16	28.967578000	8.395992000	-12.400329000
6	28.280359000	6.839626000	-12.039234000
1	28.556624000	5.971662000	-12.617660000

6	27.393011000	6.906636000	-10.995809000
1	26.851390000	6.051689000	-10.616199000
1	26.588384000	8.527165000	-9.673294000
6	27.252856000	8.237268000	-10.475579000
1	27.411996000	10.871997000	-10.076588000
1	29.149210000	10.896337000	-10.487714000

Figure S14. X-Y coordinates for **4** at level: B3LYP /3-21G*.

8	27.818598000	20.207289000	-12.814916000
6	30.516512000	17.661224000	-13.284203000
6	29.464159000	16.830880000	-14.016376000
6	28.339319000	17.852903000	-14.259083000
6	29.114841000	19.145839000	-14.528750000
6	28.353382000	20.404324000	-14.165297000
8	30.313620000	19.055434000	-13.657366000
1	31.523891000	17.324026000	-13.518417000
1	29.163567000	15.962144000	-13.440567000
8	29.978516000	16.440262000	-15.335187000
1	29.210843000	16.672905000	-15.942121000
1	27.669248000	17.978917000	-13.412177000
1	29.418455000	19.169596000	-15.579601000
1	27.548677000	20.536284000	-14.899170000
1	29.031560000	21.264333000	-14.212655000
8	27.597696000	17.480942000	-15.468118000
7	30.316328000	17.512471000	-11.820648000
6	30.913586000	16.353044000	-11.218349000
8	31.585551000	15.592344000	-11.946285000
7	30.697882000	16.163650000	-9.878524000
6	29.941279000	17.018999000	-9.182892000
7	29.782405000	16.774674000	-7.860679000
6	29.315404000	18.160231000	-9.782078000
6	29.526971000	18.368782000	-11.110242000
1	30.158768000	15.910374000	-7.487166000
1	29.136360000	17.307658000	-7.291516000
1	28.677875000	18.815613000	-9.208954000
1	29.065049000	19.180805000	-11.663430000
8	26.816346000	15.386134000	-14.261443000
6	28.386182000	13.914493000	-11.361939000
6	27.404303000	12.740453000	-11.412001000
6	26.732285000	12.951046000	-12.779325000
6	27.914068000	13.366321000	-13.659048000
6	27.566541000	14.263568000	-14.830309000
8	28.777902000	14.168879000	-12.734111000
1	29.260181000	13.706361000	-10.746905000
1	26.684398000	12.781488000	-10.601713000

8	28.145650000	11.492623000	-11.427461000
1	26.033794000	13.783155000	-12.696061000
1	28.455145000	12.472803000	-13.979440000
1	26.955083000	13.719641000	-15.556521000
1	28.486089000	14.629521000	-15.298610000
8	26.087511000	11.774694000	-13.331615000
7	26.772485000	15.528294000	-6.922939000
6	27.671383000	14.531309000	-7.245563000
7	28.166927000	13.778326000	-6.240066000
7	28.060288000	14.291662000	-8.497260000
6	27.501239000	15.126256000	-9.402180000
6	26.576580000	16.151701000	-9.181612000
6	26.099815000	16.362741000	-7.861982000
8	25.171069000	17.107322000	-7.455594000
7	26.182468000	16.714050000	-10.405671000
6	26.847867000	16.042458000	-11.337135000
7	27.685943000	15.065003000	-10.763833000
1	26.302574000	15.506929000	-6.002060000
1	27.833844000	13.854713000	-5.286755000
1	28.768045000	12.999621000	-6.483128000
1	26.752229000	16.145282000	-12.402487000
15	26.189517000	16.610087000	-15.174726000
8	25.737115000	16.090462000	-16.500711000
8	25.361143000	17.394172000	-14.204928000
8	25.529940000	9.891155000	-11.811855000
6	24.980659000	9.515887000	-7.987799000
6	23.448475000	9.500948000	-8.119452000
6	23.286922000	9.591035000	-9.646866000
6	24.339537000	8.580494000	-10.100161000
6	24.791966000	8.658955000	-11.546405000
8	25.502407000	8.920339000	-9.214312000
1	25.342220000	8.964151000	-7.121641000
1	22.979955000	10.333203000	-7.600194000
8	22.922681000	8.215467000	-7.684297000
1	23.563080000	10.585568000	-9.994200000
1	23.978602000	7.574967000	-9.866872000
1	23.907198000	8.599834000	-12.189333000
1	25.468116000	7.828353000	-11.763266000

8	21.962143000	9.266762000	-10.123661000
7	25.310074000	12.746238000	-4.147849000
6	25.602573000	11.429223000	-4.227300000
7	25.659526000	10.669802000	-5.345862000
6	25.441168000	11.388728000	-6.462955000
6	25.132834000	12.749688000	-6.514824000
6	25.018321000	13.424733000	-5.287471000
7	24.649675000	14.738241000	-5.216189000
7	24.900732000	13.135381000	-7.846074000
6	25.042332000	12.031531000	-8.576310000
7	25.384493000	10.921835000	-7.779474000
1	25.804433000	10.922702000	-3.291716000
1	24.175762000	15.075840000	-6.061002000
1	24.115915000	15.026170000	-4.375295000
1	24.896461000	11.991586000	-9.657451000
15	24.785839000	11.184357000	-12.501452000
8	23.736422000	10.715318000	-13.461479000
8	24.470511000	12.181533000	-11.403810000
8	20.628448000	10.100243000	-8.124229000
6	19.290097000	10.590977000	-4.633991000
6	18.000207000	11.051996000	-5.320081000
6	18.209466000	10.535299000	-6.749590000
6	18.973066000	9.213556000	-6.595183000
6	19.854727000	8.899998000	-7.779552000
8	19.795177000	9.421902000	-5.355981000
1	19.121485000	10.339037000	-3.585705000
1	17.899958000	12.133639000	-5.310116000
8	16.792416000	10.592862000	-4.648434000
1	18.872172000	11.229797000	-7.262070000
1	18.298112000	8.374277000	-6.427477000
1	19.198687000	8.650657000	-8.618909000
1	20.541638000	8.079691000	-7.578386000
8	16.980090000	10.354017000	-7.486046000
7	20.352307000	15.327425000	-3.156259000
6	19.180985000	14.608190000	-3.038164000
7	18.098405000	15.234189000	-2.527317000
7	19.082287000	13.336652000	-3.421052000
6	20.178994000	12.884589000	-4.071039000

6	21.396763000	13.544531000	-4.273951000
6	21.576618000	14.836619000	-3.702485000
8	22.595929000	15.560634000	-3.617374000
7	22.236201000	12.758002000	-5.076605000
6	21.548114000	11.656745000	-5.336931000
7	20.291946000	11.671484000	-4.716754000
1	20.334375000	16.336516000	-3.018892000
1	18.116822000	16.185590000	-2.181956000
1	17.229210000	14.715743000	-2.476987000
1	21.814733000	10.870456000	-6.010575000
15	20.799805000	10.403855000	-9.746722000
8	19.571060000	9.974144000	-10.486530000
8	21.406642000	11.775640000	-9.814185000
8	15.270118000	12.127125000	-8.060690000
6	17.752852000	15.162097000	-6.049793000
6	16.769981000	15.960730000	-6.952063000
6	15.878350000	14.853531000	-7.545142000
6	15.777369000	13.896997000	-6.365216000
6	15.158683000	12.538047000	-6.661958000
8	17.212772000	13.795328000	-5.978519000
1	17.766046000	15.617125000	-5.062960000
1	17.238821000	16.567920000	-7.722680000
8	15.926929000	16.758531000	-6.055546000
1	16.430627000	14.331037000	-8.329035000
1	15.224531000	14.386817000	-5.555854000
1	14.085322000	12.635934000	-6.480850000
1	15.572366000	11.783965000	-5.987463000
8	14.552199000	15.259252000	-7.962037000
7	19.133298000	15.124195000	-6.534115000
6	19.983289000	16.194642000	-6.107254000
8	19.517309000	17.052985000	-5.304650000
7	21.255684000	16.213874000	-6.581573000
6	21.713114000	15.230212000	-7.378943000
7	22.995777000	15.327192000	-7.799433000
6	20.881008000	14.142345000	-7.804497000
6	19.586348000	14.142640000	-7.380360000
1	23.530617000	16.186730000	-7.633086000
1	23.523046000	14.528979000	-8.177470000

1	21.227273000	13.366780000	-8.481220000
1	18.851357000	13.421810000	-7.739876000
15	16.603530000	11.426543000	-8.708566000
8	16.131470000	10.653400000	-9.897071000
8	17.718681000	12.442867000	-8.809064000
8	13.421030000	17.347696000	-8.796003000
6	14.615866000	20.972448000	-8.268559000
6	13.154315000	21.373509000	-8.090999000
6	12.439525000	20.014081000	-8.058735000
6	13.406257000	19.189354000	-7.198169000
6	13.372778000	17.693525000	-7.370634000
8	14.763875000	19.713513000	-7.564118000
1	15.284753000	21.724650000	-7.852257000
1	12.805811000	22.065762000	-8.856917000
8	13.070571000	21.921984000	-6.738844000
1	12.165324000	21.611749000	-6.432171000
1	12.333217000	19.565737000	-9.048923000
1	13.228915000	19.434859000	-6.150330000
1	12.428864000	17.325129000	-6.946171000
1	14.208160000	17.248758000	-6.827348000
8	11.172294000	20.264362000	-7.380715000
7	14.952271000	20.755771000	-9.704112000
6	14.985031000	21.899351000	-10.511588000
8	14.695870000	23.024564000	-10.069063000
7	15.356590000	21.646875000	-11.819355000
6	15.728860000	20.401108000	-12.408202000
8	16.041254000	20.357174000	-13.610013000
6	15.689733000	19.314130000	-11.460921000
1	15.964277000	18.314418000	-11.754708000
6	15.319222000	19.520325000	-10.177227000
1	15.377073000	22.456764000	-12.435900000
1	15.306519000	18.690604000	-9.489584000
15	14.435222000	16.166542000	-9.346488000
8	13.697092000	15.411314000	-10.409726000
8	15.807935000	16.749971000	-9.613627000
1	27.333602000	21.027771000	-12.537209000
1	10.773384000	19.398594000	-7.101614000
1	17.606798000	17.931473000	-5.549003000

6	16.542844000	18.090556000	-5.758891000
1	16.394022000	18.748174000	-6.615222000
6	15.809920000	18.639518000	-4.580948000
16	15.735233000	17.707846000	-3.101144000
6	14.785160000	18.935350000	-2.317751000
1	14.451907000	18.808771000	-1.299046000
6	14.535778000	19.990278000	-3.155639000
1	13.951968000	20.854268000	-2.869849000
1	14.978170000	20.516547000	-5.273294000
6	15.116524000	19.818764000	-4.458962000
6	16.469931000	9.159288000	-4.743081000
6	15.361911000	8.940208000	-3.760012000
16	15.122726000	10.119019000	-2.496919000
6	13.827557000	9.180588000	-1.813642000
1	13.295994000	9.529211000	-0.941290000
6	13.597234000	8.033716000	-2.527821000
1	12.829160000	7.314870000	-2.278400000
1	14.460813000	7.062333000	-4.340556000
6	14.481960000	7.896618000	-3.652662000
1	17.348274000	8.559514000	-4.468396000
1	16.164014000	8.915951000	-5.763144000
6	22.739277000	8.188475000	-6.210409000
6	22.258708000	6.824076000	-5.854176000
16	23.113424000	5.395694000	-6.374002000
6	21.945131000	4.365561000	-5.598873000
1	22.041758000	3.291683000	-5.647518000
6	20.954577000	5.090168000	-4.987382000
1	20.126652000	4.640100000	-4.457699000
1	20.454746000	7.268848000	-4.777102000
6	21.129625000	6.506323000	-5.141907000
1	21.967976000	8.901607000	-5.914661000
1	23.684101000	8.446781000	-5.711590000
6	27.944040000	10.769935000	-10.147465000
6	28.879181000	9.610509000	-10.137952000
16	30.518626000	9.780573000	-10.710126000
6	30.866028000	8.116708000	-10.328475000
1	31.839558000	7.696938000	-10.531393000
6	29.772633000	7.478689000	-9.801670000

1	29.773534000	6.437670000	-9.509029000
1	27.645953000	8.050505000	-9.340610000
6	28.625123000	8.337289000	-9.698836000
1	26.922480000	10.398620000	-10.087118000
1	28.148195000	11.461210000	-9.316120000

Figure S15. X-Y coordinates for **4** at level: B3LYP-GD3/3-21G*.

8	33.193965000	17.440126000	-10.992998000
6	34.378316000	13.828943000	-12.048257000
6	33.461348000	13.974682000	-13.269500000
6	33.058111000	15.438526000	-13.118209000
6	34.372215000	16.089942000	-12.688460000
6	34.230392000	17.423148000	-11.961592000
8	34.976238000	15.092033000	-11.828624000
1	35.143873000	13.068465000	-12.212603000
1	32.612950000	13.289503000	-13.230653000
8	34.249890000	13.775214000	-14.437948000
1	33.801476000	14.262188000	-15.151161000
1	32.337017000	15.512022000	-12.302813000
1	35.012377000	16.224579000	-13.570074000
1	34.065472000	18.197337000	-12.724069000
1	35.173325000	17.647788000	-11.450791000
8	32.539710000	15.998710000	-14.316223000
7	33.613109000	13.421621000	-10.839357000
6	33.229989000	12.055737000	-10.754859000
8	33.493160000	11.314513000	-11.709309000
7	32.591262000	11.634251000	-9.624864000
6	32.359124000	12.491702000	-8.632853000
7	31.807631000	11.994863000	-7.494892000
6	32.691340000	13.880157000	-8.711531000
6	33.313203000	14.302424000	-9.845279000
1	31.383996000	11.078155000	-7.547293000
1	31.412496000	12.629407000	-6.815338000
1	32.442468000	14.574759000	-7.920246000
1	33.579369000	15.337273000	-10.021182000
8	30.031329000	15.786988000	-13.845319000
6	29.632088000	12.822292000	-11.603941000
6	28.164143000	12.612500000	-12.028835000
6	28.068044000	13.650071000	-13.156332000
6	29.419948000	13.468034000	-13.848697000
6	29.908070000	14.635343000	-14.680785000
8	30.339288000	13.225195000	-12.757204000
1	30.092179000	11.924082000	-11.185406000
1	27.471540000	12.794229000	-11.206943000

8	27.951718000	11.323432000	-12.574449000
1	28.024774000	14.648655000	-12.709548000
1	29.372400000	12.577454000	-14.488712000
1	29.181093000	14.818943000	-15.481970000
1	30.872365000	14.384872000	-15.134729000
8	27.004313000	13.473840000	-14.066753000
7	28.703914000	13.736703000	-6.744322000
6	28.556032000	12.577982000	-7.472107000
7	28.091579000	11.483134000	-6.787267000
7	28.881179000	12.483773000	-8.743881000
6	29.334823000	13.653951000	-9.259950000
6	29.459413000	14.895956000	-8.635970000
6	29.114382000	15.005967000	-7.248997000
8	29.134062000	15.983505000	-6.505149000
7	29.888660000	15.853129000	-9.536684000
6	30.021042000	15.205747000	-10.674550000
7	29.710512000	13.859653000	-10.562965000
1	28.437788000	13.739078000	-5.764997000
1	27.318473000	11.664337000	-6.151211000
1	27.923313000	10.685185000	-7.389492000
1	30.303580000	15.638406000	-11.621279000
15	31.167621000	16.937413000	-14.178308000
8	30.954328000	17.555220000	-15.523656000
8	31.250122000	17.748483000	-12.903899000
8	24.963108000	13.562664000	-12.507967000
6	25.275596000	12.106036000	-9.099870000
6	23.759438000	11.902643000	-8.965467000
6	23.315156000	12.296548000	-10.380876000
6	24.392871000	11.622197000	-11.228598000
6	24.642248000	12.176027000	-12.613226000
8	25.595794000	11.797140000	-10.433225000
1	25.850588000	11.466493000	-8.428412000
1	23.322301000	12.545777000	-8.202253000
8	23.452916000	10.540775000	-8.735175000
1	23.408754000	13.382173000	-10.477279000
1	24.177356000	10.551339000	-11.314290000
1	23.740837000	12.030324000	-13.222228000
1	25.475974000	11.628039000	-13.065133000

8	22.009748000	11.893556000	-10.740326000
7	25.767017000	15.423850000	-5.237667000
6	25.556594000	14.100024000	-5.273143000
7	25.484668000	13.291073000	-6.339134000
6	25.628841000	13.983078000	-7.484027000
6	25.834096000	15.359406000	-7.611524000
6	25.911509000	16.087396000	-6.404891000
7	26.087458000	17.430866000	-6.376161000
7	25.946293000	15.719483000	-8.944480000
6	25.805252000	14.587922000	-9.604490000
7	25.626672000	13.494772000	-8.771965000
1	25.442332000	13.617489000	-4.304767000
1	26.460815000	17.871520000	-7.206166000
1	26.366009000	17.837437000	-5.492758000
1	25.805433000	14.474088000	-10.679660000
15	25.598920000	14.344298000	-13.825229000
8	24.763317000	14.076002000	-15.041714000
8	25.933711000	15.720744000	-13.324770000
8	20.643999000	12.336297000	-8.598368000
6	20.142068000	12.258135000	-5.068697000
6	18.607912000	12.266042000	-5.229550000
6	18.425522000	11.745390000	-6.675468000
6	19.670861000	10.879624000	-6.935314000
6	20.237718000	10.989999000	-8.337609000
8	20.649915000	11.258857000	-5.930547000
1	20.426498000	12.012199000	-4.041451000
1	18.190947000	13.262821000	-5.115828000
8	17.963867000	11.507752000	-4.216399000
1	18.420550000	12.599446000	-7.356951000
1	19.418854000	9.826882000	-6.765143000
1	19.449396000	10.685832000	-9.038002000
1	21.094354000	10.323221000	-8.463291000
8	17.250231000	10.971898000	-6.833172000
7	20.116880000	17.361849000	-4.515399000
6	19.228429000	16.440110000	-4.018029000
7	18.193703000	16.938367000	-3.256691000
7	19.351997000	15.143058000	-4.207038000
6	20.412609000	14.815838000	-4.986542000

6	21.351864000	15.673375000	-5.562203000
6	21.207791000	17.085925000	-5.376776000
8	21.879043000	18.004271000	-5.851304000
7	22.279167000	14.964458000	-6.305146000
6	21.903846000	13.714731000	-6.179665000
7	20.763120000	13.553074000	-5.415183000
1	19.904129000	18.347075000	-4.402459000
1	17.719689000	17.724115000	-3.701016000
1	17.530661000	16.207880000	-3.018394000
1	22.389704000	12.862569000	-6.613112000
15	20.750558000	12.831433000	-10.173181000
8	19.534884000	12.400365000	-10.936991000
8	21.210018000	14.266983000	-10.108779000
8	14.783663000	11.595943000	-6.921689000
6	15.994053000	15.646964000	-6.045270000
6	14.555833000	15.842138000	-6.612525000
6	14.030517000	14.393697000	-6.695334000
6	14.820925000	13.702521000	-5.586618000
6	14.858088000	12.179393000	-5.620889000
8	16.135925000	14.258852000	-5.743476000
1	16.089346000	16.248810000	-5.140431000
1	14.550001000	16.329147000	-7.589931000
8	13.785580000	16.574449000	-5.675276000
1	14.356183000	13.963349000	-7.648211000
1	14.412847000	14.006469000	-4.609509000
1	13.966193000	11.823107000	-5.095754000
1	15.743033000	11.827721000	-5.080102000
8	12.641676000	14.214014000	-6.489854000
7	17.087130000	16.041255000	-6.920898000
6	17.771463000	17.259398000	-6.679844000
8	17.298710000	18.065370000	-5.852448000
7	18.935645000	17.472877000	-7.337595000
6	19.377222000	16.587435000	-8.237262000
7	20.615380000	16.757256000	-8.752658000
6	18.582272000	15.474657000	-8.663253000
6	17.462138000	15.216548000	-7.943854000
1	21.238522000	17.352555000	-8.216943000
1	21.021983000	15.948043000	-9.229472000

1	18.906088000	14.816745000	-9.456063000
1	16.860307000	14.326466000	-8.111104000
15	16.055344000	11.317622000	-7.936827000
8	15.724065000	10.046164000	-8.663756000
8	16.417159000	12.565421000	-8.703781000
8	10.380939000	15.283738000	-6.815742000
6	9.601417000	19.149512000	-7.244724000
6	8.240624000	18.834630000	-6.603868000
6	8.437221000	17.381710000	-6.158916000
6	9.901592000	17.403212000	-5.700817000
6	10.624222000	16.073633000	-5.648037000
8	10.549826000	18.300626000	-6.636966000
1	9.867151000	20.196607000	-7.085997000
1	7.411081000	18.966411000	-7.306686000
8	8.101030000	19.682958000	-5.472937000
1	7.586150000	19.175290000	-4.820058000
1	8.325719000	16.701692000	-7.012042000
1	9.949623000	17.854133000	-4.700912000
1	10.241205000	15.521221000	-4.778363000
1	11.691168000	16.242450000	-5.494776000
8	7.504266000	17.094780000	-5.130052000
7	9.596240000	18.915496000	-8.713645000
6	8.932187000	19.871246000	-9.478189000
8	8.362604000	20.836480000	-8.977846000
7	8.965806000	19.635744000	-10.837773000
6	9.590836000	18.571374000	-11.519298000
8	9.524507000	18.506513000	-12.744941000
6	10.266378000	17.652696000	-10.630716000
1	10.800749000	16.809102000	-11.046196000
6	10.249095000	17.852715000	-9.290434000
1	8.480633000	20.319673000	-11.408478000
1	10.771237000	17.183885000	-8.617513000
15	11.602207000	14.632387000	-7.723690000
8	11.022855000	13.394419000	-8.349898000
8	12.273807000	15.684279000	-8.573434000
1	32.363893000	17.554368000	-11.516512000
1	7.651429000	16.189604000	-4.813562000
1	14.901014000	18.264842000	-6.155318000

6	13.885353000	18.002311000	-5.835135000
1	13.165968000	18.334421000	-6.593462000
6	13.566454000	18.653088000	-4.529524000
16	14.642495000	18.476269000	-3.157113000
6	13.598927000	19.438128000	-2.152152000
1	13.861818000	19.625173000	-1.119101000
6	12.496222000	19.866862000	-2.838508000
1	11.718935000	20.480051000	-2.395304000
1	11.686379000	19.631425000	-4.904527000
6	12.476928000	19.413466000	-4.195273000
6	18.245332000	10.098785000	-4.145102000
6	17.601179000	9.558842000	-2.911267000
16	18.078663000	10.104209000	-1.317699000
6	16.922131000	9.051274000	-0.557574000
1	16.829273000	9.036736000	0.520552000
6	16.215476000	8.330046000	-1.479980000
1	15.442238000	7.616912000	-1.215754000
1	16.158159000	8.163421000	-3.700277000
6	16.602219000	8.625867000	-2.824695000
1	19.330400000	9.929498000	-4.128817000
1	17.829140000	9.583875000	-5.016003000
6	23.588782000	10.149306000	-7.358881000
6	23.161077000	8.726588000	-7.220459000
16	23.934690000	7.440664000	-8.119511000
6	22.893743000	6.248139000	-7.398165000
1	22.990782000	5.206778000	-7.676176000
6	22.010863000	6.814216000	-6.520375000
1	21.271503000	6.245581000	-5.967003000
1	21.559480000	8.874601000	-5.788809000
6	22.162076000	8.232924000	-6.422790000
1	22.940420000	10.763335000	-6.723156000
1	24.625720000	10.296387000	-7.027339000
6	28.036098000	10.259053000	-11.607590000
6	27.027430000	9.200282000	-11.920250000
16	26.989514000	8.401352000	-13.477444000
6	25.642172000	7.412551000	-12.993882000
1	25.213275000	6.703578000	-13.689959000
6	25.255813000	7.683398000	-11.710210000

1	24.431176000	7.185232000	-11.212467000
1	25.878291000	9.085972000	-10.098568000
6	26.047083000	8.706563000	-11.100075000
1	27.842849000	10.640567000	-10.600628000
1	29.054882000	9.847133000	-11.627995000

Figure S16. X-Y coordinates for **4** at level: B3LYP-GD3/6-31G*.

8	31.183368000	20.259201000	-13.222177000
6	32.447651000	16.754468000	-12.608286000
6	31.216986000	16.255906000	-13.354812000
6	30.647293000	17.564771000	-13.915775000
6	31.922305000	18.282854000	-14.370554000
6	31.802715000	19.788353000	-14.462334000
8	32.920629000	17.935741000	-13.318670000
1	33.226021000	15.998147000	-12.532773000
1	30.544367000	15.666178000	-12.740654000
8	31.670364000	15.475605000	-14.519800000
1	31.081964000	15.822641000	-15.254656000
1	30.101971000	18.157082000	-13.186186000
1	32.249216000	17.873756000	-15.329947000
1	31.176929000	20.019380000	-15.333779000
1	32.799632000	20.220326000	-14.610340000
8	29.798512000	17.274137000	-15.069825000
7	32.046039000	17.155543000	-11.226885000
6	31.928575000	16.130746000	-10.260945000
8	32.142775000	14.938675000	-10.628761000
7	31.584277000	16.480745000	-8.992593000
6	31.245593000	17.757233000	-8.681107000
7	30.874331000	18.020981000	-7.428780000
6	31.308467000	18.785884000	-9.677302000
6	31.729701000	18.454611000	-10.922652000
1	30.868956000	17.265927000	-6.708415000
1	30.381484000	18.880481000	-7.210826000
1	31.036167000	19.801673000	-9.435196000
1	31.785221000	19.174426000	-11.731760000
8	29.668528000	10.561014000	-1.136866000
6	29.126401000	10.403325000	-4.806843000
6	30.163664000	9.281691000	-4.874444000
6	30.341028000	8.894631000	-3.392188000
6	28.901832000	9.038987000	-2.851057000
6	28.810649000	9.386396000	-1.385409000
8	28.283906000	10.137802000	-3.648607000
1	28.522133000	10.449147000	-5.715949000
1	31.076510000	9.599760000	-5.381171000

8	29.594712000	8.068340000	-5.469387000
1	29.639374000	8.122928000	-6.465946000
1	30.989665000	9.599437000	-2.872560000
1	28.361439000	8.110332000	-3.043234000
1	29.173922000	8.542836000	-0.788815000
1	27.785725000	9.644851000	-1.114604000
8	30.852257000	7.552435000	-3.248492000
7	31.113916000	14.432772000	-7.190878000
6	30.985579000	13.140091000	-7.653718000
7	31.363082000	12.898410000	-8.925200000
7	30.523283000	12.132661000	-6.891881000
6	30.291471000	12.501797000	-5.614594000
6	30.494369000	13.756899000	-5.030236000
6	30.857530000	14.842039000	-5.867712000
8	30.942076000	16.060454000	-5.543687000
7	30.167954000	13.718620000	-3.662943000
6	29.758676000	12.480877000	-3.437448000
7	29.795382000	11.697656000	-4.607912000
1	31.338167000	15.211944000	-7.886170000
1	31.724421000	13.643388000	-9.557432000
1	31.309204000	11.936302000	-9.242003000
1	29.530156000	12.022453000	-2.493142000
8	28.167792000	15.752420000	-13.824453000
6	28.924342000	13.886855000	-10.955451000
6	27.668335000	13.016845000	-11.105196000
6	27.226762000	13.358839000	-12.535975000
6	28.553760000	13.478781000	-13.286589000
6	28.554852000	14.472989000	-14.427368000
8	29.500930000	14.017994000	-12.271875000
1	29.652825000	13.418548000	-10.298896000
1	26.920238000	13.264003000	-10.359518000
8	28.068087000	11.610931000	-11.014885000
1	26.743451000	14.338143000	-12.512717000
1	28.879650000	12.486088000	-13.608575000
1	27.848360000	14.170198000	-15.206641000
1	29.569032000	14.538225000	-14.826814000
8	26.375167000	12.375959000	-13.174078000
7	27.812349000	15.544240000	-6.449608000

6	27.821407000	14.275583000	-6.986511000
7	27.479481000	13.236540000	-6.216643000
7	28.157849000	14.055696000	-8.261629000
6	28.310430000	15.174766000	-8.981738000
6	28.200975000	16.502811000	-8.570609000
6	28.022666000	16.740784000	-7.171490000
8	28.051057000	17.845767000	-6.554463000
7	28.355752000	17.345149000	-9.691270000
6	28.567693000	16.538028000	-10.730716000
7	28.575944000	15.186044000	-10.332467000
1	27.638501000	15.655355000	-5.408620000
1	27.155451000	13.344673000	-5.233257000
1	27.476882000	12.330405000	-6.667838000
1	28.608976000	16.836142000	-11.763191000
15	28.161557000	17.149387000	-14.693977000
8	27.457328000	16.966586000	-15.999082000
8	27.849053000	18.207620000	-13.675225000
8	27.687425000	14.882697000	1.901686000
6	26.118218000	13.508295000	-1.134215000
6	27.045065000	12.290143000	-1.085734000
6	27.699729000	12.467539000	0.298303000
6	26.523592000	12.916546000	1.165872000
6	26.852220000	13.775604000	2.372661000
8	25.709963000	13.745770000	0.234264000
1	25.227673000	13.360316000	-1.731306000
1	27.731738000	12.263743000	-1.920179000
8	26.237951000	11.067541000	-1.054049000
1	28.434541000	13.273447000	0.239008000
1	25.948187000	12.037020000	1.464155000
1	27.391037000	13.162083000	3.103449000
1	25.925541000	14.165355000	2.803035000
8	28.299538000	11.278184000	0.861516000
7	26.834604000	14.685253000	-1.697683000
6	26.985557000	14.668027000	-3.096564000
8	26.683415000	13.592207000	-3.695124000
7	27.426575000	15.782738000	-3.717386000
6	27.763747000	16.892923000	-3.014470000
7	28.118620000	17.970003000	-3.719120000

6	27.737139000	16.871684000	-1.579357000
6	27.260315000	15.756274000	-0.964669000
1	28.073268000	17.950369000	-4.759151000
1	28.335202000	18.840944000	-3.247520000
1	28.063338000	17.692232000	-0.960213000
1	27.250083000	15.659530000	0.107604000
15	29.887574000	11.004343000	0.447616000
8	30.320131000	9.814545000	1.246495000
8	30.619859000	12.311080000	0.399670000
8	24.994137000	11.741704000	-11.133860000
6	24.475582000	11.041542000	-7.467720000
6	23.086574000	10.484929000	-7.798411000
6	23.150951000	10.539185000	-9.329725000
6	24.521141000	9.920595000	-9.606794000
6	25.117796000	10.293364000	-10.946161000
8	25.360862000	10.475348000	-8.491405000
1	24.824583000	10.761808000	-6.475017000
1	22.268932000	11.035608000	-7.343772000
8	23.008365000	9.049962000	-7.473847000
1	23.159887000	11.580783000	-9.645312000
1	24.464398000	8.837305000	-9.493030000
1	24.546713000	9.792677000	-11.732820000
1	26.174016000	10.022407000	-11.005698000
8	22.099564000	9.845523000	-10.040644000
7	24.326327000	15.367363000	-4.761845000
6	24.044589000	14.094540000	-4.401980000
7	24.058844000	13.025854000	-5.213375000
6	24.371836000	13.354934000	-6.482306000
6	24.653065000	14.636009000	-6.973937000
6	24.660742000	15.691514000	-6.044303000
7	24.980329000	16.953763000	-6.338523000
7	24.946641000	14.583120000	-8.340495000
6	24.854562000	13.298865000	-8.667783000
7	24.506873000	12.504423000	-7.560676000
1	23.780907000	13.958985000	-3.365667000
1	25.222392000	17.186935000	-7.294365000
1	25.015472000	17.685603000	-5.605112000
1	25.002331000	12.853920000	-9.639799000

15	24.793493000	12.354084000	-12.666358000
8	24.095709000	11.329387000	-13.508306000
8	24.323614000	13.761510000	-12.465796000
8	25.364356000	19.930814000	2.095080000
6	23.532744000	16.954977000	0.687336000
6	24.549197000	16.071934000	1.391239000
6	25.320216000	17.116623000	2.195631000
6	24.183281000	17.957485000	2.784459000
6	24.515685000	19.387627000	3.156418000
8	23.237704000	18.026954000	1.618748000
1	22.613612000	16.447000000	0.408896000
1	25.145538000	15.485969000	0.708595000
8	23.870465000	15.192831000	2.352089000
1	25.889215000	17.741459000	1.509241000
1	23.697476000	17.424704000	3.603396000
1	25.045396000	19.393917000	4.115446000
1	23.591543000	19.968937000	3.226081000
8	26.224990000	16.563975000	3.183111000
7	24.122802000	17.488234000	-0.556176000
6	24.078554000	16.609614000	-1.641152000
8	23.717464000	15.413684000	-1.494932000
7	24.454903000	17.154291000	-2.830583000
6	24.875210000	18.463906000	-3.063861000
8	25.136224000	18.841495000	-4.236762000
6	24.989868000	19.273945000	-1.873153000
1	25.365752000	20.283002000	-1.903192000
6	24.606518000	18.767003000	-0.679060000
1	24.399055000	16.457943000	-3.665871000
1	24.709083000	19.335811000	0.229704000
15	27.794365000	16.355078000	2.663218000
8	28.643354000	16.256105000	3.890374000
8	28.069067000	17.320765000	1.538437000
8	20.196393000	10.928830000	-8.797130000
6	20.126049000	12.170607000	-5.548867000
6	18.603360000	12.309977000	-5.764606000
6	18.275639000	11.233982000	-6.819724000
6	19.380203000	10.172339000	-6.697834000
6	19.875248000	9.706494000	-8.052072000

8	20.516450000	10.843824000	-5.988404000
1	20.366209000	12.297378000	-4.493016000
1	18.372198000	13.305005000	-6.121483000
8	17.846472000	12.204626000	-4.536978000
1	18.325126000	11.680563000	-7.812427000
1	19.032587000	9.333709000	-6.090871000
1	19.082590000	9.147294000	-8.561935000
1	20.774401000	9.093706000	-7.963219000
8	16.973515000	10.625978000	-6.604157000
7	21.516369000	16.810226000	-4.495506000
6	21.153075000	15.763225000	-3.670961000
7	20.981451000	16.022016000	-2.366662000
7	20.944636000	14.519341000	-4.138320000
6	21.092670000	14.411179000	-5.470716000
6	21.443636000	15.399567000	-6.378894000
6	21.717031000	16.707663000	-5.884928000
8	22.086947000	17.704778000	-6.556893000
7	21.403764000	14.886442000	-7.686484000
6	21.030343000	13.611681000	-7.573834000
7	20.842282000	13.265448000	-6.217124000
1	21.703220000	17.766925000	-4.065461000
1	21.155317000	16.960594000	-1.956697000
1	20.847089000	15.224535000	-1.755600000
1	20.899342000	12.917787000	-8.387102000
15	20.769786000	10.800254000	-10.344574000
8	19.839969000	9.985594000	-11.185008000
8	21.221924000	12.196557000	-10.672796000
8	23.262395000	24.178930000	-0.571220000
6	20.994606000	21.034297000	-0.197903000
6	22.003068000	20.620889000	0.873163000
6	22.884504000	21.870520000	0.903018000
6	21.823724000	22.973868000	0.957924000
6	22.311080000	24.344677000	0.530693000
8	20.787596000	22.470974000	-0.008246000
1	20.051379000	20.508387000	-0.125123000
1	22.502036000	19.688500000	0.648815000
8	21.352756000	20.578287000	2.189083000
1	23.434867000	21.953704000	-0.030946000

1	21.382210000	23.008102000	1.955210000
1	22.821935000	24.803333000	1.382979000
1	21.461435000	24.960359000	0.228120000
8	23.817324000	21.960496000	2.005742000
7	21.553420000	20.814036000	-1.569087000
6	21.607200000	19.501196000	-2.084728000
8	21.356030000	18.533963000	-1.297363000
7	21.917966000	19.338257000	-3.397619000
6	22.305873000	20.389625000	-4.176091000
7	22.533296000	20.188736000	-5.468938000
6	22.439907000	21.693660000	-3.590864000
6	22.009772000	21.865359000	-2.317485000
1	22.384169000	19.251946000	-5.898901000
1	22.690152000	20.994449000	-6.085006000
1	22.872081000	22.530322000	-4.114050000
1	22.005516000	22.823421000	-1.835157000
15	25.393198000	21.536984000	1.679757000
8	26.256656000	22.309479000	2.626982000
8	25.611242000	21.529422000	0.189276000
8	15.728978000	12.837024000	-6.391030000
6	15.408282000	16.425980000	-5.183338000
6	14.023496000	16.413061000	-5.845640000
6	13.909588000	14.929296000	-6.188683000
6	14.429541000	14.257779000	-4.922716000
6	14.952758000	12.858367000	-5.140208000
8	15.565171000	15.144374000	-4.518909000
1	15.531312000	17.239389000	-4.471150000
1	13.965861000	17.081145000	-6.697155000
8	12.992576000	16.736614000	-4.858624000
1	14.589871000	14.720965000	-7.011033000
1	13.665169000	14.279144000	-4.142459000
1	14.116358000	12.164518000	-5.243638000
1	15.611659000	12.569955000	-4.322017000
8	12.597040000	14.436291000	-6.540187000
7	16.464519000	16.575455000	-6.215565000
6	16.768600000	17.881905000	-6.629931000
8	15.975126000	18.814530000	-6.272035000
7	17.891373000	18.076777000	-7.361471000

6	18.654511000	17.030770000	-7.779587000
7	19.824118000	17.274373000	-8.364848000
6	18.207246000	15.684504000	-7.541370000
6	17.144838000	15.498346000	-6.719954000
1	20.230367000	18.229727000	-8.314913000
1	20.472451000	16.486515000	-8.501374000
1	18.761103000	14.850384000	-7.938656000
1	16.767574000	14.520276000	-6.445516000
15	15.711821000	11.456934000	-7.313442000
8	14.472014000	10.674212000	-7.005485000
8	16.131762000	11.878620000	-8.688473000
8	23.107380000	26.759419000	-5.072273000
6	19.758556000	24.991193000	-5.345186000
6	20.015348000	24.421051000	-3.937911000
6	21.266716000	25.198614000	-3.563179000
6	20.922221000	26.610318000	-4.053190000
6	22.132080000	27.496947000	-4.247456000
8	20.284227000	26.343879000	-5.372495000
1	18.694968000	24.973884000	-5.577907000
1	20.151562000	23.339105000	-3.945475000
8	18.862947000	24.817697000	-3.131962000
1	22.104198000	24.843855000	-4.160562000
1	20.202604000	27.064804000	-3.366122000
1	22.599165000	27.652255000	-3.272065000
1	21.847675000	28.442384000	-4.716150000
8	21.619218000	25.129679000	-2.161716000
7	18.817261000	20.640422000	-7.392874000
6	17.950041000	21.641198000	-7.008844000
7	16.647784000	21.344547000	-6.924798000
7	18.376743000	22.880363000	-6.705448000
6	19.713673000	23.010795000	-6.775249000
6	20.655592000	22.082986000	-7.198844000
6	20.201636000	20.793320000	-7.591061000
8	20.891343000	19.846329000	-8.060425000
7	21.949987000	22.609131000	-7.041417000
6	21.790929000	23.815973000	-6.504220000
7	20.421636000	24.117206000	-6.330771000
1	18.429154000	19.653317000	-7.517532000

1	16.316218000	20.363585000	-6.852026000
1	15.992051000	22.099299000	-6.765774000
1	22.578370000	24.526578000	-6.314249000
15	23.277209000	25.153850000	-1.891581000
8	23.674394000	26.561025000	-1.537328000
8	23.942283000	24.369046000	-2.986502000
8	11.454678000	15.892839000	-8.272609000
6	12.343909000	19.537717000	-7.998792000
6	11.129103000	19.744218000	-8.910608000
6	10.388166000	18.393538000	-8.843455000
6	10.634887000	17.961473000	-7.382261000
6	10.691294000	16.463411000	-7.154411000
8	11.981493000	18.497220000	-7.052032000
1	12.589824000	20.471996000	-7.497360000
1	11.416419000	20.040819000	-9.923928000
8	10.280977000	20.718019000	-8.239671000
1	9.357057000	20.360696000	-8.418689000
1	10.795165000	17.650103000	-9.528136000
1	9.889913000	18.438423000	-6.739854000
1	9.677098000	16.048674000	-7.133029000
1	11.205783000	16.268821000	-6.212240000
8	8.990030000	18.714722000	-9.111252000
7	13.556961000	19.099482000	-8.717444000
6	14.508972000	20.090845000	-9.005768000
8	14.289358000	21.299105000	-8.771323000
7	15.668074000	19.621109000	-9.563590000
6	16.015075000	18.295315000	-9.824623000
8	17.144237000	18.025330000	-10.312712000
6	14.982724000	17.338356000	-9.492017000
1	15.117287000	16.278012000	-9.631164000
6	13.811211000	17.767259000	-8.966424000
1	16.377255000	20.387745000	-9.816083000
1	13.024983000	17.068117000	-8.716706000
15	12.247705000	14.435899000	-8.165979000
8	11.300513000	13.307267000	-8.424001000
8	13.524111000	14.632883000	-8.942187000
8	23.749680000	25.571311000	-9.774111000
6	19.876348000	26.130763000	-9.878260000

6	20.037153000	26.598776000	-8.423239000
6	21.553418000	26.675510000	-8.316597000
6	21.951372000	27.285881000	-9.666106000
6	23.381909000	26.944673000	-10.088020000
8	20.988103000	26.695650000	-10.632112000
1	18.913854000	26.432905000	-10.293372000
1	19.582751000	25.898926000	-7.728240000
8	19.498272000	27.945912000	-8.324435000
1	20.023819000	28.350153000	-7.575604000
1	21.968255000	25.678997000	-8.225712000
1	21.796081000	28.366888000	-9.617113000
1	24.051572000	27.659176000	-9.588299000
1	23.467764000	27.083389000	-11.169104000
8	21.993721000	27.545408000	-7.237740000
7	17.368285000	21.613835000	-10.157985000
6	16.898372000	22.864190000	-9.928495000
7	17.628541000	23.989139000	-9.852358000
6	18.950652000	23.753246000	-10.018532000
6	19.551779000	22.505673000	-10.255784000
6	18.702794000	21.379377000	-10.313388000
7	19.126437000	20.118394000	-10.481684000
7	20.940262000	22.643508000	-10.360573000
6	21.177204000	23.942022000	-10.196098000
7	19.989704000	24.662997000	-9.978526000
1	15.834182000	22.914056000	-9.740667000
1	20.113793000	19.922242000	-10.346271000
1	18.448940000	19.335349000	-10.435050000
1	22.143566000	24.435744000	-10.182977000
15	23.485067000	27.225704000	-6.585659000
8	24.282966000	28.488740000	-6.615089000
8	24.006381000	25.946817000	-7.233082000
1	30.463460000	7.087376000	-4.049480000
1	31.161651000	21.251707000	-13.228769000
1	8.419004000	17.931656000	-8.897923000
1	23.942189000	25.590505000	-8.751562000
1	13.757236000	18.701011000	-5.115980000
6	13.059188000	18.166641000	-4.462632000
1	12.062708000	18.588925000	-4.595978000

6	13.519247000	18.238017000	-3.034782000
16	13.772736000	16.764499000	-2.137800000
6	14.220536000	17.659902000	-0.715574000
1	14.499955000	17.149102000	0.193366000
6	14.173608000	19.013689000	-0.932013000
1	14.424421000	19.755862000	-0.188280000
1	13.694405000	20.357468000	-2.640600000
6	13.771550000	19.345267000	-2.269180000
6	18.032235000	10.986260000	-3.735391000
6	18.135729000	11.485868000	-2.321297000
16	18.350392000	13.205653000	-2.090706000
6	18.547716000	12.987717000	-0.382211000
1	18.736818000	13.823354000	0.274360000
6	18.445509000	11.669196000	-0.015216000
1	18.549801000	11.325502000	1.004145000
1	18.111019000	9.727304000	-1.060154000
6	18.200714000	10.802576000	-1.134795000
1	18.959499000	10.472475000	-4.021350000
1	17.189653000	10.310507000	-3.900549000
6	22.766522000	8.713554000	-6.052765000
6	24.055747000	8.318828000	-5.383532000
16	25.490238000	8.110875000	-6.348700000
6	26.435483000	7.682082000	-4.959288000
1	27.506511000	7.569714000	-5.062562000
6	25.670148000	7.663083000	-3.820794000
1	26.060712000	7.432590000	-2.838640000
1	23.546554000	8.095762000	-3.293427000
6	24.299926000	8.027520000	-4.065175000
1	22.071778000	7.866568000	-6.075434000
1	22.277131000	9.543821000	-5.539199000
6	28.106540000	11.249947000	-9.565578000
6	28.693264000	9.896558000	-9.389315000
16	30.286951000	9.491086000	-9.977476000
6	30.236056000	7.939869000	-9.191395000
1	31.050174000	7.239305000	-9.297122000
6	29.045655000	7.745918000	-8.531042000
1	28.780489000	6.819087000	-8.037666000
1	27.180524000	8.956177000	-8.204679000

6	28.163013000	8.876226000	-8.643533000
1	27.089626000	11.241750000	-9.170566000
1	28.678264000	11.997315000	-9.011431000
6	18.683672000	23.962153000	-1.948336000
1	19.633675000	23.789378000	-1.435656000
1	18.027644000	24.537766000	-1.285529000
6	17.630640000	22.229151000	-3.562535000
6	18.040956000	22.643527000	-2.321418000
16	17.736032000	21.412914000	-1.111980000
6	17.058355000	20.343213000	-2.308523000
6	17.074188000	20.899840000	-3.557456000
1	17.732888000	22.828384000	-4.455001000
1	16.662228000	19.384598000	-2.019509000
1	16.708677000	20.384425000	-4.436300000
6	20.697685000	19.285404000	2.509213000
1	21.349292000	18.475246000	2.184036000
1	20.647223000	19.284104000	3.602061000
6	18.996266000	18.389652000	0.788607000
6	19.330868000	19.096300000	1.920406000
16	17.912686000	19.804962000	2.656467000
6	16.876270000	19.114704000	1.449175000
6	17.587117000	18.392330000	0.523189000
1	19.743798000	17.964092000	0.135310000
1	15.809919000	19.267164000	1.488274000
1	17.122935000	17.879731000	-0.306796000
6	23.115443000	14.106505000	1.662590000
1	23.220360000	14.227211000	0.580184000
1	23.554977000	13.145654000	1.942714000
6	20.928980000	13.122035000	2.619933000
6	21.679912000	14.144846000	2.095956000
16	20.727465000	15.603921000	1.948315000
6	19.317445000	14.812895000	2.582350000
6	19.571832000	13.502491000	2.896678000
1	21.328722000	12.133949000	2.804730000
1	18.393248000	15.358111000	2.699544000
1	18.832045000	12.832550000	3.311817000
6	25.453447000	10.900235000	-2.309973000
1	25.643549000	9.893373000	-2.685537000

1	25.792521000	11.616577000	-3.065090000
6	23.522627000	11.484949000	-0.728880000
6	24.003407000	11.124338000	-1.963911000
16	22.702175000	10.965195000	-3.117408000
6	21.520410000	11.367838000	-1.912237000
6	22.098313000	11.636937000	-0.699783000
1	24.176662000	11.669404000	0.105025000
1	20.470898000	11.392166000	-2.147709000
1	21.530763000	11.937696000	0.169086000

Figure S17. X-Y coordinates for **3:4** at level: B3LYP-GD3/3-21G*.

8	6.904432000	-8.452132000	-5.706569000
6	9.730015000	-6.250765000	-4.448114000
6	9.499290000	-6.813064000	-3.040277000
6	8.516833000	-7.956309000	-3.337005000
6	9.065575000	-8.493144000	-4.663576000
6	8.076033000	-9.243808000	-5.529842000
8	9.560250000	-7.322703000	-5.353185000
1	10.730203000	-5.826367000	-4.546158000
1	9.118984000	-6.059843000	-2.348328000
8	10.730890000	-7.349146000	-2.564046000
1	10.498318000	-8.191009000	-2.130711000
1	7.499555000	-7.580170000	-3.472735000
1	9.910539000	-9.161360000	-4.451334000
1	7.844617000	-10.191698000	-5.021813000
1	8.550100000	-9.478419000	-6.493119000
8	8.553843000	-8.972001000	-2.345102000
7	8.765596000	-5.163904000	-4.770483000
6	9.031950000	-3.887726000	-4.239519000
8	10.016566000	-3.758400000	-3.483404000
7	8.214271000	-2.860385000	-4.570622000
6	7.121698000	-3.067899000	-5.323933000
7	6.352826000	-2.010392000	-5.615682000
6	6.807358000	-4.367322000	-5.836073000
6	7.661551000	-5.381464000	-5.544026000
1	6.545770000	-1.094835000	-5.192000000
1	5.439162000	-2.157084000	-6.019198000
1	5.928240000	-4.537322000	-6.444971000
1	7.511962000	-6.396727000	-5.890949000
8	8.197481000	6.557957000	-0.261111000
6	8.712527000	3.002793000	0.616626000
6	10.214195000	3.262942000	0.817430000
6	10.268026000	4.798174000	0.849075000
6	8.933057000	5.154386000	1.533255000
6	8.361993000	6.506517000	1.157744000
8	8.015122000	4.110448000	1.144569000
1	8.408676000	2.089394000	1.134511000
1	10.815095000	2.816228000	0.020575000

8	10.645801000	2.816906000	2.101379000
1	10.874443000	1.871906000	2.053125000
1	10.261506000	5.188255000	-0.172110000
1	9.066694000	5.120320000	2.623463000
1	9.060075000	7.284800000	1.491432000
1	7.395513000	6.659664000	1.649549000
8	11.403718000	5.319795000	1.503658000
7	8.416548000	-0.409234000	-3.053003000
6	9.175599000	-0.426508000	-1.906120000
7	9.865750000	-1.557347000	-1.655470000
7	9.238686000	0.596302000	-1.059014000
6	8.513269000	1.653939000	-1.477965000
6	7.780429000	1.809676000	-2.657452000
6	7.667291000	0.683065000	-3.524721000
8	7.004774000	0.579650000	-4.572933000
7	7.204322000	3.072826000	-2.713260000
6	7.564450000	3.650906000	-1.591869000
7	8.358933000	2.835505000	-0.794929000
1	8.375098000	-1.274373000	-3.628614000
1	9.950858000	-2.313251000	-2.344971000
1	10.498064000	-1.539192000	-0.868090000
1	7.347999000	4.664331000	-1.293397000
8	7.631387000	-7.543675000	-0.435973000
6	8.312355000	-3.924408000	0.281619000
6	7.759370000	-4.088920000	1.709938000
6	7.601355000	-5.610713000	1.751537000
6	8.855504000	-6.082272000	1.016838000
6	8.779272000	-7.463935000	0.409005000
8	9.033227000	-5.099826000	-0.029012000
1	8.971193000	-3.057439000	0.208036000
1	6.817345000	-3.562381000	1.856168000
8	8.730617000	-3.649214000	2.657457000
1	6.731247000	-5.866794000	1.137833000
1	9.715776000	-6.045549000	1.698987000
1	8.716993000	-8.205004000	1.214045000
1	9.693147000	-7.649604000	-0.167595000
8	7.489357000	-6.202956000	3.028120000
7	5.241365000	-0.379571000	-1.406360000

6	6.062428000	-0.400236000	-0.304860000
7	6.121120000	0.715197000	0.449362000
7	6.802831000	-1.450877000	0.021968000
6	6.616016000	-2.493553000	-0.809714000
6	5.758322000	-2.613363000	-1.903814000
6	5.006474000	-1.457320000	-2.280857000
8	4.220203000	-1.320908000	-3.236074000
7	5.827580000	-3.897310000	-2.429443000
6	6.716671000	-4.519343000	-1.686121000
7	7.241506000	-3.706284000	-0.691781000
1	4.724808000	0.500774000	-1.610766000
1	5.425672000	1.468921000	0.361239000
1	6.623815000	0.636104000	1.321832000
1	7.015385000	-5.553386000	-1.768868000
15	7.318606000	-8.979162000	-1.202182000
8	7.634034000	-10.135593000	-0.302107000
8	6.005299000	-8.787569000	-1.899577000
8	3.414657000	7.804525000	-3.095923000
6	3.662943000	5.385311000	-0.301598000
6	5.044549000	5.889712000	0.150272000
6	5.191960000	7.116031000	-0.770766000
6	3.772908000	7.692341000	-0.730657000
6	3.317451000	8.557919000	-1.889684000
8	2.932021000	6.523353000	-0.678496000
1	3.125937000	4.864922000	0.483050000
1	5.819019000	5.132437000	0.026809000
8	5.024321000	6.354165000	1.493750000
1	5.416055000	6.770560000	-1.786512000
1	3.655200000	8.263447000	0.199773000
1	3.947980000	9.455107000	-1.939248000
1	2.278571000	8.855464000	-1.711815000
8	6.136404000	8.080745000	-0.355404000
7	3.756275000	4.415098000	-1.427468000
6	4.085837000	3.100569000	-1.064767000
8	4.444409000	2.897194000	0.113741000
7	3.991966000	2.122789000	-1.991396000
6	3.615351000	2.400413000	-3.249181000
7	3.515213000	1.373149000	-4.102277000

6	3.334104000	3.743618000	-3.659289000
6	3.415664000	4.716265000	-2.712152000
1	3.695274000	0.412782000	-3.789459000
1	3.172678000	1.520957000	-5.039654000
1	3.059532000	3.995371000	-4.675852000
1	3.227423000	5.758921000	-2.928995000
15	7.686840000	7.974099000	-0.960305000
8	8.419576000	9.140812000	-0.364537000
8	7.637928000	7.685860000	-2.433469000
8	5.396221000	-4.995972000	3.880537000
6	4.714147000	-1.365782000	3.186457000
6	3.905693000	-1.186187000	4.485077000
6	4.129882000	-2.565282000	5.122683000
6	5.608938000	-2.793814000	4.815170000
6	6.110453000	-4.219050000	4.841436000
8	5.765147000	-2.253934000	3.484948000
1	5.123924000	-0.417066000	2.835568000
1	2.857970000	-0.949580000	4.297231000
8	4.517601000	-0.191171000	5.294709000
1	3.530398000	-3.298194000	4.571888000
1	6.209606000	-2.203116000	5.519640000
1	5.966793000	-4.621435000	5.852330000
1	7.180913000	-4.229037000	4.606717000
8	3.880132000	-2.666093000	6.507871000
7	1.659702000	0.142776000	-0.535745000
6	2.109136000	0.763047000	0.566883000
7	2.861541000	0.245034000	1.536050000
6	3.125949000	-1.051153000	1.306897000
6	2.695721000	-1.835689000	0.232283000
6	1.944089000	-1.160541000	-0.757969000
7	1.494183000	-1.734542000	-1.895759000
7	3.188635000	-3.128799000	0.348201000
6	3.905776000	-3.113406000	1.454001000
7	3.906764000	-1.878209000	2.078402000
1	1.833538000	1.808395000	0.654126000
1	2.005925000	-2.541391000	-2.226959000
1	1.148290000	-1.100067000	-2.619162000
1	4.441267000	-3.950658000	1.881066000

15	5.949605000	-6.535254000	3.589436000
8	6.158073000	-7.266281000	4.883473000
8	5.096039000	-7.054334000	2.468057000
8	-1.602235000	6.070142000	-5.807081000
6	-0.852002000	5.329847000	-2.207306000
6	0.328700000	6.308992000	-2.140129000
6	0.242819000	6.926427000	-3.546303000
6	-1.271235000	7.123695000	-3.672005000
6	-1.873031000	7.251488000	-5.055850000
8	-1.812181000	5.947345000	-3.025223000
1	-1.287649000	5.114942000	-1.232506000
1	1.266711000	5.809334000	-1.926109000
8	0.069102000	7.339883000	-1.202488000
1	0.584705000	6.189444000	-4.280164000
1	-1.555150000	8.010484000	-3.091627000
1	-1.441633000	8.133729000	-5.546267000
1	-2.955540000	7.391543000	-4.959974000
8	0.929783000	8.148184000	-3.724278000
7	-0.451062000	4.008418000	-2.766090000
6	0.198458000	3.149231000	-1.881513000
8	0.521498000	3.508009000	-0.746126000
7	0.446218000	1.891097000	-2.366488000
6	0.146790000	1.404360000	-3.635810000
8	0.431314000	0.238047000	-3.940848000
6	-0.487972000	2.370436000	-4.505337000
1	-0.747013000	2.086403000	-5.516503000
6	-0.766321000	3.614155000	-4.043456000
1	0.901737000	1.225896000	-1.697048000
1	-1.239591000	4.368863000	-4.658973000
15	2.453034000	8.151357000	-4.405227000
8	2.680440000	9.566806000	-4.847726000
8	2.610688000	6.956920000	-5.305114000
8	1.533670000	-1.665923000	6.672730000
6	0.135746000	1.306521000	4.929558000
6	-1.070641000	1.239605000	5.891053000
6	-0.519702000	0.349410000	7.025969000
6	0.985040000	0.638412000	7.028537000
6	1.868189000	-0.517028000	7.450501000

8	1.300832000	1.000754000	5.666186000
1	0.221107000	2.300302000	4.489369000
1	-1.927675000	0.783505000	5.398984000
8	-1.551709000	2.512530000	6.282593000
1	-0.667789000	-0.697151000	6.741770000
1	1.197397000	1.490017000	7.688158000
1	1.706483000	-0.717636000	8.516503000
1	2.919532000	-0.252283000	7.289054000
8	-1.087464000	0.603752000	8.295581000
7	-1.744914000	0.886399000	0.286390000
6	-1.710051000	1.971847000	1.131298000
7	-2.347964000	3.086022000	0.723692000
7	-1.127558000	1.940998000	2.327414000
6	-0.622190000	0.726545000	2.628862000
6	-0.634970000	-0.440531000	1.870228000
6	-1.220164000	-0.387088000	0.568617000
8	-1.301714000	-1.303072000	-0.260694000
7	-0.055757000	-1.487262000	2.572447000
6	0.296784000	-0.965649000	3.728276000
7	-0.004870000	0.385256000	3.808560000
1	-2.185292000	0.992100000	-0.650255000
1	-2.719130000	3.175599000	-0.230028000
1	-2.196391000	3.926606000	1.262670000
1	0.750972000	-1.489248000	4.557822000
15	2.337315000	-3.082808000	6.993248000
8	2.433423000	-3.294179000	8.475555000
8	1.756722000	-4.087821000	6.041016000
8	-5.385524000	2.405954000	-7.463371000
6	-5.241391000	3.655543000	-3.884502000
6	-4.360748000	4.823983000	-4.341724000
6	-4.419330000	4.625379000	-5.858880000
6	-5.900250000	4.283969000	-6.054859000
6	-6.260849000	3.522631000	-7.312847000
8	-6.222378000	3.484089000	-4.887316000
1	-5.719970000	3.851143000	-2.929793000
1	-3.358931000	4.773575000	-3.927728000
8	-4.969998000	6.073436000	-4.034180000
1	-3.816964000	3.749523000	-6.119035000

1	-6.490818000	5.208221000	-6.022432000
1	-6.158309000	4.196768000	-8.172531000
1	-7.306848000	3.202098000	-7.252424000
8	-4.022845000	5.736662000	-6.637981000
7	-4.452327000	2.400697000	-3.712487000
6	-3.635844000	2.306539000	-2.570112000
8	-3.535267000	3.312793000	-1.836088000
7	-3.003726000	1.138164000	-2.312256000
6	-3.106017000	0.095004000	-3.158334000
7	-2.485539000	-1.043868000	-2.840849000
6	-3.855382000	0.207311000	-4.375498000
6	-4.530205000	1.365896000	-4.595246000
1	-2.042213000	-1.149747000	-1.920397000
1	-2.680969000	-1.884569000	-3.376408000
1	-3.898645000	-0.607436000	-5.085548000
1	-5.153179000	1.534019000	-5.461783000
15	-2.454027000	5.783992000	-7.207418000
8	-2.400826000	6.992092000	-8.095676000
8	-2.021387000	4.410200000	-7.634501000
8	-3.455950000	0.033667000	7.520469000
6	-5.945816000	0.130180000	4.638013000
6	-6.992058000	-0.437999000	5.621566000
6	-6.227815000	-0.308427000	6.943720000
6	-5.505081000	1.027751000	6.765092000
6	-4.269627000	1.204758000	7.623063000
8	-5.158169000	1.055377000	5.359692000
1	-6.417365000	0.623477000	3.786629000
1	-7.267431000	-1.459884000	5.365020000
8	-8.150299000	0.376258000	5.691685000
1	-5.484610000	-1.108874000	6.994669000
1	-6.201072000	1.850886000	6.972401000
1	-4.584603000	1.350548000	8.661346000
1	-3.699620000	2.079736000	7.292510000
8	-7.006891000	-0.295533000	8.122604000
7	-5.068729000	-0.925795000	4.065655000
6	-5.514739000	-1.602209000	2.917764000
8	-6.707443000	-1.455799000	2.569973000
7	-4.629570000	-2.359004000	2.224766000

6	-3.375887000	-2.536016000	2.674674000
7	-2.497407000	-3.188825000	1.896987000
6	-2.983452000	-2.042983000	3.962076000
6	-3.842866000	-1.207973000	4.599020000
1	-2.724374000	-3.310679000	0.905013000
1	-1.511338000	-3.044401000	2.106054000
1	-2.010464000	-2.263685000	4.377101000
1	-3.605709000	-0.730466000	5.541404000
15	-2.387114000	-0.357015000	8.728822000
8	-2.865041000	0.182545000	10.044631000
8	-2.034011000	-1.797553000	8.495934000
8	-5.655652000	-3.044460000	-8.112552000
6	-7.492620000	-2.421836000	-4.903524000
6	-7.314015000	-0.896759000	-5.052388000
6	-6.786608000	-0.800832000	-6.492036000
6	-7.579390000	-1.916304000	-7.191167000
6	-6.944986000	-2.511477000	-8.432459000
8	-7.709223000	-2.951552000	-6.193608000
1	-8.336253000	-2.647398000	-4.248051000
1	-6.611289000	-0.503488000	-4.313748000
8	-8.598686000	-0.308563000	-4.893328000
1	-5.725537000	-1.063276000	-6.507825000
1	-8.573384000	-1.525911000	-7.450504000
1	-6.836790000	-1.727814000	-9.189852000
1	-7.600226000	-3.289998000	-8.835360000
8	-6.984406000	0.475860000	-7.063601000
7	-5.378560000	-3.175084000	-0.441575000
6	-6.704300000	-3.013756000	-0.763787000
7	-7.573720000	-2.876702000	0.264384000
7	-7.152849000	-3.018456000	-2.013510000
6	-6.165627000	-3.149889000	-2.921154000
6	-4.809301000	-3.379449000	-2.706732000
6	-4.335679000	-3.406096000	-1.356365000
8	-3.176150000	-3.585770000	-0.954732000
7	-4.126360000	-3.417174000	-3.915690000
6	-5.043755000	-3.195768000	-4.831779000
7	-6.313038000	-3.036944000	-4.287448000
1	-5.099995000	-3.031845000	0.549394000

1	-7.244005000	-2.486927000	1.157234000
1	-8.512252000	-2.615091000	-0.006167000
1	-4.884880000	-3.169443000	-5.900732000
15	-5.916553000	1.040051000	-8.232594000
8	-6.745197000	1.421003000	-9.426676000
8	-4.728272000	0.126812000	-8.301559000
8	-8.257910000	-2.513220000	7.947128000
6	-9.648240000	-3.696385000	4.633682000
6	-10.504662000	-4.714437000	5.403586000
6	-10.337731000	-4.242716000	6.854773000
6	-10.276995000	-2.715008000	6.675578000
6	-9.550259000	-1.937432000	7.752119000
8	-9.593430000	-2.524876000	5.418384000
1	-10.093131000	-3.488796000	3.660317000
1	-10.163116000	-5.743967000	5.240149000
8	-11.849358000	-4.539167000	4.982732000
1	-12.401885000	-4.743386000	5.758848000
1	-9.392983000	-4.610257000	7.271810000
1	-11.302803000	-2.333541000	6.588904000
1	-10.130583000	-1.974901000	8.683565000
1	-9.453660000	-0.892744000	7.436506000
8	-11.449776000	-4.699601000	7.606406000
7	-8.272386000	-4.171701000	4.367812000
6	-8.060368000	-4.820222000	3.148543000
8	-8.978490000	-5.058225000	2.366864000
7	-6.756183000	-5.175644000	2.903026000
6	-5.660897000	-4.999458000	3.744319000
8	-4.537808000	-5.389159000	3.398994000
6	-5.973420000	-4.357125000	5.001953000
1	-5.181023000	-4.179387000	5.716515000
6	-7.247137000	-3.976229000	5.263409000
1	-6.592356000	-5.648412000	1.987141000
1	-7.522334000	-3.484237000	6.189524000
15	-7.195741000	-1.723436000	8.957417000
8	-7.889576000	-1.347647000	10.233343000
8	-5.930626000	-2.531562000	8.901384000
8	-3.372348000	-7.250219000	-6.775615000
6	-6.716673000	-7.399401000	-4.683873000

6	-7.149470000	-6.170103000	-5.501336000
6	-6.052826000	-6.136041000	-6.566081000
6	-5.814778000	-7.624349000	-6.839914000
6	-4.432423000	-7.957970000	-7.398997000
8	-6.016928000	-8.263507000	-5.560369000
1	-7.584887000	-7.902491000	-4.248681000
1	-7.176590000	-5.268163000	-4.884649000
8	-8.417642000	-6.442312000	-6.077642000
1	-8.505647000	-5.808522000	-6.811710000
1	-5.155733000	-5.689649000	-6.132918000
1	-6.584033000	-7.982005000	-7.537398000
1	-4.453727000	-7.759835000	-8.480613000
1	-4.247517000	-9.028818000	-7.260858000
8	-6.446453000	-5.451959000	-7.742696000
7	-6.321807000	-6.377276000	0.353545000
6	-7.395464000	-6.591264000	-0.427393000
7	-7.426617000	-6.826330000	-1.739936000
6	-6.186904000	-6.838679000	-2.263057000
6	-4.983523000	-6.630763000	-1.577830000
6	-5.082653000	-6.372605000	-0.192649000
7	-4.011986000	-6.145368000	0.597021000
7	-3.902401000	-6.715265000	-2.438023000
6	-4.439248000	-6.966627000	-3.611637000
7	-5.821648000	-7.053763000	-3.573448000
1	-8.350511000	-6.540870000	0.090063000
1	-3.176014000	-5.807142000	0.137743000
1	-4.171251000	-5.826427000	1.557054000
1	-3.901330000	-7.109589000	-4.541238000
15	-5.303639000	-4.579834000	-8.592092000
8	-5.624412000	-4.767162000	-10.043781000
8	-3.936424000	-4.863492000	-8.009935000
1	11.583462000	4.705059000	2.238785000
1	6.317138000	-8.913720000	-6.324541000
1	-11.366071000	-4.383935000	8.519870000
1	-3.412699000	-6.338851000	-7.157446000
1	-8.689424000	-0.474691000	3.857272000
6	-8.986424000	0.336742000	4.529531000
1	-10.001709000	0.119369000	4.880377000

6	-8.951242000	1.648744000	3.795812000
16	-8.482698000	3.115613000	4.625608000
6	-8.827543000	4.077244000	3.216743000
1	-8.660916000	5.146409000	3.233731000
6	-9.272266000	3.305295000	2.178417000
1	-9.530766000	3.702403000	1.203027000
1	-9.646545000	1.143587000	1.811493000
6	-9.335329000	1.914300000	2.508580000
6	-0.635697000	3.472274000	6.810326000
6	-1.092315000	4.832874000	6.367316000
16	-2.144149000	4.990849000	4.979886000
6	-2.072297000	6.724168000	5.064886000
1	-2.618342000	7.320007000	4.345847000
6	-1.285417000	7.145690000	6.101957000
1	-1.110358000	8.190982000	6.333927000
1	-0.074822000	6.188614000	7.707916000
6	-0.728188000	6.060684000	6.850754000
1	0.381273000	3.292241000	6.437410000
1	-0.601817000	3.402996000	7.905074000
6	4.318562000	1.150701000	4.813703000
6	5.618699000	1.889610000	4.700422000
16	7.057809000	1.147655000	4.020765000
6	7.941766000	2.645188000	4.114442000
1	8.960416000	2.693329000	3.750679000
6	7.176482000	3.640748000	4.651365000
1	7.536173000	4.653083000	4.801847000
1	5.097568000	3.852497000	5.424269000
6	5.854678000	3.206569000	4.991496000
1	3.655130000	1.682188000	5.502505000
1	3.810225000	1.126501000	3.841700000
6	8.678515000	-2.228883000	2.889358000
6	10.033900000	-1.591554000	2.872194000
16	11.251092000	-2.019773000	1.690984000
6	12.288853000	-0.722864000	2.207381000
1	13.261059000	-0.591278000	1.751078000
6	11.733489000	-0.021198000	3.243709000
1	12.234053000	0.801655000	3.743846000
1	9.841917000	-0.097535000	4.418449000

6	10.445334000	-0.521448000	3.622703000
1	8.214183000	-2.034516000	3.861352000
1	8.046139000	-1.757484000	2.129167000
6	-8.583861000	1.040037000	-4.420828000
1	-7.867719000	1.643379000	-4.989309000
1	-9.586096000	1.428217000	-4.635392000
6	-8.105940000	0.099143000	-2.048829000
6	-8.281937000	1.123604000	-2.940639000
16	-8.063215000	2.672976000	-2.152529000
6	-7.708182000	1.905148000	-0.630990000
6	-7.766875000	0.544678000	-0.729401000
1	-8.190632000	-0.944704000	-2.321372000
1	-7.480565000	2.507586000	0.235378000
1	-7.563527000	-0.119245000	0.104845000
6	-4.805852000	6.527480000	-2.679040000
1	-3.859992000	6.169811000	-2.270341000
1	-4.748808000	7.619229000	-2.756175000
6	-5.804858000	5.390120000	-0.594323000
6	-5.909907000	6.134901000	-1.741111000
16	-7.555481000	6.690223000	-1.965661000
6	-8.071808000	5.919389000	-0.494427000
6	-7.034433000	5.277502000	0.126060000
1	-4.879056000	4.912843000	-0.297351000
1	-9.105693000	5.983607000	-0.180859000
1	-7.140962000	4.743050000	1.062864000
6	0.126762000	6.956195000	0.186478000
1	0.234427000	5.870906000	0.282359000
1	1.013420000	7.406115000	0.640338000
6	-1.197661000	8.543862000	1.724240000
6	-1.095530000	7.463590000	0.888405000
16	-2.672019000	6.748514000	0.622242000
6	-3.442701000	7.918038000	1.650482000
6	-2.535355000	8.805789000	2.160927000
1	-0.337940000	9.139418000	2.013860000
1	-4.512314000	7.876586000	1.809563000
1	-2.806730000	9.620442000	2.823691000
6	4.815010000	5.343037000	2.495551000
1	5.400615000	5.673261000	3.359108000

1	5.221157000	4.382466000	2.163625000
6	2.504921000	6.278384000	3.134641000
6	3.354188000	5.234307000	2.862230000
16	2.472651000	3.724184000	2.819791000
6	0.969327000	4.530360000	3.147639000
6	1.143843000	5.879749000	3.302560000
1	2.845499000	7.307897000	3.174532000
1	0.050407000	3.960588000	3.173778000
1	0.326853000	6.560339000	3.514258000

Figure S18. X-Y coordinates for **3:4** at level: B3LYP-GD3/6-31G*.

8	31.203463000	20.200535000	-13.363155000
6	32.498168000	16.662604000	-12.732798000
6	31.248413000	16.171334000	-13.458743000
6	30.681724000	17.483984000	-14.024858000
6	31.957466000	18.197028000	-14.493729000
6	31.846585000	19.706180000	-14.592461000
8	32.982328000	17.840012000	-13.455587000
1	33.275660000	15.900396000	-12.652931000
1	30.573684000	15.598096000	-12.824511000
8	31.666697000	15.371634000	-14.633477000
1	31.055320000	15.751762000	-15.346611000
1	30.128678000	18.081313000	-13.299999000
1	32.270998000	17.785018000	-15.461547000
1	31.233049000	19.933896000	-15.480128000
1	32.852244000	20.132946000	-14.729738000
8	29.832723000	17.183402000	-15.188159000
7	32.112622000	17.077554000	-11.342796000
6	32.019324000	16.061123000	-10.352319000
8	32.260812000	14.861509000	-10.702683000
7	31.674229000	16.430373000	-9.084003000
6	31.329794000	17.718330000	-8.790913000
7	30.977474000	18.002665000	-7.532284000
6	31.374970000	18.731479000	-9.806762000
6	31.786104000	18.380939000	-11.058147000
1	30.967797000	17.251969000	-6.793999000
1	30.516511000	18.885194000	-7.323979000
1	31.096517000	19.753774000	-9.580068000
1	31.827651000	19.089893000	-11.883795000
8	29.864952000	10.570857000	-1.156285000
6	29.211042000	10.413073000	-4.805376000
6	30.246443000	9.289768000	-4.909423000
6	30.468413000	8.895482000	-3.431154000
6	29.040885000	9.037109000	-2.844442000
6	28.993050000	9.392198000	-1.375012000
8	28.385416000	10.136703000	-3.632638000
1	28.583131000	10.479549000	-5.700885000
1	31.147026000	9.608682000	-5.445300000

8	29.657997000	8.068498000	-5.490818000
1	29.692970000	8.126608000	-6.494223000
1	31.133084000	9.601035000	-2.925297000
1	28.491392000	8.103828000	-3.016498000
1	29.372676000	8.543455000	-0.786500000
1	27.971973000	9.652276000	-1.075139000
8	30.991740000	7.547804000	-3.313302000
7	31.165945000	14.446408000	-7.251757000
6	31.035632000	13.144471000	-7.699585000
7	31.409062000	12.885473000	-8.973568000
7	30.580444000	12.132972000	-6.920701000
6	30.361024000	12.517994000	-5.641951000
6	30.566811000	13.788195000	-5.067431000
6	30.918868000	14.870015000	-5.922499000
8	31.012526000	16.099031000	-5.605377000
7	30.272856000	13.757621000	-3.683215000
6	29.875520000	12.506378000	-3.437034000
7	29.894553000	11.710864000	-4.610393000
1	31.401156000	15.220008000	-7.967877000
1	31.788671000	13.622723000	-9.615448000
1	31.358388000	11.914070000	-9.271253000
1	29.685125000	12.049238000	-2.477626000
8	28.176298000	15.692673000	-13.862851000
6	28.938918000	13.779422000	-10.990726000
6	27.670975000	12.925153000	-11.133474000
6	27.215785000	13.303852000	-12.552974000
6	28.534516000	13.395400000	-13.327721000
6	28.542472000	14.396571000	-14.465258000
8	29.523953000	13.894405000	-12.313586000
1	29.669803000	13.316535000	-10.324885000
1	26.933975000	13.164852000	-10.369290000
8	28.064323000	11.504342000	-11.066656000
1	26.769343000	14.303521000	-12.497327000
1	28.834610000	12.395336000	-13.667748000
1	27.820443000	14.103349000	-15.240434000
1	29.557950000	14.450525000	-14.875515000
8	26.303065000	12.370824000	-13.199057000
7	27.816443000	15.491299000	-6.474366000

6	27.816321000	14.214860000	-7.002766000
7	27.462621000	13.183278000	-6.221982000
7	28.150994000	13.974882000	-8.285894000
6	28.322798000	15.090456000	-9.014245000
6	28.227686000	16.432234000	-8.610400000
6	28.034494000	16.686456000	-7.211776000
8	28.050157000	17.807291000	-6.605013000
7	28.399281000	17.273728000	-9.739649000
6	28.612559000	16.449922000	-10.780433000
7	28.596208000	15.092909000	-10.373320000
1	27.639682000	15.604218000	-5.424154000
1	27.132591000	13.304649000	-5.234997000
1	27.443636000	12.273825000	-6.671241000
1	28.668322000	16.735618000	-11.818641000
15	28.176795000	17.069806000	-14.789056000
8	27.474001000	16.842837000	-16.098831000
8	27.870821000	18.168045000	-13.799199000
8	27.835052000	14.905126000	1.883501000
6	26.186333000	13.454246000	-1.102484000
6	27.134705000	12.249070000	-1.063030000
6	27.829340000	12.458859000	0.298329000
6	26.672801000	12.905734000	1.198049000
6	27.032686000	13.778954000	2.388135000
8	25.809822000	13.715084000	0.277091000
1	25.279278000	13.285750000	-1.677390000
1	27.799857000	12.216452000	-1.920663000
8	26.344515000	11.005074000	-0.984187000
1	28.554624000	13.274563000	0.200422000
1	26.113885000	12.021527000	1.527792000
1	27.614491000	13.170573000	3.097922000
1	26.116662000	14.154894000	2.861159000
8	28.467668000	11.283590000	0.868742000
7	26.876835000	14.638921000	-1.701971000
6	26.997635000	14.608521000	-3.112476000
8	26.676298000	13.523584000	-3.697466000
7	27.436471000	15.718506000	-3.754729000
6	27.795834000	16.837578000	-3.062417000
7	28.171949000	17.902774000	-3.784634000

6	27.773910000	16.837149000	-1.625566000
6	27.302688000	15.725149000	-0.984423000
1	28.113582000	17.877038000	-4.831436000
1	28.390246000	18.779517000	-3.318002000
1	28.103045000	17.674274000	-1.023761000
1	27.304730000	15.641660000	0.094931000
15	30.075696000	11.066510000	0.428800000
8	30.565556000	9.914465000	1.266444000
8	30.756979000	12.408284000	0.325149000
8	24.852550000	11.869229000	-11.142227000
6	24.440321000	11.103175000	-7.490177000
6	23.047699000	10.534158000	-7.790591000
6	23.079344000	10.598419000	-9.324110000
6	24.452478000	9.999758000	-9.643442000
6	25.006884000	10.410957000	-10.992034000
8	25.319773000	10.540031000	-8.528019000
1	24.815623000	10.830352000	-6.500413000
1	22.234483000	11.082355000	-7.315993000
8	22.985716000	9.091305000	-7.455425000
1	23.074117000	11.649143000	-9.626301000
1	24.416025000	8.908937000	-9.551824000
1	24.412340000	9.917240000	-11.772997000
1	26.069204000	10.163430000	-11.098075000
8	22.021836000	9.898599000	-10.034844000
7	24.273393000	15.373112000	-4.682052000
6	23.988396000	14.086259000	-4.359675000
7	23.999151000	13.031103000	-5.206078000
6	24.311970000	13.400878000	-6.469939000
6	24.590565000	14.702702000	-6.930689000
6	24.606145000	15.733442000	-5.965179000
7	24.938238000	17.004781000	-6.218446000
7	24.876689000	14.689195000	-8.308286000
6	24.788700000	13.401157000	-8.673487000
7	24.447333000	12.574413000	-7.576891000
1	23.727635000	13.914196000	-3.324160000
1	25.203201000	17.260423000	-7.165457000
1	24.993195000	17.712663000	-5.450967000
1	24.921756000	12.979329000	-9.663347000

15	24.707243000	12.498361000	-12.688317000
8	23.924285000	11.534844000	-13.543332000
8	24.360889000	13.949280000	-12.476140000
8	25.428397000	19.897640000	2.142579000
6	23.577544000	16.887668000	0.838743000
6	24.621046000	16.015970000	1.521075000
6	25.407930000	17.075579000	2.293123000
6	24.283750000	17.919928000	2.910866000
6	24.627231000	19.357510000	3.252507000
8	23.280098000	17.962534000	1.778219000
1	22.656975000	16.366524000	0.573397000
1	25.206716000	15.424705000	0.825094000
8	23.970169000	15.138767000	2.517510000
1	25.955942000	17.697060000	1.580320000
1	23.829612000	17.398388000	3.760587000
1	25.206324000	19.370471000	4.188816000
1	23.705044000	19.942434000	3.362270000
8	26.351138000	16.542574000	3.266763000
7	24.137080000	17.433566000	-0.421262000
6	24.060425000	16.559415000	-1.521951000
8	23.675381000	15.364597000	-1.380627000
7	24.430558000	17.117395000	-2.714608000
6	24.877395000	18.428324000	-2.934660000
8	25.149187000	18.822780000	-4.110369000
6	25.005254000	19.227183000	-1.737273000
1	25.386107000	20.239075000	-1.765967000
6	24.627493000	18.712741000	-0.535590000
1	24.356596000	16.423792000	-3.568384000
1	24.746095000	19.273164000	0.384818000
15	27.922006000	16.378634000	2.679054000
8	28.807962000	16.274597000	3.891236000
8	28.144378000	17.373225000	1.556965000
8	20.143276000	11.041989000	-8.758210000
6	20.050595000	12.262010000	-5.456184000
6	18.520701000	12.377343000	-5.650561000
6	18.237681000	11.355085000	-6.771796000
6	19.321967000	10.274635000	-6.647216000
6	19.821695000	9.816022000	-8.005161000

8	20.460073000	10.932359000	-5.903610000
1	20.315220000	12.393986000	-4.402424000
1	18.256530000	13.387502000	-5.952679000
8	17.761469000	12.187848000	-4.419268000
1	18.374133000	11.859635000	-7.733043000
1	18.962589000	9.426162000	-6.052626000
1	19.020562000	9.259440000	-8.515156000
1	20.722288000	9.197194000	-7.920878000
8	16.910990000	10.748384000	-6.713150000
7	21.440050000	16.921669000	-4.399246000
6	21.083712000	15.865944000	-3.575908000
7	20.918325000	16.112276000	-2.264269000
7	20.871383000	14.613567000	-4.050336000
6	21.004356000	14.519597000	-5.387827000
6	21.351041000	15.518130000	-6.301692000
6	21.635013000	16.825553000	-5.799315000
8	22.010991000	17.831672000	-6.470457000
7	21.299727000	15.007311000	-7.618986000
6	20.920190000	13.721301000	-7.505797000
7	20.742954000	13.370972000	-6.141722000
1	21.632194000	17.884934000	-3.954052000
1	21.091174000	17.056347000	-1.843633000
1	20.810207000	15.301061000	-1.661023000
1	20.787768000	13.018760000	-8.316556000
15	20.688799000	10.883111000	-10.328005000
8	19.732641000	10.057079000	-11.144661000
8	21.149507000	12.279350000	-10.682169000
8	23.310335000	24.211626000	-0.415034000
6	21.050522000	21.057758000	-0.001797000
6	22.083789000	20.642288000	1.045701000
6	22.957176000	21.899396000	1.076556000
6	21.892021000	23.003033000	1.149544000
6	22.368242000	24.377446000	0.705715000
8	20.822212000	22.494320000	0.207815000
1	20.116716000	20.509647000	0.082030000
1	22.589991000	19.711532000	0.807057000
8	21.445769000	20.575485000	2.377463000
1	23.499967000	21.990633000	0.133683000

1	21.469452000	23.044313000	2.159870000
1	22.893549000	24.841146000	1.553072000
1	21.509711000	24.992918000	0.413304000
8	23.904933000	21.988827000	2.177442000
7	21.579766000	20.859236000	-1.392074000
6	21.571932000	19.550050000	-1.941374000
8	21.280807000	18.581876000	-1.163209000
7	21.857790000	19.405651000	-3.268120000
6	22.260912000	20.471534000	-4.032572000
7	22.472282000	20.286377000	-5.337403000
6	22.430067000	21.762505000	-3.424644000
6	22.037431000	21.919344000	-2.128953000
1	22.306966000	19.348745000	-5.776576000
1	22.613189000	21.105161000	-5.950187000
1	22.863272000	22.604284000	-3.946413000
1	22.065035000	22.869595000	-1.623055000
15	25.481495000	21.538666000	1.803904000
8	26.365957000	22.249444000	2.793709000
8	25.692109000	21.592271000	0.305651000
8	15.718699000	12.992726000	-6.511647000
6	15.210123000	16.512269000	-5.288435000
6	13.843514000	16.453504000	-5.995006000
6	13.767073000	14.962006000	-6.318995000
6	14.300561000	14.303300000	-5.047272000
6	14.882002000	12.926793000	-5.294544000
8	15.393612000	15.237640000	-4.599066000
1	15.289299000	17.340361000	-4.581089000
1	13.810031000	17.104058000	-6.867270000
8	12.752903000	16.782476000	-5.063817000
1	14.452915000	14.756478000	-7.143366000
1	13.520842000	14.273849000	-4.276230000
1	14.063565000	12.219907000	-5.480046000
1	15.516061000	12.605526000	-4.463613000
8	12.459016000	14.422727000	-6.654052000
7	16.300506000	16.685479000	-6.294525000
6	16.632876000	18.004759000	-6.678366000
8	15.839265000	18.944024000	-6.317736000
7	17.785145000	18.200086000	-7.376334000

6	18.555829000	17.144120000	-7.783862000
7	19.743218000	17.382930000	-8.350473000
6	18.097175000	15.798642000	-7.565411000
6	16.999441000	15.609186000	-6.781496000
1	20.150646000	18.343718000	-8.294034000
1	20.394231000	16.583075000	-8.447655000
1	18.662010000	14.958209000	-7.944886000
1	16.611797000	14.622155000	-6.533913000
15	15.757963000	11.668210000	-7.532801000
8	14.457206000	10.914350000	-7.423053000
8	16.365996000	12.167490000	-8.818587000
8	23.104908000	26.682609000	-5.078974000
6	19.736181000	25.054940000	-5.180260000
6	20.003702000	24.475138000	-3.778814000
6	21.278690000	25.228637000	-3.414055000
6	20.975302000	26.652167000	-3.914291000
6	22.220167000	27.473872000	-4.186667000
8	20.238415000	26.420883000	-5.199271000
1	18.669771000	25.027617000	-5.418463000
1	20.117988000	23.387188000	-3.790653000
8	18.857426000	24.890060000	-2.954802000
1	22.110798000	24.843976000	-4.008093000
1	20.320499000	27.156419000	-3.190473000
1	22.749327000	27.603184000	-3.232714000
1	21.964989000	28.440421000	-4.639373000
8	21.627038000	25.168059000	-2.002876000
7	18.730778000	20.749432000	-7.384921000
6	17.878657000	21.752425000	-6.962039000
7	16.564232000	21.478728000	-6.884997000
7	18.322927000	22.983423000	-6.606190000
6	19.665295000	23.095075000	-6.668883000
6	20.599336000	22.166024000	-7.136924000
6	20.126837000	20.894629000	-7.580774000
8	20.811754000	19.949669000	-8.080092000
7	21.910683000	22.668684000	-6.960549000
6	21.766516000	23.865110000	-6.366136000
7	20.397420000	24.180215000	-6.179959000
1	18.329963000	19.754329000	-7.513919000

1	16.215709000	20.492524000	-6.837535000
1	15.957039000	22.234752000	-6.579400000
1	22.561923000	24.561064000	-6.147210000
15	23.299804000	25.221208000	-1.730388000
8	23.666616000	26.638569000	-1.344281000
8	23.998655000	24.460811000	-2.832753000
8	11.398104000	15.790755000	-8.542228000
6	12.098027000	19.489554000	-8.335701000
6	10.958795000	19.600095000	-9.359508000
6	10.271497000	18.217000000	-9.284305000
6	10.409666000	17.858069000	-7.785805000
6	10.530597000	16.370706000	-7.496337000
8	11.687963000	18.501856000	-7.344709000
1	12.292390000	20.462483000	-7.878741000
1	11.330466000	19.853473000	-10.362860000
8	10.005940000	20.570455000	-8.825284000
1	9.123031000	20.120806000	-9.051932000
1	10.761560000	17.457815000	-9.899614000
1	9.577919000	18.306936000	-7.226529000
1	9.535089000	15.900745000	-7.524382000
1	10.995675000	16.234073000	-6.514575000
8	8.878789000	18.460739000	-9.691403000
7	13.377847000	19.044982000	-8.942723000
6	14.331824000	20.054220000	-9.218782000
8	14.073497000	21.269580000	-9.033866000
7	15.527029000	19.583374000	-9.711564000
6	15.899003000	18.247315000	-9.930253000
8	17.049961000	17.972848000	-10.388724000
6	14.869945000	17.283854000	-9.600096000
1	15.031159000	16.218648000	-9.703069000
6	13.664172000	17.708830000	-9.129719000
1	16.256824000	20.360897000	-9.934042000
1	12.874084000	17.001657000	-8.884318000
15	12.146025000	14.304021000	-8.298427000
8	11.151378000	13.188090000	-8.470969000
8	13.441328000	14.402458000	-9.075522000
8	23.721198000	25.479248000	-9.760073000
6	19.827444000	26.064731000	-9.849990000

6	20.009992000	26.539181000	-8.398702000
6	21.531879000	26.620357000	-8.315103000
6	21.918630000	27.212111000	-9.678318000
6	23.343877000	26.845077000	-10.115415000
8	20.924597000	26.630650000	-10.636442000
1	18.852916000	26.352534000	-10.257960000
1	19.573447000	25.831217000	-7.691826000
8	19.464969000	27.891003000	-8.282571000
1	20.051004000	28.293929000	-7.570625000
1	21.958430000	25.625908000	-8.201729000
1	21.781114000	28.300667000	-9.640938000
1	24.024572000	27.577964000	-9.646675000
1	23.412643000	26.948440000	-11.206287000
8	21.961427000	27.520985000	-7.246934000
7	17.270186000	21.558016000	-10.195669000
6	16.813032000	22.817361000	-9.959489000
7	17.559191000	23.942207000	-9.849213000
6	18.886838000	23.684926000	-9.990500000
6	19.481956000	22.425539000	-10.229738000
6	18.614660000	21.308626000	-10.321632000
7	19.022661000	20.042343000	-10.510774000
7	20.881799000	22.549087000	-10.321116000
6	21.131608000	23.856550000	-10.144111000
7	19.940965000	24.588798000	-9.933704000
1	15.740725000	22.883754000	-9.803827000
1	20.009417000	19.837431000	-10.364937000
1	18.328888000	19.263300000	-10.479527000
1	22.106296000	24.345652000	-10.120804000
15	23.470324000	27.219166000	-6.588983000
8	24.221138000	28.520516000	-6.567702000
8	24.039500000	25.962621000	-7.256225000
1	30.568730000	7.103931000	-4.118511000
1	31.315918000	21.191096000	-13.336903000
1	8.317646000	17.700010000	-9.374441000
1	23.917837000	25.556002000	-8.726322000
1	13.468611000	18.773068000	-5.382688000
6	12.835138000	18.221917000	-4.674761000
1	11.811464000	18.609858000	-4.722737000

6	13.416356000	18.305350000	-3.291491000
16	13.415279000	16.874686000	-2.288907000
6	14.120039000	17.753326000	-0.959821000
1	14.347071000	17.252008000	-0.026413000
6	14.346513000	19.076187000	-1.282921000
1	14.800848000	19.796306000	-0.612126000
1	14.070512000	20.369557000	-3.082111000
6	13.946278000	19.392149000	-2.628013000
6	18.074292000	10.966021000	-3.641948000
6	18.211782000	11.435104000	-2.218362000
16	18.403268000	13.152498000	-1.946765000
6	18.645314000	12.897435000	-0.245534000
1	18.834115000	13.726301000	0.426472000
6	18.572626000	11.560085000	0.092991000
1	18.706848000	11.192334000	1.104908000
1	18.244401000	9.634253000	-0.998729000
6	18.316351000	10.716746000	-1.044593000
1	19.021058000	10.525646000	-3.990382000
1	17.267965000	10.231702000	-3.771285000
6	22.762516000	8.796066000	-6.012486000
6	24.056640000	8.397695000	-5.349345000
16	25.501882000	8.257304000	-6.313487000
6	26.446909000	7.770112000	-4.940084000
1	27.521949000	7.665540000	-5.050917000
6	25.672585000	7.686365000	-3.799623000
1	26.064393000	7.405956000	-2.826027000
1	23.532170000	8.067451000	-3.264887000
6	24.296391000	8.046039000	-4.034964000
1	22.051299000	7.956690000	-5.999370000
1	22.293597000	9.653850000	-5.515110000
6	28.116951000	11.157056000	-9.601474000
6	28.734653000	9.821012000	-9.408469000
16	30.360623000	9.460530000	-9.943092000
6	30.332588000	7.907728000	-9.155829000
1	31.175768000	7.232412000	-9.237270000
6	29.119734000	7.674593000	-8.529356000
1	28.869151000	6.736261000	-8.041279000
1	27.204278000	8.830328000	-8.265469000

6	28.205653000	8.778153000	-8.675492000
1	27.096177000	11.131939000	-9.204761000
1	28.669952000	11.934608000	-9.060060000
6	18.667654000	23.982368000	-1.802624000
1	19.610283000	23.822326000	-1.264408000
1	17.968818000	24.523069000	-1.146289000
6	17.625255000	22.285606000	-3.486104000
6	18.080918000	22.654415000	-2.235675000
16	17.930111000	21.335144000	-1.091891000
6	17.269383000	20.285819000	-2.314671000
6	17.165080000	20.919336000	-3.533176000
1	17.646763000	22.939981000	-4.349556000
1	16.967528000	19.278879000	-2.064037000
1	16.769737000	20.430521000	-4.418317000
6	20.735793000	19.283337000	2.616746000
1	21.365663000	18.461029000	2.264181000
1	20.662644000	19.237652000	3.712217000
6	18.963735000	18.341735000	0.976969000
6	19.375029000	19.184198000	1.994567000
16	18.052593000	20.186273000	2.553275000
6	16.946150000	19.441895000	1.439165000
6	17.567910000	18.480678000	0.665470000
1	19.651371000	17.701572000	0.439773000
1	15.909152000	19.751136000	1.408447000
1	17.049968000	17.900643000	-0.091170000
6	23.210016000	14.037128000	1.836509000
1	23.302792000	14.158932000	0.749624000
1	23.660555000	13.077247000	2.119220000
6	21.020869000	13.021744000	2.784308000
6	21.777544000	14.063588000	2.281076000
16	20.823434000	15.525690000	2.159075000
6	19.405266000	14.720305000	2.761582000
6	19.658511000	13.395496000	3.055968000
1	21.424750000	12.027891000	2.953148000
1	18.479152000	15.269153000	2.884172000
1	18.910844000	12.716377000	3.452931000
6	25.516829000	10.836801000	-2.221708000
1	25.672227000	9.812532000	-2.578780000

1	25.861009000	11.531848000	-2.998512000
6	23.609934000	11.384647000	-0.578594000
6	24.080093000	11.099477000	-1.846836000
16	22.769732000	11.052884000	-3.005469000
6	21.597827000	11.399353000	-1.770310000
6	22.186955000	11.568978000	-0.535263000
1	24.273328000	11.482402000	0.267601000
1	20.545432000	11.457262000	-2.006902000
1	21.623333000	11.824778000	0.354732000

Figure S19. X-Y coordinates for **3:4** at level: B97D3/3-21G*.

8	-7.010434000	-7.543660000	6.895802000
6	-9.879937000	-5.535133000	5.363685000
6	-9.653422000	-6.292992000	4.047487000
6	-8.677071000	-7.395636000	4.496971000
6	-9.201109000	-7.724845000	5.902280000
6	-8.196034000	-8.342119000	6.856914000
8	-9.699216000	-6.461295000	6.420961000
1	-10.881982000	-5.096133000	5.410992000
1	-9.256223000	-5.643676000	3.260186000
8	-10.888217000	-6.884386000	3.636125000
1	-10.635133000	-7.782235000	3.332923000
1	-7.648266000	-7.021117000	4.547621000
1	-10.049485000	-8.422497000	5.809109000
1	-7.980145000	-9.360762000	6.487336000
1	-8.654548000	-8.430209000	7.856544000
8	-8.755434000	-8.548718000	3.662620000
7	-8.912380000	-4.405602000	5.509862000
6	-9.189361000	-3.213228000	4.797969000
8	-10.204097000	-3.184657000	4.062159000
7	-8.348638000	-2.157604000	4.949081000
6	-7.228245000	-2.267472000	5.694155000
7	-6.443108000	-1.181959000	5.806795000
6	-6.908575000	-3.481311000	6.384981000
6	-7.784723000	-4.521640000	6.273756000
1	-6.638059000	-0.339677000	5.241827000
1	-5.507863000	-1.288896000	6.179082000
1	-6.009402000	-3.572417000	6.988179000
1	-7.637592000	-5.479835000	6.766602000
8	-8.254497000	6.436260000	-0.746166000
6	-8.825859000	2.788308000	-1.143527000
6	-10.329133000	3.041830000	-1.356352000
6	-10.363419000	4.564470000	-1.578989000
6	-9.037191000	4.808789000	-2.336083000
6	-8.429094000	6.186253000	-2.146982000
8	-8.122252000	3.789671000	-1.853241000
1	-8.539698000	1.796182000	-1.517330000
1	-10.928746000	2.703214000	-0.502027000

8	-10.784676000	2.450595000	-2.577800000
1	-11.018711000	1.517074000	-2.405594000
1	-10.327099000	5.081466000	-0.612315000
1	-9.199471000	4.648747000	-3.415043000
1	-9.112446000	6.930092000	-2.586773000
1	-7.459422000	6.246150000	-2.661289000
8	-11.514864000	5.015796000	-2.268637000
7	-8.512623000	0.003022000	3.060348000
6	-9.291578000	-0.191647000	1.939175000
7	-10.006195000	-1.337785000	1.887026000
7	-9.354457000	0.679430000	0.925160000
6	-8.601894000	1.779264000	1.148700000
6	-7.831663000	2.111960000	2.278315000
6	-7.723175000	1.145342000	3.325562000
8	-7.039145000	1.211602000	4.371089000
7	-7.229519000	3.359058000	2.114488000
6	-7.607750000	3.760090000	0.912978000
7	-8.445063000	2.840358000	0.276658000
1	-8.480451000	-0.760062000	3.776922000
1	-10.096176000	-1.966430000	2.700034000
1	-10.660359000	-1.428917000	1.119147000
1	-7.380863000	4.710280000	0.447926000
8	-7.757206000	-7.404611000	1.570186000
6	-8.379266000	-3.868685000	0.333734000
6	-7.821315000	-4.247146000	-1.053731000
6	-7.678460000	-5.762745000	-0.870775000
6	-8.945170000	-6.110574000	-0.082800000
6	-8.899758000	-7.401641000	0.706227000
8	-9.123661000	-4.978251000	0.810580000
1	-9.029920000	-2.988885000	0.281573000
1	-6.870804000	-3.754257000	-1.274173000
8	-8.790059000	-3.942430000	-2.063380000
1	-6.811740000	-5.932394000	-0.216768000
1	-9.805357000	-6.162044000	-0.771496000
1	-8.846182000	-8.240064000	-0.004283000
1	-9.825424000	-7.499867000	1.292588000
8	-7.560229000	-6.541292000	-2.048546000
7	-5.223636000	-0.142341000	1.440425000

6	-6.063623000	-0.316612000	0.363274000
7	-6.106635000	0.667845000	-0.559635000
7	-6.837175000	-1.394260000	0.212467000
6	-6.660426000	-2.298960000	1.197079000
6	-5.792328000	-2.258257000	2.301744000
6	-5.007493000	-1.072147000	2.484059000
8	-4.204093000	-0.799751000	3.404556000
7	-5.876988000	-3.448421000	3.024518000
6	-6.786022000	-4.173277000	2.388663000
7	-7.304373000	-3.516002000	1.272928000
1	-4.682127000	0.752541000	1.489151000
1	-5.393034000	1.416716000	-0.594539000
1	-6.620345000	0.462980000	-1.407521000
1	-7.100247000	-5.179396000	2.635727000
15	-7.509386000	-8.754144000	2.520448000
8	-7.887186000	-10.011634000	1.781104000
8	-6.181431000	-8.528678000	3.196532000
8	-3.448176000	8.189217000	1.824752000
6	-3.640359000	5.380138000	-0.624040000
6	-5.039389000	5.777534000	-1.134761000
6	-5.220847000	7.116582000	-0.388898000
6	-3.816582000	7.725172000	-0.513538000
6	-3.384675000	8.757791000	0.512841000
8	-2.930647000	6.580280000	-0.435112000
1	-3.092920000	4.748605000	-1.321760000
1	-5.792580000	5.020551000	-0.897221000
8	-5.042532000	6.054862000	-2.534506000
1	-5.440339000	6.903243000	0.666943000
1	-3.720754000	8.177172000	-1.514041000
1	-4.051614000	9.632181000	0.436366000
1	-2.356096000	9.069658000	0.285551000
8	-6.193922000	7.993903000	-0.929335000
7	-3.713767000	4.588867000	0.644827000
6	-4.038310000	3.223372000	0.494032000
8	-4.391705000	2.833090000	-0.643426000
7	-3.945860000	2.406017000	1.570059000
6	-3.578814000	2.888822000	2.774329000
7	-3.509066000	2.014223000	3.792840000

6	-3.291140000	4.280686000	2.960863000
6	-3.371534000	5.094492000	1.864963000
1	-3.684673000	1.010572000	3.637084000
1	-3.141151000	2.308669000	4.687934000
1	-3.021032000	4.692191000	3.929200000
1	-3.188987000	6.164841000	1.907765000
15	-7.738070000	7.952229000	-0.262478000
8	-8.500457000	9.027136000	-0.997102000
8	-7.648946000	7.862785000	1.241718000
8	-5.385382000	-5.533192000	-3.029361000
6	-4.720738000	-1.796649000	-2.933620000
6	-3.897250000	-1.822615000	-4.237129000
6	-4.093482000	-3.294760000	-4.636448000
6	-5.577653000	-3.493055000	-4.313582000
6	-6.075616000	-4.908548000	-4.117986000
8	-5.766405000	-2.732248000	-3.091072000
1	-5.144926000	-0.805020000	-2.739006000
1	-2.852256000	-1.541157000	-4.077012000
8	-4.511495000	-0.982710000	-5.212927000
1	-3.487650000	-3.913662000	-3.959783000
1	-6.178378000	-3.034933000	-5.116821000
1	-5.909632000	-5.462960000	-5.055829000
1	-7.154852000	-4.885151000	-3.910139000
8	-3.816395000	-3.625580000	-5.985043000
7	-1.571398000	0.297551000	0.451179000
6	-2.008142000	0.712742000	-0.753213000
7	-2.792330000	0.045510000	-1.611991000
6	-3.094740000	-1.180150000	-1.145234000
6	-2.669348000	-1.770932000	0.059457000
6	-1.890577000	-0.942417000	0.909472000
7	-1.440725000	-1.313407000	2.132801000
7	-3.195091000	-3.056390000	0.183325000
6	-3.933448000	-3.225899000	-0.907678000
7	-3.910064000	-2.118761000	-1.749489000
1	-1.698018000	1.715721000	-1.040277000
1	-1.981598000	-2.026558000	2.609817000
1	-1.075933000	-0.558609000	2.727008000
1	-4.496143000	-4.114409000	-1.171814000

15	-6.002362000	-7.001693000	-2.508862000
8	-6.212292000	-7.928204000	-3.681012000
8	-5.184212000	-7.358022000	-1.291269000
8	1.572039000	7.005709000	4.781432000
6	0.899210000	5.740351000	1.289534000
6	-0.295122000	6.681148000	1.061127000
6	-0.245403000	7.499365000	2.365932000
6	1.266028000	7.734016000	2.496866000
6	1.836539000	8.069897000	3.862138000
8	1.844644000	6.486380000	2.020414000
1	1.355318000	5.387945000	0.360920000
1	-1.228385000	6.141598000	0.904021000
8	-0.030855000	7.574477000	-0.015429000
1	-0.603429000	6.872177000	3.193906000
1	1.555133000	8.540120000	1.804403000
1	1.373547000	9.008507000	4.208184000
1	2.920894000	8.223685000	3.767918000
8	-0.948119000	8.730148000	2.345662000
7	0.508891000	4.503921000	2.036219000
6	-0.115000000	3.502120000	1.278635000
8	-0.410873000	3.674630000	0.088413000
7	-0.365802000	2.332877000	1.959622000
6	-0.080832000	2.055503000	3.302159000
8	-0.371740000	0.947826000	3.793206000
6	0.543145000	3.151006000	4.012025000
1	0.796119000	3.034327000	5.061446000
6	0.815522000	4.317704000	3.362243000
1	-0.812998000	1.557566000	1.398502000
1	1.273714000	5.170216000	3.857547000
15	-2.477898000	8.811244000	3.042913000
8	-2.742802000	10.286980000	3.205239000
8	-2.591465000	7.801525000	4.160716000
8	-1.447985000	-2.637688000	-6.298956000
6	-0.046102000	0.555021000	-5.086680000
6	1.169252000	0.321186000	-6.012366000
6	0.609713000	-0.725921000	-7.004352000
6	-0.895159000	-0.431233000	-7.062985000
6	-1.777271000	-1.648038000	-7.278511000

8	-1.218304000	0.177367000	-5.783792000
1	-0.109246000	1.607366000	-4.791822000
1	2.014725000	-0.076721000	-5.447423000
8	1.690672000	1.513809000	-6.584766000
1	0.743859000	-1.718233000	-6.552848000
1	-1.105931000	0.294488000	-7.865440000
1	-1.597580000	-2.035996000	-8.293380000
1	-2.835304000	-1.364532000	-7.182962000
8	1.189983000	-0.686158000	-8.298558000
7	1.874598000	0.880827000	-0.452270000
6	1.851943000	1.804012000	-1.476640000
7	2.527872000	2.957257000	-1.283323000
7	1.248718000	1.577873000	-2.650408000
6	0.716465000	0.338926000	-2.728349000
6	0.714776000	-0.686196000	-1.772622000
6	1.313466000	-0.415610000	-0.500572000
8	1.378873000	-1.174127000	0.484635000
7	0.098451000	-1.827289000	-2.281885000
6	-0.261168000	-1.505141000	-3.518080000
7	0.070825000	-0.188106000	-3.830914000
1	2.333095000	1.147194000	0.451885000
1	2.882951000	3.220469000	-0.349570000
1	2.373842000	3.691052000	-1.964196000
1	-0.738195000	-2.154142000	-4.244158000
15	-2.243642000	-4.107779000	-6.352934000
8	-2.316805000	-4.611265000	-7.772572000
8	-1.661606000	-4.895042000	-5.204158000
8	5.363159000	3.659589000	6.960890000
6	5.298017000	4.401165000	3.238407000
6	4.403436000	5.616358000	3.510863000
6	4.437354000	5.638822000	5.044339000
6	5.918682000	5.332707000	5.316234000
6	6.254815000	4.741418000	6.673033000
8	6.279863000	4.391519000	4.260550000
1	5.780369000	4.454551000	2.262558000
1	3.405895000	5.499722000	3.088962000
8	5.009840000	6.820939000	3.036112000
1	3.827191000	4.805909000	5.417881000

1	6.512028000	6.250988000	5.180432000
1	6.146400000	5.529920000	7.434927000
1	7.301782000	4.405248000	6.673264000
8	4.026465000	6.853133000	5.652671000
7	4.522537000	3.119571000	3.250656000
6	3.750197000	2.811325000	2.104954000
8	3.667835000	3.677102000	1.201443000
7	3.145458000	1.598139000	2.032553000
6	3.215631000	0.723228000	3.063364000
7	2.595276000	-0.457518000	2.937111000
6	3.923328000	1.057257000	4.264201000
6	4.584542000	2.251375000	4.300654000
1	2.155303000	-0.718107000	2.039793000
1	2.773888000	-1.193938000	3.618858000
1	3.945213000	0.383473000	5.114874000
1	5.176032000	2.578256000	5.148608000
15	2.441569000	6.950424000	6.216471000
8	2.372283000	8.284884000	6.915856000
8	2.031904000	5.641751000	6.848258000
8	3.545860000	-1.251384000	-7.417376000
6	6.037992000	-0.705132000	-4.569270000
6	7.080360000	-1.448464000	-5.436475000
6	6.326974000	-1.529787000	-6.772096000
6	5.618733000	-0.172286000	-6.827271000
6	4.388003000	-0.128460000	-7.711630000
8	5.276021000	0.112864000	-5.440343000
1	6.511613000	-0.091019000	-3.796278000
1	7.332497000	-2.423793000	-5.011538000
8	8.262190000	-0.680204000	-5.634083000
1	5.573969000	-2.324355000	-6.697065000
1	6.325591000	0.597844000	-7.175678000
1	4.716902000	-0.173218000	-8.759622000
1	3.831288000	0.805639000	-7.549083000
8	7.120068000	-1.722122000	-7.931443000
7	5.130555000	-1.640935000	-3.838178000
6	5.546612000	-2.116971000	-2.573425000
8	6.738964000	-1.920015000	-2.230400000
7	4.634182000	-2.734977000	-1.778524000

6	3.378102000	-2.964217000	-2.218075000
7	2.478672000	-3.485438000	-1.359338000
6	3.008388000	-2.672749000	-3.572969000
6	3.900096000	-1.974015000	-4.333256000
1	2.705406000	-3.456393000	-0.356472000
1	1.495495000	-3.325571000	-1.593564000
1	2.029043000	-2.931051000	-3.961077000
1	3.685126000	-1.648259000	-5.347547000
15	2.448760000	-1.778184000	-8.566495000
8	2.949205000	-1.470351000	-9.955263000
8	2.027746000	-3.152305000	-8.106489000
8	5.645039000	-1.655417000	8.499977000
6	7.468460000	-1.553990000	5.235184000
6	7.282363000	-0.025834000	5.122656000
6	6.776700000	0.314636000	6.536955000
6	7.574303000	-0.669692000	7.411795000
6	6.933884000	-1.064554000	8.731427000
8	7.739419000	-1.854748000	6.591105000
1	8.292994000	-1.892981000	4.597904000
1	6.560061000	0.234239000	4.340552000
8	8.567629000	0.526784000	4.831981000
1	5.711164000	0.064580000	6.607552000
1	8.564648000	-0.229922000	7.620475000
1	6.813885000	-0.162276000	9.348549000
1	7.594861000	-1.761239000	9.264646000
8	6.979251000	1.672536000	6.892643000
7	5.372712000	-3.162516000	0.981592000
6	6.698448000	-2.942264000	1.281614000
7	7.584952000	-2.996045000	0.252392000
7	7.138914000	-2.712882000	2.522264000
6	6.140494000	-2.662278000	3.428902000
6	4.776420000	-2.929675000	3.248976000
6	4.312870000	-3.213066000	1.919776000
8	3.150812000	-3.459821000	1.544431000
7	4.079089000	-2.715959000	4.439029000
6	4.994121000	-2.311152000	5.309365000
7	6.275076000	-2.272015000	4.754452000
1	5.097016000	-3.171596000	-0.027141000

1	7.249287000	-2.739325000	-0.691985000
1	8.502805000	-2.630913000	0.486069000
1	4.824857000	-2.078867000	6.355008000
15	5.868780000	2.407638000	7.943883000
8	6.671222000	2.956002000	9.099579000
8	4.658719000	1.521895000	8.100454000
8	8.268872000	-3.970586000	-7.406337000
6	9.691442000	-4.705588000	-3.958690000
6	10.449116000	-5.895427000	-4.575581000
6	10.265175000	-5.643206000	-6.081458000
6	10.315342000	-4.102005000	-6.149149000
6	9.601019000	-3.453058000	-7.318771000
8	9.706749000	-3.658240000	-4.907753000
1	10.165182000	-4.388228000	-3.024809000
1	10.032785000	-6.860061000	-4.244657000
8	11.821970000	-5.768956000	-4.217292000
1	12.318631000	-6.093764000	-4.995697000
1	9.281441000	-6.004259000	-6.415885000
1	11.370578000	-3.783537000	-6.159759000
1	10.157470000	-3.669470000	-8.245341000
1	9.576669000	-2.363931000	-7.170488000
8	11.320930000	-6.298324000	-6.777473000
7	8.286185000	-5.040510000	-3.608281000
6	8.065853000	-5.517619000	-2.305507000
8	8.993547000	-5.701997000	-1.511166000
7	6.744717000	-5.765615000	-2.002297000
6	5.642205000	-5.660220000	-2.858402000
8	4.503193000	-5.970150000	-2.460546000
6	5.965921000	-5.192608000	-4.189253000
1	5.171011000	-5.067822000	-4.918115000
6	7.258919000	-4.908538000	-4.512936000
1	6.569391000	-6.086381000	-1.014342000
1	7.549190000	-4.556106000	-5.500907000
15	7.243933000	-3.280980000	-8.544534000
8	7.965855000	-3.123709000	-9.858875000
8	5.939088000	-4.021604000	-8.379331000
8	3.368916000	-6.039738000	7.922560000
6	6.715839000	-6.546533000	5.854464000

6	7.148220000	-5.191950000	6.444865000
6	6.057564000	-4.981098000	7.500076000
6	5.822100000	-6.403717000	8.025794000
6	4.439855000	-6.638047000	8.642650000
8	6.027407000	-7.260524000	6.870947000
1	7.581222000	-7.118157000	5.494385000
1	7.156165000	-4.408241000	5.676647000
8	8.429357000	-5.344812000	7.048968000
1	8.476895000	-4.618525000	7.701854000
1	5.153077000	-4.608982000	7.006626000
1	6.596173000	-6.638317000	8.775306000
1	4.476395000	-6.260577000	9.680369000
1	4.250240000	-7.720258000	8.687728000
8	6.463749000	-4.106261000	8.544810000
7	6.302451000	-6.477579000	0.700205000
6	7.380740000	-6.549578000	1.507992000
7	7.416921000	-6.526121000	2.850111000
6	6.174971000	-6.420104000	3.367985000
6	4.962525000	-6.326392000	2.655078000
6	5.059945000	-6.347795000	1.241102000
7	3.988671000	-6.279644000	0.417099000
7	3.880644000	-6.239534000	3.523401000
6	4.422247000	-6.277779000	4.732471000
7	5.809990000	-6.388106000	4.703301000
1	8.337405000	-6.614568000	0.987217000
1	3.153958000	-5.850699000	0.802780000
1	4.157893000	-6.136714000	-0.588049000
1	3.886109000	-6.244718000	5.678032000
15	5.301820000	-3.101947000	9.235503000
8	5.622225000	-3.046659000	10.705922000
8	3.928174000	-3.476104000	8.700970000
1	-11.709115000	4.301597000	-2.910251000
1	-6.433348000	-7.912060000	7.586718000
1	11.247414000	-6.076086000	-7.722336000
1	3.438372000	-5.070055000	8.140549000
1	8.800216000	-1.274676000	-3.694382000
6	9.083660000	-0.543179000	-4.463174000
1	10.111475000	-0.772652000	-4.782980000

6	9.007550000	0.849311000	-3.897766000
16	8.591518000	2.195726000	-4.938971000
6	8.882552000	3.339692000	-3.656816000
1	8.726122000	4.399619000	-3.833212000
6	9.272963000	2.711117000	-2.496160000
1	9.487116000	3.238974000	-1.569031000
1	9.611181000	0.611332000	-1.824501000
6	9.337160000	1.286618000	-2.633133000
6	0.784653000	2.428587000	-7.215045000
6	1.255267000	3.825821000	-6.919110000
16	2.295964000	4.123349000	-5.541347000
6	2.254239000	5.839392000	-5.817427000
1	2.805818000	6.503295000	-5.158960000
6	1.483234000	6.158882000	-6.912236000
1	1.329365000	7.179768000	-7.259084000
1	0.274327000	5.045528000	-8.424256000
6	0.917126000	5.005429000	-7.545687000
1	-0.239216000	2.292613000	-6.831378000
1	0.754923000	2.245953000	-8.301574000
6	-4.321972000	0.426312000	-4.944662000
6	-5.623191000	1.168911000	-4.992446000
16	-7.056530000	0.578398000	-4.164182000
6	-7.967964000	1.997169000	-4.603698000
1	-8.994892000	2.097745000	-4.265578000
6	-7.211951000	2.864487000	-5.355498000
1	-7.592326000	3.810464000	-5.737547000
1	-5.125966000	2.929216000	-6.153252000
6	-5.879185000	2.387967000	-5.582523000
1	-3.639972000	0.844445000	-5.697407000
1	-3.835066000	0.552121000	-3.965171000
6	-8.733414000	-2.554388000	-2.466958000
6	-10.095251000	-1.947544000	-2.594929000
16	-11.335534000	-2.208119000	-1.384399000
6	-12.396902000	-1.051610000	-2.137481000
1	-13.388005000	-0.881118000	-1.728624000
6	-11.830893000	-0.513916000	-3.272885000
1	-12.346877000	0.194147000	-3.920096000
1	-9.902014000	-0.728559000	-4.379214000

6	-10.517083000	-1.028255000	-3.532338000
1	-8.219829000	-2.474995000	-3.434852000
1	-8.139453000	-1.986040000	-1.735502000
6	8.525188000	1.762718000	4.107905000
1	7.844594000	2.475098000	4.595620000
1	9.544368000	2.169763000	4.187872000
6	7.868401000	0.412429000	1.967402000
6	8.132624000	1.576170000	2.657246000
16	7.897997000	2.973166000	1.622001000
6	7.406359000	1.970001000	0.285243000
6	7.442943000	0.636862000	0.616095000
1	7.958618000	-0.576723000	2.407478000
1	7.142329000	2.427827000	-0.660848000
1	7.181349000	-0.154863000	-0.084283000
6	4.889806000	7.041998000	1.614230000
1	3.939126000	6.640528000	1.246700000
1	4.862861000	8.136787000	1.510296000
6	5.918219000	5.595241000	-0.273617000
6	6.007114000	6.470474000	0.789425000
16	7.672519000	6.960375000	1.044456000
6	8.221241000	5.992190000	-0.294847000
6	7.176557000	5.330037000	-0.899941000
1	4.980716000	5.133073000	-0.568411000
1	9.278428000	5.956095000	-0.540106000
1	7.302406000	4.666319000	-1.752376000
6	-0.062490000	6.973229000	-1.334779000
1	-0.175352000	5.884849000	-1.256554000
1	-0.941162000	7.355360000	-1.869042000
6	1.333668000	8.381005000	-2.997075000
6	1.176487000	7.358913000	-2.084063000
16	2.720245000	6.596732000	-1.754770000
6	3.554396000	7.662350000	-2.845774000
6	2.686024000	8.554175000	-3.435171000
1	0.499101000	8.994315000	-3.334406000
1	4.625601000	7.556410000	-2.988257000
1	3.002087000	9.306621000	-4.155633000
6	-4.783288000	4.916971000	-3.385884000
1	-5.361104000	5.115362000	-4.298937000

1	-5.173683000	3.997481000	-2.929820000
6	-2.452538000	5.810156000	-4.071158000
6	-3.312538000	4.792260000	-3.704412000
16	-2.429771000	3.296021000	-3.485592000
6	-0.917712000	4.063442000	-3.862397000
6	-1.086937000	5.397290000	-4.163236000
1	-2.793154000	6.832486000	-4.228086000
1	0.001282000	3.490339000	-3.797429000
1	-0.259344000	6.054514000	-4.420954000

Figure S20. X-Y coordinates for **3:4** at level: B97D3/6-31G*.

8	8.961004000	4.403460000	3.170512000
6	10.771215000	2.986171000	0.240688000
6	9.449728000	3.195354000	-0.513124000
6	8.670499000	4.187685000	0.383859000
6	9.787972000	5.035974000	1.009769000
6	9.460081000	5.546383000	2.400495000
8	10.962434000	4.139500000	1.109719000
1	11.588717000	2.872081000	-0.468825000
1	8.923289000	2.263938000	-0.720212000
8	9.754120000	3.909526000	-1.759790000
1	9.107549000	4.682344000	-1.729197000
1	8.061566000	3.714213000	1.150913000
1	10.014944000	5.873435000	0.343583000
1	8.696830000	6.328457000	2.308701000
1	10.362839000	5.975158000	2.850143000
8	7.862213000	5.070896000	-0.463250000
7	10.752887000	1.763620000	1.076394000
6	11.228284000	0.556279000	0.455366000
8	11.577001000	0.609207000	-0.743440000
7	11.267189000	-0.570838000	1.231521000
6	10.859065000	-0.540261000	2.504466000
7	10.922268000	-1.693918000	3.205517000
6	10.372573000	0.655422000	3.130269000
6	10.346977000	1.790705000	2.379955000
1	11.270223000	-2.525943000	2.741639000
1	10.631835000	-1.753614000	4.173605000
1	10.046768000	0.659091000	4.159613000
1	9.992082000	2.744126000	2.761685000
8	6.346638000	3.157024000	-1.150522000
6	7.040382000	-0.514438000	-1.471413000
6	5.753270000	-0.673935000	-2.289265000
6	5.347830000	0.793784000	-2.548190000
6	6.708503000	1.450214000	-2.812596000
6	6.789133000	2.933181000	-2.535866000
8	7.645351000	0.744688000	-1.885009000
1	7.726226000	-1.348952000	-1.615476000
1	5.001286000	-1.253641000	-1.759000000

8	6.081117000	-1.255899000	-3.586161000
1	5.553059000	-0.680849000	-4.220474000
1	4.823094000	1.254394000	-1.714454000
1	7.003459000	1.245183000	-3.845280000
1	6.139327000	3.478434000	-3.226527000
1	7.824360000	3.267288000	-2.649489000
8	4.540088000	0.859263000	-3.763874000
7	5.517213000	-3.263040000	2.493278000
6	6.143798000	-3.677031000	1.332389000
7	6.302960000	-5.001027000	1.134832000
7	6.588479000	-2.816862000	0.417644000
6	6.384391000	-1.520720000	0.744750000
6	5.785352000	-1.005835000	1.898749000
6	5.221224000	-1.912169000	2.834465000
8	4.506568000	-1.673257000	3.839254000
7	5.726826000	0.393860000	1.833413000
6	6.262601000	0.712401000	0.663124000
7	6.681217000	-0.430984000	-0.044342000
1	5.106498000	-3.954775000	3.119655000
1	5.984063000	-5.700152000	1.793456000
1	6.755741000	-5.304947000	0.281000000
1	6.360682000	1.696216000	0.231191000
15	6.222963000	4.707327000	-0.580745000
8	5.690190000	5.602539000	-1.652481000
8	5.670963000	4.578752000	0.802586000
8	2.880641000	-0.957713000	-3.108744000
6	1.742061000	-4.573077000	-2.028994000
6	0.377896000	-4.088608000	-2.523456000
6	0.724237000	-2.789701000	-3.272650000
6	2.072618000	-3.133303000	-3.917028000
6	2.961393000	-1.942445000	-4.209491000
8	2.748145000	-4.005976000	-2.919199000
1	1.785998000	-5.663180000	-2.008901000
1	-0.356056000	-3.973093000	-1.726343000
8	-0.094642000	-5.041833000	-3.539138000
1	-0.373260000	-4.434134000	-4.291352000
1	0.802783000	-1.913635000	-2.634542000
1	1.902045000	-3.702628000	-4.835841000

1	2.620239000	-1.454826000	-5.125189000
1	4.002531000	-2.261197000	-4.301765000
8	-0.275331000	-2.567635000	-4.321737000
7	1.441549000	-5.535690000	3.048383000
6	1.004499000	-6.235298000	1.981200000
7	1.126796000	-5.907632000	0.676747000
6	1.751237000	-4.724686000	0.509972000
6	2.250068000	-3.891214000	1.525824000
6	2.090754000	-4.349928000	2.853968000
7	2.551878000	-3.699149000	3.938565000
7	2.821644000	-2.736659000	0.966990000
6	2.671603000	-2.879497000	-0.347132000
7	2.029717000	-4.074594000	-0.677288000
1	0.500382000	-7.170155000	2.196565000
1	3.126391000	-2.843341000	3.898461000
1	2.324801000	-4.100171000	4.843450000
1	2.964089000	-2.181460000	-1.114618000
15	2.879139000	0.652636000	-3.534990000
8	2.281290000	0.818473000	-4.896711000
8	2.481147000	1.414210000	-2.311959000
8	-2.276516000	-2.287846000	-2.761119000
6	-2.579724000	-3.432950000	0.571045000
6	-4.065916000	-3.013582000	0.532273000
6	-4.411074000	-2.979881000	-0.985271000
6	-3.442727000	-4.001623000	-1.608368000
6	-2.907118000	-3.593023000	-2.966954000
8	-2.288230000	-4.113067000	-0.678668000
1	-2.417819000	-4.099639000	1.418882000
1	-4.227253000	-2.058280000	1.030305000
8	-4.845052000	-4.078859000	1.149252000
1	-5.520536000	-4.297972000	0.434371000
1	-4.312253000	-1.988744000	-1.429454000
1	-3.952288000	-4.966996000	-1.667516000
1	-3.727775000	-3.525098000	-3.689214000
1	-2.167236000	-4.324812000	-3.298927000
8	-5.761028000	-3.525789000	-1.176220000
7	-0.015451000	-0.981576000	4.158896000
6	-0.567950000	-2.248371000	4.177844000

7	-0.506766000	-2.953662000	5.325473000
7	-1.164064000	-2.781691000	3.111089000
6	-1.126733000	-1.991817000	2.014276000
6	-0.550365000	-0.731158000	1.887042000
6	0.024993000	-0.099113000	3.028662000
8	0.496883000	1.046743000	3.156398000
7	-0.717254000	-0.258254000	0.577435000
6	-1.388175000	-1.206757000	-0.068757000
7	-1.678237000	-2.289370000	0.778043000
1	0.393317000	-0.594856000	5.008142000
1	-0.060157000	-2.605975000	6.164781000
1	-0.901660000	-3.886669000	5.331902000
1	-1.631037000	-1.201291000	-1.117909000
15	-1.475353000	-1.452735000	-3.937975000
8	-2.314402000	-1.307811000	-5.164799000
8	-0.826716000	-0.323050000	-3.192709000
8	-6.842402000	-1.748440000	0.274238000
6	-6.822798000	0.722759000	3.259521000
6	-8.065097000	1.241962000	2.505453000
6	-8.518914000	0.039410000	1.632708000
6	-7.985037000	-1.195565000	2.373465000
6	-7.543994000	-2.319515000	1.448832000
8	-6.809391000	-0.735302000	3.139831000
1	-6.857377000	1.053728000	4.296559000
1	-7.849561000	2.137141000	1.921083000
8	-9.131546000	1.519531000	3.471927000
1	-9.890711000	0.952857000	3.123346000
1	-8.120776000	0.075252000	0.623040000
1	-8.756818000	-1.559940000	3.059930000
1	-8.409467000	-2.874782000	1.083650000
1	-6.844925000	-2.987103000	1.957825000
8	-9.985167000	-0.022750000	1.624926000
7	-5.547414000	1.217218000	2.718331000
6	-4.781352000	2.144659000	3.514879000
8	-5.297318000	2.600772000	4.557955000
7	-3.516821000	2.442322000	3.080307000
6	-3.039746000	1.929986000	1.939258000
7	-1.765120000	2.210179000	1.581139000

6	-3.825751000	1.068083000	1.097045000
6	-5.051565000	0.702478000	1.550684000
1	-1.157046000	2.607634000	2.293895000
1	-1.299191000	1.583901000	0.908587000
1	-3.451487000	0.707662000	0.152551000
1	-5.668243000	-0.022509000	1.032846000
15	-7.071652000	-2.479312000	-1.197216000
8	-8.276906000	-3.362891000	-1.156063000
8	-6.824655000	-1.431799000	-2.242135000
8	-10.047921000	1.949087000	0.036157000
6	-7.583113000	4.779570000	-0.306273000
6	-8.610174000	5.406836000	-1.262760000
6	-9.899380000	4.599344000	-1.007538000
6	-9.798158000	4.298130000	0.502331000
6	-10.487274000	3.026055000	0.944872000
8	-8.342279000	4.134267000	0.760529000
1	-6.924295000	5.556530000	0.077450000
1	-8.274393000	5.383361000	-2.303978000
8	-8.856361000	6.752910000	-0.768891000
1	-9.846598000	6.862776000	-0.913060000
1	-9.942993000	3.670102000	-1.576056000
1	-10.171950000	5.163080000	1.058065000
1	-11.574821000	3.128087000	0.887251000
1	-10.194727000	2.781530000	1.970688000
8	-10.987529000	5.513246000	-1.334009000
7	-6.717676000	3.765999000	-0.942961000
6	-5.401788000	4.157548000	-1.235382000
8	-4.993360000	5.316237000	-1.058821000
7	-4.611345000	3.130064000	-1.721255000
6	-4.964814000	1.771682000	-1.903559000
8	-4.093224000	0.943369000	-2.233734000
6	-6.357510000	1.494828000	-1.628204000
1	-6.695448000	0.471658000	-1.774380000
6	-7.156619000	2.465840000	-1.133576000
1	-3.639860000	3.373280000	-1.907424000
1	-8.172682000	2.270735000	-0.808254000
15	-10.757634000	0.456913000	0.211284000
8	-12.196532000	0.630995000	0.578949000

8	-10.249908000	-0.371748000	-0.923880000
1	8.770018000	4.701061000	4.098712000
1	-11.854872000	5.122416000	-1.051579000

Figure S21. X-Y coordinates for **1** at level: B3LYP/3-21G*.

8	-6.111461000	3.643926000	-3.589524000
6	-8.077327000	3.700753000	-0.432405000
6	-6.736425000	3.918612000	0.272671000
6	-5.803224000	4.331922000	-0.887510000
6	-6.737826000	5.120761000	-1.811791000
6	-6.340169000	5.056758000	-3.272747000
8	-8.068833000	4.489900000	-1.655638000
1	-8.900954000	3.982622000	0.221242000
1	-6.423260000	3.038373000	0.826586000
8	-6.858773000	5.080013000	1.161679000
1	-6.066422000	5.642016000	0.904045000
1	-5.360046000	3.487414000	-1.411124000
1	-6.776994000	6.159493000	-1.471229000
1	-5.425906000	5.649133000	-3.401202000
1	-7.140814000	5.487285000	-3.885184000
8	-4.784500000	5.273331000	-0.403058000
7	-8.249397000	2.271884000	-0.786550000
6	-8.761535000	1.425093000	0.252966000
8	-8.980748000	1.938885000	1.370391000
7	-8.979582000	0.109689000	-0.062053000
6	-8.693023000	-0.351929000	-1.282649000
7	-8.932893000	-1.662076000	-1.524524000
6	-8.147172000	0.477326000	-2.316140000
6	-7.933950000	1.788209000	-2.023413000
1	-9.266837000	-2.244884000	-0.764892000
1	-8.694349000	-2.098555000	-2.405950000
1	-7.877717000	0.069803000	-3.278518000
1	-7.478085000	2.484590000	-2.719144000
8	-3.942215000	3.420340000	1.091275000
6	-5.502116000	0.276560000	2.014982000
6	-4.180357000	-0.092602000	2.702898000
6	-3.447868000	1.258262000	2.803400000
6	-4.587277000	2.249266000	3.052455000
6	-4.327177000	3.631812000	2.492125000
8	-5.760586000	1.677228000	2.329843000
1	-6.316041000	-0.358792000	2.365245000
1	-3.600551000	-0.835394000	2.163315000

8	-4.496816000	-0.515443000	4.069974000
1	-3.831501000	0.012471000	4.610670000
1	-2.894583000	1.465244000	1.895092000
1	-4.805676000	2.295850000	4.122744000
1	-3.511447000	4.116661000	3.035665000
1	-5.235893000	4.239401000	2.529218000
8	-2.571997000	1.253058000	3.982234000
7	-6.075011000	-3.005555000	-1.832939000
6	-6.460450000	-3.129115000	-0.506848000
7	-7.023420000	-4.290810000	-0.120707000
7	-6.298220000	-2.149054000	0.380567000
6	-5.750457000	-1.029915000	-0.133877000
6	-5.349377000	-0.813016000	-1.451851000
6	-5.438799000	-1.868838000	-2.376580000
8	-5.001892000	-1.915876000	-3.568573000
7	-4.764029000	0.456251000	-1.576156000
6	-4.804514000	0.984972000	-0.356224000
7	-5.413294000	0.119751000	0.555056000
1	-6.080889000	-3.824653000	-2.441518000
1	-7.160530000	-5.074609000	-0.746469000
1	-7.289868000	-4.390753000	0.851743000
1	-4.378036000	1.917685000	-0.038524000
15	-3.346449000	4.604563000	0.124840000
8	-2.650911000	5.649064000	0.933112000
8	-2.743048000	3.853335000	-1.034451000
8	-1.329575000	-0.781823000	3.146548000
6	-1.616335000	-4.541686000	1.742516000
6	-0.077796000	-4.385345000	1.861709000
6	0.091076000	-3.213019000	2.873260000
6	-1.229122000	-3.170487000	3.639610000
6	-1.603733000	-1.806483000	4.177131000
8	-2.244922000	-3.581365000	2.647802000
1	-1.860101000	-5.579951000	1.985337000
1	0.411061000	-4.189836000	0.906786000
8	0.460654000	-5.606486000	2.463067000
1	0.899635000	-5.252439000	3.300018000
1	0.275296000	-2.261046000	2.380003000
1	-1.189002000	-3.895742000	4.461357000

1	-1.006172000	-1.585145000	5.064126000
1	-2.670515000	-1.784293000	4.413385000
8	1.143546000	-3.570666000	3.838982000
7	-3.087755000	-6.451162000	-2.835494000
6	-2.455348000	-7.032797000	-1.792344000
7	-2.070705000	-6.453560000	-0.632779000
6	-2.380000000	-5.142435000	-0.598005000
6	-3.024310000	-4.413060000	-1.611483000
6	-3.401585000	-5.124839000	-2.770085000
7	-4.075626000	-4.568547000	-3.797795000
7	-3.193822000	-3.082048000	-1.211403000
6	-2.672531000	-3.010686000	0.009361000
7	-2.161526000	-4.237474000	0.426345000
1	-2.233708000	-8.088010000	-1.897992000
1	-4.314894000	-3.566182000	-3.828584000
1	-4.284062000	-5.160162000	-4.596179000
1	-2.630750000	-2.138947000	0.633749000
15	-0.995158000	0.739806000	3.684353000
8	-0.325467000	0.671826000	5.022065000
8	-0.454712000	1.578735000	2.563045000
8	2.740728000	-3.419315000	1.904415000
6	2.221994000	-3.094053000	-1.585319000
6	3.704554000	-2.774279000	-1.760166000
6	4.369499000	-3.340586000	-0.479418000
6	3.462378000	-4.526954000	-0.089114000
6	3.274137000	-4.691285000	1.411351000
8	2.136331000	-4.274059000	-0.711897000
1	1.759111000	-3.317807000	-2.546400000
1	3.879835000	-1.712389000	-1.918906000
8	4.191505000	-3.567568000	-2.895480000
1	4.987168000	-4.045912000	-2.506495000
1	4.455698000	-2.626234000	0.331389000
1	3.889424000	-5.439899000	-0.515043000
1	4.233164000	-4.911988000	1.888305000
1	2.540887000	-5.473729000	1.621218000
8	5.684095000	-3.912365000	-0.814744000
7	-2.080337000	-0.386356000	-1.865168000
6	-1.533730000	-1.232250000	-2.804421000

7	-2.255529000	-1.451805000	-3.929034000
7	-0.338946000	-1.816458000	-2.642745000
6	0.244153000	-1.524668000	-1.457132000
6	-0.277305000	-0.753986000	-0.416111000
6	-1.573466000	-0.198291000	-0.553275000
8	-2.282723000	0.355736000	0.315202000
7	0.608758000	-0.734630000	0.667243000
6	1.644986000	-1.458045000	0.292028000
7	1.472392000	-1.990076000	-0.999637000
1	-3.029331000	0.009034000	-2.005990000
1	-3.283691000	-1.391450000	-3.891059000
1	-1.856591000	-2.113462000	-4.587397000
1	2.483114000	-1.702033000	0.907681000
15	2.673391000	-2.997607000	3.478946000
8	3.634943000	-3.775278000	4.312830000
8	2.530017000	-1.491032000	3.503521000
8	6.268109000	-1.557662000	-1.580214000
6	4.094018000	1.653742000	-2.935974000
6	5.390670000	2.324623000	-2.413654000
6	6.408201000	1.154894000	-2.338773000
6	5.818893000	0.101633000	-3.273108000
6	6.314539000	-1.301950000	-3.034717000
8	4.375265000	0.192161000	-2.978123000
1	3.872147000	2.037963000	-3.931169000
1	5.248748000	2.806236000	-1.448702000
8	5.875428000	3.314015000	-3.383508000
1	6.787682000	2.948615000	-3.616846000
1	6.486541000	0.732967000	-1.342727000
1	6.018796000	0.394918000	-4.313033000
1	7.340712000	-1.393373000	-3.396396000
1	5.670844000	-2.024904000	-3.540992000
8	7.703034000	1.602575000	-2.858161000
7	2.918965000	1.888950000	-2.133142000
6	1.753115000	2.469504000	-2.773893000
8	1.823093000	2.732704000	-3.998186000
7	0.658432000	2.688630000	-1.999433000
6	0.657707000	2.387559000	-0.682548000
7	-0.452292000	2.574184000	0.027602000

6	1.832684000	1.861252000	-0.018684000
6	2.915324000	1.601486000	-0.781614000
1	-1.295409000	2.950180000	-0.442350000
1	-0.526875000	2.170760000	0.987117000
1	1.791180000	1.647435000	1.035395000
1	3.816271000	1.148854000	-0.389123000
15	7.025958000	-2.927190000	-1.055974000
8	7.750902000	-3.547298000	-2.215186000
8	7.702045000	-2.614831000	0.247071000
8	8.010957000	2.861704000	-0.666478000
6	5.209062000	3.566248000	1.614301000
6	6.220463000	4.290535000	2.511583000
6	7.455954000	4.471735000	1.605246000
6	6.810702000	4.726235000	0.225476000
6	7.640531000	4.253846000	-0.955408000
8	5.543248000	3.947771000	0.243265000
1	4.193904000	3.864261000	1.867059000
1	6.427479000	3.735790000	3.431988000
8	5.680053000	5.621094000	2.744503000
1	6.502568000	6.200033000	2.708578000
1	8.096312000	3.590075000	1.574973000
1	6.577131000	5.791452000	0.143191000
1	8.540611000	4.868632000	-1.060671000
1	7.046184000	4.297772000	-1.872606000
8	8.143832000	5.647622000	2.129589000
7	5.264359000	2.100348000	1.748124000
6	4.195883000	1.466164000	2.419970000
8	3.242606000	2.113724000	2.897775000
7	4.293921000	0.100336000	2.471240000
6	5.319971000	-0.696523000	1.944952000
8	5.264339000	-1.941902000	2.081153000
6	6.352448000	0.026161000	1.237621000
1	7.120646000	-0.548785000	0.744002000
6	6.281363000	1.371428000	1.153523000
1	3.508596000	-0.467315000	2.940305000
1	6.985899000	1.944916000	0.563174000
15	8.894687000	1.941475000	-1.726379000
8	9.887926000	2.812943000	-2.426455000

8	9.214632000	0.690872000	-0.970954000
1	-5.860552000	3.564974000	-4.546916000
1	8.829013000	5.951043000	1.478676000

Figure S22. X-Y coordinates for **1** at level: B3LYP-GD3/3-21G*.

8	5.304315000	-4.744259000	-3.129358000
6	7.978655000	-3.742235000	-0.694463000
6	6.926338000	-3.793167000	0.423026000
6	5.763719000	-4.530505000	-0.265390000
6	6.499761000	-5.500663000	-1.196249000
6	5.730125000	-5.913487000	-2.434560000
8	7.719192000	-4.825256000	-1.564910000
1	8.981488000	-3.827553000	-0.271614000
1	6.667808000	-2.798341000	0.789451000
8	7.439937000	-4.596248000	1.482077000
1	6.698284000	-5.167864000	1.756120000
1	5.138643000	-3.845015000	-0.842924000
1	6.752635000	-6.405636000	-0.628001000
1	4.873012000	-6.519562000	-2.106079000
1	6.373284000	-6.542263000	-3.066248000
8	4.986595000	-5.273693000	0.668522000
7	7.947339000	-2.468614000	-1.457722000
6	8.556411000	-1.344684000	-0.835563000
8	8.971928000	-1.471619000	0.322878000
7	8.651097000	-0.186684000	-1.548906000
6	8.152530000	-0.123292000	-2.780026000
7	8.306182000	1.050403000	-3.459250000
6	7.509795000	-1.226788000	-3.418771000
6	7.433913000	-2.388777000	-2.714843000
1	8.573672000	1.849440000	-2.898071000
1	7.643859000	1.254860000	-4.197295000
1	7.093211000	-1.147523000	-4.414802000
1	6.961875000	-3.285347000	-3.097369000
8	4.007163000	-3.189764000	1.773075000
6	5.611957000	0.176519000	2.111019000
6	4.347098000	0.633574000	2.864856000
6	3.652814000	-0.703169000	3.190707000
6	4.847829000	-1.646514000	3.387977000
6	4.583080000	-3.104305000	3.076029000
8	5.881637000	-1.152091000	2.512340000
1	6.451513000	0.832270000	2.356941000
1	3.728050000	1.307880000	2.265861000

8	4.759580000	1.269711000	4.068498000
1	4.172600000	0.909188000	4.760433000
1	3.022089000	-1.026645000	2.361685000
1	5.192821000	-1.567727000	4.427648000
1	3.897331000	-3.516757000	3.824366000
1	5.528407000	-3.659583000	3.116688000
8	2.917277000	-0.623960000	4.409279000
7	6.035618000	3.050751000	-2.040591000
6	6.338555000	3.354030000	-0.731973000
7	6.842807000	4.595516000	-0.483346000
7	6.214037000	2.486936000	0.255753000
6	5.749219000	1.287001000	-0.152498000
6	5.394738000	0.887345000	-1.440685000
6	5.469380000	1.840874000	-2.486584000
8	5.111552000	1.734743000	-3.677749000
7	4.896932000	-0.405679000	-1.431461000
6	4.950484000	-0.775589000	-0.171115000
7	5.469513000	0.207780000	0.652164000
1	6.058914000	3.787499000	-2.740361000
1	6.621854000	5.351429000	-1.118572000
1	6.855389000	4.858243000	0.493756000
1	4.601288000	-1.709685000	0.237755000
15	3.517878000	-4.646223000	1.169715000
8	3.048617000	-5.552902000	2.265279000
8	2.696642000	-4.303274000	-0.044531000
8	1.135336000	1.028510000	3.599483000
6	1.564389000	4.550024000	1.644652000
6	0.012376000	4.469338000	1.640480000
6	-0.289846000	3.507801000	2.830214000
6	1.041189000	3.447439000	3.590927000
6	1.314187000	2.198201000	4.401735000
8	2.039791000	3.588442000	2.570481000
1	1.856632000	5.569087000	1.927427000
1	-0.358357000	4.069745000	0.693972000
8	-0.547721000	5.754581000	1.849117000
1	-1.032458000	5.687056000	2.695506000
1	-0.554829000	2.513643000	2.470560000
1	1.089100000	4.307753000	4.277537000

1	0.631821000	2.178901000	5.257862000
1	2.344006000	2.249372000	4.777303000
8	-1.306063000	4.062317000	3.660139000
7	3.137235000	6.458235000	-2.878017000
6	2.588689000	7.045322000	-1.801044000
7	2.213733000	6.493158000	-0.641683000
6	2.436452000	5.169630000	-0.640949000
6	2.979824000	4.411666000	-1.686413000
6	3.360561000	5.126459000	-2.843023000
7	3.982103000	4.543786000	-3.897981000
7	3.051581000	3.074582000	-1.337619000
6	2.567581000	3.026317000	-0.116491000
7	2.186166000	4.260978000	0.366362000
1	2.431844000	8.118841000	-1.887876000
1	4.067126000	3.533360000	-3.963063000
1	4.089393000	5.085612000	-4.744456000
1	2.469561000	2.139867000	0.490423000
15	1.249746000	-0.443147000	4.349711000
8	0.820274000	-0.334020000	5.781720000
8	0.684775000	-1.468184000	3.406817000
8	-3.059220000	3.456952000	1.867549000
6	-2.179491000	3.021457000	-1.758926000
6	-3.622169000	2.654406000	-2.133198000
6	-4.350927000	2.967903000	-0.804323000
6	-3.619483000	4.242073000	-0.349451000
6	-3.618278000	4.553344000	1.137305000
8	-2.267593000	4.100357000	-0.835473000
1	-1.622606000	3.330990000	-2.645826000
1	-3.707385000	1.600947000	-2.418793000
8	-3.985935000	3.535799000	-3.181014000
1	-4.971703000	3.488023000	-3.300251000
1	-4.176581000	2.147224000	-0.103690000
1	-4.092090000	5.090051000	-0.863123000
1	-4.649528000	4.725603000	1.458852000
1	-3.022503000	5.456411000	1.305518000
8	-5.746528000	3.223497000	-0.833009000
7	2.049193000	0.171125000	-1.980736000
6	1.515427000	0.995309000	-2.940921000

7	2.236736000	1.124360000	-4.095669000
7	0.345752000	1.605346000	-2.817417000
6	-0.237582000	1.383163000	-1.616609000
6	0.249878000	0.619069000	-0.556258000
6	1.528029000	-0.000024000	-0.679961000
8	2.183828000	-0.581509000	0.188127000
7	-0.585164000	0.702862000	0.540268000
6	-1.561661000	1.479953000	0.156855000
7	-1.416921000	1.932961000	-1.149615000
1	3.004977000	-0.184657000	-2.089658000
1	3.255003000	1.117375000	-4.000685000
1	1.898836000	1.873313000	-4.688064000
1	-2.374221000	1.803894000	0.783954000
15	-2.883002000	3.514170000	3.502250000
8	-3.731200000	4.580318000	4.121916000
8	-2.894300000	2.071137000	3.954193000
8	-6.185154000	1.063202000	-2.086183000
6	-3.694255000	-2.111455000	-2.918323000
6	-4.945179000	-2.952728000	-2.548812000
6	-6.081090000	-1.903115000	-2.531197000
6	-5.521478000	-0.823944000	-3.458008000
6	-6.178063000	0.534399000	-3.417374000
8	-4.144157000	-0.754336000	-3.067660000
1	-3.276073000	-2.481677000	-3.854728000
1	-4.820893000	-3.438969000	-1.578738000
8	-5.179255000	-3.924962000	-3.560509000
1	-6.144105000	-3.903860000	-3.713316000
1	-6.211691000	-1.487685000	-1.531938000
1	-5.603045000	-1.188397000	-4.495864000
1	-7.204231000	0.411445000	-3.785555000
1	-5.648256000	1.216817000	-4.089093000
8	-7.281889000	-2.480479000	-3.027716000
7	-2.625621000	-2.168240000	-1.941638000
6	-1.367530000	-2.740619000	-2.315111000
8	-1.170752000	-3.028504000	-3.503390000
7	-0.446227000	-2.945306000	-1.339586000
6	-0.699958000	-2.607276000	-0.069176000
7	0.239495000	-2.876838000	0.850257000

6	-1.949863000	-2.008781000	0.330661000
6	-2.871420000	-1.810510000	-0.639353000
1	1.139455000	-3.221155000	0.505598000
1	0.252115000	-2.381897000	1.743641000
1	-2.126490000	-1.702246000	1.352640000
1	-3.833642000	-1.347437000	-0.453698000
15	-6.827539000	2.579063000	-1.893986000
8	-6.693384000	3.303789000	-3.223826000
8	-8.147723000	2.527314000	-1.184041000
8	-8.103481000	-3.033239000	-0.660832000
6	-5.265730000	-3.005595000	1.833664000
6	-6.179055000	-3.702905000	2.856694000
6	-7.388171000	-4.099899000	1.997608000
6	-6.706574000	-4.456672000	0.664211000
6	-7.570014000	-4.352732000	-0.578794000
8	-5.607592000	-3.528611000	0.562392000
1	-4.218753000	-3.203865000	2.058520000
1	-6.441487000	-3.039714000	3.690413000
8	-5.498536000	-4.863578000	3.309272000
1	-6.189832000	-5.522640000	3.501903000
1	-8.061152000	-3.245098000	1.862232000
1	-6.315665000	-5.480097000	0.739138000
1	-8.379601000	-5.092417000	-0.517796000
1	-6.968777000	-4.588818000	-1.464252000
8	-8.049288000	-5.185668000	2.624609000
7	-5.420003000	-1.536779000	1.821744000
6	-4.524948000	-0.790881000	2.597254000
8	-3.602426000	-1.318222000	3.219691000
7	-4.755252000	0.561522000	2.608151000
6	-5.818381000	1.247125000	2.002434000
8	-5.972615000	2.451875000	2.198954000
6	-6.662290000	0.407994000	1.171010000
1	-7.446463000	0.870145000	0.585186000
6	-6.445539000	-0.925294000	1.126167000
1	-4.071120000	1.129559000	3.155217000
1	-7.052076000	-1.589609000	0.523349000
15	-8.686516000	-2.469647000	-2.111787000
8	-9.568810000	-3.496053000	-2.757140000

8	-9.110209000	-1.058860000	-1.837206000
1	4.812973000	-5.022560000	-3.917438000
1	-8.781029000	-5.480676000	2.059819000

Figure S23. X-Y coordinates for **1** at level: B3LYP-GD3/6-31G*.

8	3.478722000	7.114682000	-2.713727000
6	6.613295000	5.354294000	-1.631517000
6	6.903655000	5.095937000	-3.110942000
6	5.856592000	5.985933000	-3.812488000
6	5.866444000	7.232761000	-2.913351000
6	4.587935000	8.043337000	-2.932009000
8	6.082765000	6.703958000	-1.538226000
1	7.504003000	5.234009000	-1.017828000
1	6.901355000	4.040979000	-3.374819000
8	8.209587000	5.700914000	-3.415845000
1	8.021417000	6.210884000	-4.261628000
1	4.862350000	5.549277000	-3.885664000
1	6.712223000	7.865506000	-3.193210000
1	4.514366000	8.533074000	-3.910911000
1	4.635893000	8.810980000	-2.150836000
8	6.350389000	6.370948000	-5.134350000
7	5.573864000	4.406021000	-1.128762000
6	6.000608000	3.107072000	-0.766285000
8	7.223278000	2.824218000	-0.921399000
7	5.074947000	2.237285000	-0.276591000
6	3.770557000	2.590734000	-0.160549000
7	2.913800000	1.689712000	0.322678000
6	3.334695000	3.900304000	-0.549290000
6	4.259305000	4.774570000	-1.022390000
1	3.237710000	0.732857000	0.587505000
1	1.928803000	1.919493000	0.402733000
1	2.294594000	4.179859000	-0.475976000
1	4.001056000	5.763489000	-1.385240000
8	6.134488000	-7.544649000	2.837903000
6	8.267206000	-4.858625000	1.109938000
6	9.116811000	-4.913506000	2.393017000
6	8.657568000	-6.211507000	3.093793000
6	8.355587000	-7.130748000	1.889920000
6	7.283867000	-8.170500000	2.143848000
8	7.886158000	-6.231109000	0.803876000
1	8.829729000	-4.405439000	0.290585000
1	9.021769000	-4.012209000	3.000884000

8	10.507797000	-5.226676000	2.050351000
1	11.015682000	-4.385731000	1.908366000
1	7.747557000	-6.063466000	3.672963000
1	9.283117000	-7.621533000	1.578251000
1	7.676745000	-8.964847000	2.782388000
1	6.925664000	-8.572347000	1.193710000
8	9.695275000	-6.735162000	3.948709000
7	5.940943000	-0.382054000	0.272839000
6	7.247063000	-0.746291000	0.003025000
7	8.043668000	0.184238000	-0.553903000
7	7.733416000	-1.965686000	0.291808000
6	6.826854000	-2.780891000	0.868960000
6	5.489616000	-2.505293000	1.175343000
6	4.969919000	-1.221790000	0.852188000
8	3.792396000	-0.806081000	1.039324000
7	4.879057000	-3.624291000	1.765406000
6	5.825782000	-4.549201000	1.817537000
7	7.041752000	-4.080034000	1.288850000
1	5.622861000	0.605205000	0.044438000
1	7.742022000	1.167830000	-0.707185000
1	9.008900000	-0.078544000	-0.718973000
1	5.741587000	-5.553649000	2.201551000
8	6.454392000	3.990640000	-6.024769000
6	7.584642000	0.782686000	-4.299616000
6	7.864565000	0.154869000	-5.667459000
6	7.687792000	1.355330000	-6.624365000
6	8.342643000	2.479600000	-5.811328000
6	7.920565000	3.891399000	-6.125669000
8	7.967676000	2.186222000	-4.400610000
1	8.136246000	0.285254000	-3.500553000
1	7.232567000	-0.706209000	-5.876247000
8	9.287152000	-0.198933000	-5.716234000
1	9.570351000	0.161837000	-6.610886000
1	6.652446000	1.573882000	-6.878348000
1	9.427733000	2.395853000	-5.921152000
1	8.242913000	4.168411000	-7.133075000
1	8.381763000	4.552217000	-5.387651000
8	8.489470000	1.128632000	-7.827292000

7	3.998576000	-2.199871000	-2.347475000
6	5.320194000	-2.476714000	-2.642790000
7	5.769119000	-3.717656000	-2.401125000
7	6.150446000	-1.559015000	-3.163830000
6	5.546616000	-0.381040000	-3.410812000
6	4.213926000	-0.014946000	-3.189726000
6	3.347787000	-0.969258000	-2.575865000
8	2.140234000	-0.822145000	-2.237289000
7	3.996445000	1.300086000	-3.638216000
6	5.167252000	1.709992000	-4.109372000
7	6.153149000	0.715876000	-3.978910000
1	3.404442000	-2.953571000	-1.894115000
1	5.141007000	-4.497559000	-2.118910000
1	6.742532000	-3.899234000	-2.617653000
1	5.393681000	2.646743000	-4.590394000
15	5.780148000	5.452826000	-6.427107000
8	6.460511000	6.009367000	-7.636299000
8	4.303608000	5.282654000	-6.263684000
8	0.503155000	-8.297718000	2.392480000
6	2.955813000	-7.754412000	-0.360757000
6	4.088800000	-7.933546000	0.646766000
6	3.357110000	-8.486802000	1.894758000
6	2.303750000	-9.406548000	1.258379000
6	1.018440000	-9.618410000	2.035307000
8	1.936203000	-8.726518000	-0.016135000
1	3.305437000	-7.892126000	-1.381122000
1	4.648427000	-7.016611000	0.811385000
8	4.945538000	-9.016848000	0.159397000
1	5.072386000	-9.580577000	0.982870000
1	2.914955000	-7.718377000	2.525407000
1	2.767306000	-10.370449000	1.032258000
1	1.218736000	-10.220237000	2.927478000
1	0.320509000	-10.134756000	1.375232000
8	4.294537000	-9.309052000	2.663172000
7	2.376642000	-6.386558000	-0.270107000
6	3.013287000	-5.390459000	-1.038622000
8	4.069520000	-5.718603000	-1.654929000
7	2.462225000	-4.151606000	-1.071675000

6	1.331489000	-3.860009000	-0.380726000
7	0.824771000	-2.633262000	-0.526810000
6	0.727972000	-4.847865000	0.467376000
6	1.277454000	-6.090590000	0.489090000
1	1.279346000	-1.954755000	-1.173429000
1	-0.024320000	-2.368100000	-0.039534000
1	-0.141632000	-4.662139000	1.079069000
1	0.880444000	-6.875830000	1.117842000
15	5.199577000	-8.497764000	3.829941000
8	6.055571000	-9.546016000	4.467071000
8	4.288387000	-7.562757000	4.558788000
8	7.536101000	-1.154818000	-8.468727000
6	6.718870000	-4.563101000	-6.836334000
6	6.739261000	-5.167846000	-8.240553000
6	7.292326000	-4.008094000	-9.097956000
6	8.370787000	-3.437810000	-8.164435000
6	8.749090000	-1.989149000	-8.358431000
8	7.800702000	-3.585045000	-6.795411000
1	6.842131000	-5.327201000	-6.067963000
1	5.785981000	-5.583657000	-8.561179000
8	7.788949000	-6.198403000	-8.246774000
1	8.285489000	-5.996006000	-9.097447000
1	6.552306000	-3.262970000	-9.381853000
1	9.268242000	-4.057221000	-8.247369000
1	9.342115000	-1.867729000	-9.267564000
1	9.315335000	-1.665734000	-7.481922000
8	7.938276000	-4.565561000	-10.287562000
7	2.028849000	-4.626295000	-4.614112000
6	2.953781000	-5.610484000	-4.729584000
7	4.143874000	-5.525072000	-5.347476000
6	4.357522000	-4.300221000	-5.883954000
6	3.475045000	-3.212870000	-5.836923000
6	2.256403000	-3.390597000	-5.149715000
7	1.345568000	-2.427325000	-4.995111000
7	4.017516000	-2.102065000	-6.485674000
6	5.209375000	-2.505408000	-6.913485000
7	5.464523000	-3.840881000	-6.576007000
1	2.666851000	-6.547810000	-4.270294000

1	1.535148000	-1.507465000	-5.378148000
1	0.492629000	-2.590662000	-4.424867000
1	5.936180000	-1.914500000	-7.450003000
15	7.718179000	0.368491000	-9.116040000
8	8.736105000	0.319956000	-10.210594000
8	6.339413000	0.932792000	-9.237007000
8	-4.570296000	-6.501646000	0.091542000
6	-1.846759000	-8.239902000	-1.890741000
6	-1.160462000	-8.606608000	-0.582043000
6	-2.196104000	-8.138783000	0.454542000
6	-3.497873000	-8.643277000	-0.191978000
6	-4.785678000	-7.942970000	0.191538000
8	-3.273802000	-8.403975000	-1.653631000
1	-1.511973000	-8.850966000	-2.727339000
1	-0.161035000	-8.195486000	-0.486662000
8	-1.119340000	-10.074077000	-0.485903000
1	-1.417343000	-10.247921000	0.454639000
1	-2.205895000	-7.064207000	0.613826000
1	-3.601488000	-9.717243000	-0.019125000
1	-5.073283000	-8.226956000	1.208847000
1	-5.550675000	-8.258205000	-0.518815000
8	-1.937645000	-8.825354000	1.721357000
7	-1.581845000	-6.809523000	-2.223715000
6	-0.398447000	-6.514001000	-2.917956000
8	0.453040000	-7.392049000	-3.165511000
7	-0.268275000	-5.191313000	-3.276578000
6	-1.150225000	-4.141229000	-3.002596000
8	-0.907658000	-2.978386000	-3.423706000
6	-2.296071000	-4.523103000	-2.214801000
1	-3.035571000	-3.807021000	-1.890562000
6	-2.468059000	-5.820821000	-1.871073000
1	0.633497000	-4.956279000	-3.810021000
1	-3.310147000	-6.124151000	-1.264109000
15	-1.052822000	-7.952472000	2.854361000
8	-1.360276000	-8.560215000	4.183612000
8	-1.200541000	-6.490970000	2.532087000
8	5.895129000	-5.859437000	-11.104681000
6	3.248110000	-7.885819000	-9.337137000

6	2.854159000	-8.429473000	-10.723569000
6	4.048722000	-8.019182000	-11.617975000
6	5.235793000	-8.144317000	-10.657476000
6	6.404743000	-7.235632000	-10.951354000
8	4.701146000	-7.765340000	-9.323678000
1	2.891024000	-8.551001000	-8.549842000
1	1.894258000	-8.036405000	-11.054539000
8	2.851435000	-9.888635000	-10.661649000
1	3.385878000	-10.142402000	-11.476518000
1	3.967004000	-7.019356000	-12.038293000
1	5.565085000	-9.187898000	-10.640688000
1	6.915286000	-7.542110000	-11.867555000
1	7.084773000	-7.272538000	-10.098171000
8	4.214917000	-9.009439000	-12.686359000
7	-0.599284000	-5.436029000	-7.080493000
6	-0.194845000	-6.751719000	-6.938398000
7	-0.951565000	-7.547742000	-6.167445000
7	0.899886000	-7.245599000	-7.546127000
6	1.543778000	-6.337455000	-8.305637000
6	1.222552000	-4.993367000	-8.494195000
6	0.075848000	-4.463053000	-7.838973000
8	-0.354393000	-3.280411000	-7.904929000
7	2.123033000	-4.392775000	-9.387930000
6	2.978862000	-5.354580000	-9.722871000
7	2.659240000	-6.568332000	-9.092239000
1	-1.503480000	-5.121389000	-6.616943000
1	-1.865202000	-7.249397000	-5.767591000
1	-0.633162000	-8.501351000	-6.038931000
1	3.853611000	-5.265768000	-10.348518000
15	6.957006000	-4.705615000	-11.649978000
8	7.833503000	-5.290466000	-12.710679000
8	6.153523000	-3.450781000	-11.779429000
8	-8.056363000	-3.296513000	-3.560505000
6	-6.044694000	-6.381276000	-4.605104000
6	-5.747048000	-6.683208000	-3.141431000
6	-6.596938000	-5.613159000	-2.433532000
6	-7.899895000	-5.704045000	-3.246262000
6	-8.817569000	-4.504859000	-3.227169000

8	-7.422354000	-5.918291000	-4.647585000
1	-5.898564000	-7.244385000	-5.252094000
1	-4.685393000	-6.687911000	-2.916320000
8	-6.362773000	-7.976207000	-2.822343000
1	-6.804857000	-7.808257000	-1.939900000
1	-6.156791000	-4.620134000	-2.460046000
1	-8.459075000	-6.586712000	-2.926586000
1	-9.265412000	-4.394737000	-2.236795000
1	-9.617937000	-4.659046000	-3.960140000
8	-6.827420000	-6.023938000	-1.049886000
7	-5.159584000	-5.274234000	-5.089035000
6	-3.831511000	-5.596456000	-5.448742000
8	-3.439593000	-6.780603000	-5.237325000
7	-3.057461000	-4.624409000	-6.009846000
6	-3.530709000	-3.363242000	-6.190502000
7	-2.765982000	-2.462734000	-6.807628000
6	-4.843270000	-3.014497000	-5.725912000
6	-5.625402000	-3.991854000	-5.204119000
1	-1.851124000	-2.739343000	-7.220954000
1	-3.175649000	-1.566876000	-7.081110000
1	-5.201646000	-2.001841000	-5.816824000
1	-6.620962000	-3.804431000	-4.822174000
15	-5.782696000	-5.367673000	0.092901000
8	-6.517767000	-5.386876000	1.393179000
8	-5.142966000	-4.147538000	-0.507443000
8	1.859172000	-8.770370000	-13.600705000
6	-1.913271000	-8.384292000	-13.127313000
6	-1.988399000	-8.587973000	-14.644306000
6	-0.583374000	-9.120621000	-14.991984000
6	-0.244996000	-9.989332000	-13.772656000
6	1.237334000	-10.104253000	-13.478757000
8	-0.913079000	-9.317396000	-12.627203000
1	-2.885438000	-8.548420000	-12.666316000
1	-2.284122000	-7.686995000	-15.177993000
8	-2.923494000	-9.689610000	-14.898326000
1	-2.403222000	-10.276229000	-15.528520000
1	0.158469000	-8.341675000	-15.146969000
1	-0.676729000	-10.985296000	-13.907263000

1	1.710052000	-10.768583000	-14.205790000
1	1.400137000	-10.462535000	-12.459011000
8	-0.666316000	-9.985763000	-16.170785000
7	-1.478599000	-7.011489000	-12.749032000
6	-2.474101000	-6.069674000	-12.399356000
8	-3.679432000	-6.378220000	-12.627746000
7	-2.087636000	-4.904303000	-11.806269000
6	-0.776369000	-4.630300000	-11.584707000
7	-0.445895000	-3.544084000	-10.887338000
6	0.238185000	-5.532538000	-12.054003000
6	-0.148081000	-6.714476000	-12.591881000
1	-1.181621000	-2.956515000	-10.449983000
1	0.517875000	-3.443136000	-10.556782000
1	1.281059000	-5.296487000	-11.918556000
1	0.567178000	-7.464379000	-12.909273000
15	3.431397000	-8.663232000	-14.135412000
8	3.726958000	-9.816027000	-15.040935000
8	3.659229000	-7.222035000	-14.458958000
8	-8.196881000	1.576840000	-6.283471000
6	-8.325021000	-1.627622000	-8.374148000
6	-8.525703000	-2.383333000	-7.050410000
6	-8.776507000	-1.245795000	-6.044658000
6	-9.629411000	-0.286514000	-6.886140000
6	-9.604144000	1.153843000	-6.438508000
8	-9.044016000	-0.364663000	-8.250506000
1	-8.685056000	-2.219569000	-9.216288000
1	-7.670636000	-3.019736000	-6.809947000
8	-9.772271000	-3.125911000	-7.162105000
1	-10.160585000	-3.052234000	-6.238318000
1	-7.877894000	-0.757992000	-5.675701000
1	-10.656656000	-0.660762000	-6.899371000
1	-10.124969000	1.239656000	-5.481010000
1	-10.101769000	1.772033000	-7.189039000
8	-9.569603000	-1.754477000	-4.928034000
7	-4.127095000	-3.339741000	-10.664390000
6	-5.441632000	-3.753377000	-10.807822000
7	-5.678532000	-4.807662000	-11.601147000
7	-6.465918000	-3.143969000	-10.183176000

6	-6.079776000	-2.118105000	-9.402396000
6	-4.788691000	-1.630863000	-9.194279000
6	-3.704181000	-2.260522000	-9.866621000
8	-2.479431000	-1.955507000	-9.793188000
7	-4.808442000	-0.576201000	-8.267356000
6	-6.087633000	-0.419357000	-7.939411000
7	-6.906754000	-1.345228000	-8.607598000
1	-3.359415000	-3.895545000	-11.148391000
1	-4.920843000	-5.379569000	-12.032680000
1	-6.644010000	-5.107687000	-11.681821000
1	-6.505024000	0.330048000	-7.286550000
15	-8.832657000	-1.832736000	-3.420263000
8	-9.943226000	-1.974207000	-2.429260000
8	-7.757731000	-0.792872000	-3.374389000
8	-1.614286000	-8.229275000	-17.742367000
6	-4.352212000	-5.567380000	-17.655388000
6	-4.106530000	-5.475381000	-19.170365000
6	-3.300648000	-6.751658000	-19.498540000
6	-3.880695000	-7.769703000	-18.495129000
6	-2.923844000	-8.850401000	-18.037283000
8	-4.232265000	-6.972772000	-17.292396000
1	-5.335233000	-5.163153000	-17.418999000
1	-3.597064000	-4.549126000	-19.453532000
8	-5.408729000	-5.629913000	-19.799849000
1	-5.199297000	-6.202279000	-20.601456000
1	-2.228042000	-6.634261000	-19.342802000
1	-4.788435000	-8.208196000	-18.921086000
1	-2.785308000	-9.615526000	-18.804896000
1	-3.315425000	-9.294589000	-17.119033000
8	-3.635650000	-7.060702000	-20.884172000
7	-3.381214000	-4.808753000	-16.840565000
6	-3.841054000	-3.637472000	-16.203456000
8	-4.983529000	-3.179857000	-16.401675000
7	-2.934084000	-3.062705000	-15.344570000
6	-1.650730000	-3.513352000	-15.044862000
8	-0.932843000	-2.900815000	-14.211757000
6	-1.259107000	-4.716895000	-15.743239000
1	-0.285773000	-5.136957000	-15.546438000

6	-2.131451000	-5.328719000	-16.576973000
1	-3.307312000	-2.211443000	-14.803003000
1	-1.901729000	-6.278011000	-17.048544000
15	-0.298197000	-9.244284000	-17.633194000
8	-0.411949000	-10.314331000	-18.670922000
8	0.890389000	-8.360756000	-17.422576000
8	-4.924287000	4.244627000	-8.579023000
6	-6.898155000	2.595167000	-11.554581000
6	-7.876867000	2.164520000	-10.443490000
6	-7.370325000	2.990473000	-9.268858000
6	-7.031275000	4.339908000	-9.912429000
6	-5.947977000	5.111153000	-9.146629000
8	-6.537687000	3.982795000	-11.268102000
1	-7.352861000	2.498741000	-12.541188000
1	-7.878015000	1.089736000	-10.243682000
8	-9.187620000	2.671914000	-10.827890000
1	-9.624406000	2.901278000	-9.957974000
1	-6.471233000	2.548738000	-8.851357000
1	-7.943930000	4.933873000	-10.008087000
1	-6.447401000	5.692777000	-8.360140000
1	-5.461987000	5.805715000	-9.836609000
8	-8.392543000	3.164463000	-8.245873000
7	-3.959164000	-0.994065000	-13.905848000
6	-5.225859000	-0.588852000	-14.174292000
7	-5.946744000	0.311606000	-13.484366000
6	-5.256147000	0.838172000	-12.443976000
6	-3.945267000	0.505254000	-12.076958000
6	-3.282800000	-0.484112000	-12.833128000
7	-2.053673000	-0.925202000	-12.546842000
7	-3.520419000	1.276341000	-10.993578000
6	-4.550811000	2.061397000	-10.703916000
7	-5.650561000	1.816639000	-11.545037000
1	-5.679557000	-1.079729000	-15.026896000
1	-1.689396000	-0.736966000	-11.616970000
1	-1.603938000	-1.651452000	-13.134601000
1	-4.577564000	2.833234000	-9.940458000
15	-7.865795000	3.142141000	-6.663947000
8	-8.719462000	4.087849000	-5.889230000

8	-6.353008000	3.227126000	-6.681120000
1	10.526877000	-6.429062000	3.470291000
1	2.629692000	7.629254000	-2.683007000
1	-3.274350000	-7.951673000	-21.130160000
1	-5.373628000	3.821314000	-7.743524000

Figure S24. X-Y coordinates for **1:2** at level: B3LYP/3-21G*.

8	6.507218000	-6.275105000	2.337350000
6	5.073274000	-3.071945000	3.445802000
6	6.138414000	-3.079055000	4.552987000
6	7.176133000	-4.121279000	4.083802000
6	7.130018000	-3.965162000	2.545893000
6	7.409946000	-5.243677000	1.783876000
8	5.740606000	-3.527336000	2.225709000
1	4.668227000	-2.068616000	3.310706000
1	5.718194000	-3.274687000	5.538982000
8	6.900888000	-1.825960000	4.499853000
1	6.496790000	-1.169451000	5.126024000
1	6.882917000	-5.131442000	4.361599000
1	7.833726000	-3.184804000	2.244561000
1	8.450972000	-5.544802000	1.927300000
1	7.194027000	-5.108516000	0.721742000
8	8.482716000	-3.822888000	4.628160000
7	0.106766000	-3.166134000	4.494457000
6	0.959750000	-2.084422000	4.401010000
7	0.445819000	-0.851196000	4.557870000
7	2.268570000	-2.227053000	4.163334000
6	2.657436000	-3.513490000	4.019607000
6	1.870438000	-4.661997000	4.099252000
6	0.470473000	-4.535206000	4.327804000
8	-0.408089000	-5.421898000	4.373813000
7	2.651440000	-5.803723000	3.856964000
6	3.878870000	-5.349907000	3.640169000
7	3.937735000	-3.950255000	3.731777000
1	-0.888463000	-3.004125000	4.642434000
1	-0.540787000	-0.683649000	4.716559000
1	1.068184000	-0.054965000	4.476590000
1	4.741353000	-5.932493000	3.367046000
8	2.098030000	-8.521860000	0.582462000
6	3.407374000	-5.369338000	-1.043156000
6	4.659397000	-5.610532000	-0.186469000
6	4.536225000	-7.092608000	0.234709000
6	3.807698000	-7.747695000	-0.947870000
6	2.933344000	-8.928452000	-0.566707000

8	2.954315000	-6.676231000	-1.525413000
1	3.643569000	-4.701430000	-1.869356000
1	4.732733000	-4.917306000	0.649695000
8	5.840454000	-5.496114000	-1.052644000
1	6.339637000	-6.349324000	-0.867075000
1	3.984801000	-7.228835000	1.161759000
1	4.545515000	-8.066494000	-1.689278000
1	3.579322000	-9.761262000	-0.275119000
1	2.310039000	-9.219420000	-1.412343000
8	5.878081000	-7.692057000	0.316177000
7	2.304252000	-4.747666000	-0.281455000
6	2.186546000	-3.325466000	-0.323575000
8	3.086360000	-2.670203000	-0.906209000
7	1.085851000	-2.762343000	0.260670000
6	0.156108000	-3.527676000	0.857740000
7	-0.940160000	-2.936713000	1.375683000
6	0.299430000	-4.952673000	0.963667000
6	1.383471000	-5.515902000	0.373378000
1	-1.051053000	-1.936896000	1.226352000
1	-1.780258000	-3.520750000	1.549784000
1	-0.412910000	-5.563374000	1.492973000
1	1.569195000	-6.577888000	0.399220000
15	6.566097000	-7.834754000	1.829413000
8	7.983464000	-8.259131000	1.591154000
8	5.612050000	-8.567344000	2.725307000
8	-2.409507000	-6.255866000	-0.685393000
6	-1.164781000	-7.979547000	-3.669649000
6	0.061653000	-8.233351000	-2.753368000
6	-0.525680000	-8.259176000	-1.320311000
6	-2.035573000	-8.480162000	-1.478883000
6	-2.835780000	-7.658822000	-0.483851000
8	-2.374818000	-8.050162000	-2.854429000
1	-1.164694000	-8.720962000	-4.466877000
1	0.810452000	-7.447631000	-2.856692000
8	0.666582000	-9.528094000	-3.053367000
1	0.524010000	-10.048930000	-2.204003000
1	-0.336096000	-7.329707000	-0.794375000
1	-2.256023000	-9.543472000	-1.354387000

1	-2.558534000	-7.980319000	0.522917000
1	-3.904392000	-7.767828000	-0.657258000
8	0.033701000	-9.415053000	-0.608435000
7	-1.147908000	-6.650903000	-4.317859000
6	-0.672406000	-6.594989000	-5.632758000
8	-0.254447000	-7.599582000	-6.236371000
7	-0.711701000	-5.331077000	-6.189487000
6	-1.189266000	-4.141581000	-5.598967000
8	-1.153737000	-3.073442000	-6.244316000
6	-1.680573000	-4.318091000	-4.254064000
1	-2.125804000	-3.472902000	-3.750692000
6	-1.637556000	-5.536861000	-3.668992000
1	-0.363345000	-5.255973000	-7.144204000
1	-1.991279000	-5.701780000	-2.662579000
15	0.629974000	-9.184272000	0.924323000
8	0.773689000	-10.547219000	1.528586000
8	-0.172796000	-8.090218000	1.579170000
8	-5.828476000	-2.681318000	-2.936634000
6	-6.831640000	-6.369494000	-3.313301000
6	-5.616479000	-6.617458000	-2.401342000
6	-5.345612000	-5.231062000	-1.794130000
6	-6.732541000	-4.588762000	-1.690567000
6	-6.717469000	-3.076252000	-1.822287000
8	-7.509944000	-5.176445000	-2.810880000
1	-7.488211000	-7.237718000	-3.301219000
1	-4.761232000	-7.033336000	-2.935042000
8	-6.028684000	-7.514665000	-1.314122000
1	-5.782177000	-7.013873000	-0.481991000
1	-4.685501000	-4.626103000	-2.406348000
1	-7.200661000	-4.864479000	-0.741602000
1	-6.338122000	-2.626834000	-0.904728000
1	-7.728583000	-2.713453000	-2.023415000
8	-4.802630000	-5.377262000	-0.432664000
7	-6.462884000	-6.122493000	-4.724111000
6	-6.471507000	-7.240946000	-5.614245000
8	-6.675275000	-8.382001000	-5.130052000
7	-6.271090000	-6.999531000	-6.944703000
6	-6.065080000	-5.748151000	-7.393642000

7	-5.898975000	-5.554357000	-8.714557000
6	-6.024337000	-4.622793000	-6.501804000
6	-6.239760000	-4.853558000	-5.183105000
1	-5.951137000	-6.357003000	-9.334885000
1	-5.823743000	-4.606117000	-9.108632000
1	-5.853852000	-3.626535000	-6.872649000
1	-6.232355000	-4.061360000	-4.447847000
15	-3.226525000	-4.927517000	-0.194683000
8	-3.071313000	-4.722317000	1.295936000
8	-2.871034000	-3.841573000	-1.172495000
8	-3.115358000	-0.638311000	-6.757093000
6	-6.831293000	0.104259000	-7.097915000
6	-7.000816000	-0.410194000	-5.657702000
6	-5.555584000	-0.495009000	-5.150400000
6	-4.897037000	0.712793000	-5.827927000
6	-3.398358000	0.594853000	-5.988565000
8	-5.537386000	0.780303000	-7.168482000
1	-7.650666000	0.777749000	-7.350252000
1	-7.537539000	-1.361244000	-5.620093000
8	-7.664737000	0.648510000	-4.909053000
1	-7.234905000	0.597787000	-4.003899000
1	-5.055394000	-1.416479000	-5.438049000
1	-5.141982000	1.607606000	-5.250481000
1	-2.951795000	0.499025000	-4.997110000
1	-3.003015000	1.468691000	-6.507615000
8	-5.547238000	-0.287086000	-3.699039000
7	-9.742304000	-2.435482000	-10.373749000
6	-10.083436000	-1.420024000	-9.500372000
7	-11.355215000	-0.987955000	-9.490853000
7	-9.186787000	-0.860983000	-8.678954000
6	-7.951828000	-1.393954000	-8.780123000
6	-7.525674000	-2.432625000	-9.609066000
6	-8.450343000	-3.007566000	-10.524205000
8	-8.255187000	-3.870678000	-11.416287000
7	-6.154300000	-2.668117000	-9.413511000
6	-5.768091000	-1.782789000	-8.495188000
7	-6.834691000	-0.984599000	-8.080096000
1	-10.445057000	-2.790922000	-11.021267000

1	-12.074033000	-1.390570000	-10.081314000
1	-11.608758000	-0.241151000	-8.853503000
1	-4.769950000	-1.659888000	-8.116231000
15	-4.780878000	-1.419209000	-2.754490000
8	-4.831480000	-0.909008000	-1.346338000
8	-3.500317000	-1.783396000	-3.455363000
8	-2.299049000	-1.911002000	-11.393341000
6	-4.461193000	1.347986000	-11.941993000
6	-4.306141000	1.507169000	-10.416009000
6	-3.250107000	0.454371000	-10.105840000
6	-2.276381000	0.582909000	-11.287654000
6	-1.503605000	-0.703143000	-11.596769000
8	-3.157461000	0.915774000	-12.441731000
1	-4.772296000	2.283656000	-12.406423000
1	-5.237176000	1.356551000	-9.865034000
8	-3.724596000	2.827217000	-10.196075000
1	-3.155387000	2.718200000	-9.381977000
1	-3.690395000	-0.535793000	-10.098581000
1	-1.591728000	1.415396000	-11.109453000
1	-0.608856000	-0.716590000	-10.962136000
1	-1.188203000	-0.677462000	-12.642718000
8	-2.583127000	0.727119000	-8.836672000
7	-9.268412000	0.266812000	-13.627845000
6	-8.652545000	1.449625000	-13.406206000
7	-7.400999000	1.651721000	-12.939835000
6	-6.736994000	0.494684000	-12.736564000
6	-7.246741000	-0.793333000	-12.959845000
6	-8.587897000	-0.891045000	-13.386485000
7	-9.210673000	-2.073857000	-13.561425000
7	-6.263679000	-1.758537000	-12.699894000
6	-5.192425000	-1.068540000	-12.321042000
7	-5.435332000	0.309126000	-12.301958000
1	-9.235421000	2.337933000	-13.618489000
1	-8.826531000	-2.915102000	-13.122983000
1	-10.190522000	-2.066662000	-13.829960000
1	-4.223160000	-1.475433000	-12.060724000
15	-2.033075000	-0.588367000	-7.979654000
8	-0.650944000	-0.260422000	-7.511557000

8	-2.336343000	-1.833149000	-8.796716000
1	8.432709000	-2.820374000	4.726588000
1	-2.334692000	-2.021606000	-10.364256000

Figure S25. X-Y coordinates for **2** at level: B3LYP/3-21G*.

8	-8.700397000	-2.907980000	-1.823322000
6	-7.585292000	-3.258358000	1.592544000
6	-8.908318000	-3.980731000	1.892266000
6	-9.467096000	-4.311303000	0.494431000
6	-8.175076000	-4.640110000	-0.289055000
6	-8.263217000	-4.306312000	-1.764437000
8	-7.116407000	-3.786897000	0.319786000
1	-6.849790000	-3.437002000	2.379174000
1	-9.577104000	-3.391004000	2.521943000
8	-8.633625000	-5.315845000	2.430676000
1	-8.549885000	-5.267706000	3.418265000
1	-9.955548000	-3.449918000	0.042509000
1	-7.924396000	-5.692517000	-0.133880000
1	-8.997546000	-4.956944000	-2.250289000
1	-7.284160000	-4.413943000	-2.240446000
8	-10.381525000	-5.426128000	0.540745000
7	-7.085714000	1.029779000	4.208601000
6	-6.781931000	-0.267475000	4.566537000
7	-6.267937000	-0.488002000	5.794751000
7	-6.999633000	-1.300653000	3.754710000
6	-7.488417000	-0.942867000	2.545963000
6	-7.794938000	0.334717000	2.077642000
6	-7.568869000	1.459561000	2.925742000
8	-7.726558000	2.674108000	2.708582000
7	-8.256869000	0.266540000	0.754721000
6	-8.239737000	-1.020943000	0.435063000
7	-7.772320000	-1.808007000	1.507830000
1	-6.874410000	1.792507000	4.849086000
1	-6.041987000	0.258370000	6.439483000
1	-6.033971000	-1.440100000	6.048955000
1	-8.526066000	-1.463266000	-0.502778000
8	-6.315753000	1.509323000	-2.483479000
6	-4.345380000	-1.601594000	-1.773787000
6	-5.659451000	-2.333438000	-2.056812000
6	-6.505260000	-1.269367000	-2.780972000
6	-5.468954000	-0.463449000	-3.567872000
6	-5.877443000	0.980926000	-3.785402000

8	-4.236312000	-0.504492000	-2.741777000
1	-3.501260000	-2.284268000	-1.848953000
1	-6.113753000	-2.709150000	-1.143147000
8	-5.416409000	-3.420474000	-3.013410000
1	-6.123198000	-3.256071000	-3.711054000
1	-7.058899000	-0.621706000	-2.106130000
1	-5.287095000	-0.955000000	-4.528556000
1	-6.709983000	0.999798000	-4.497194000
1	-5.034081000	1.548455000	-4.179897000
8	-7.393583000	-1.923591000	-3.750254000
7	-4.354055000	-1.038567000	-0.412407000
6	-3.899439000	-1.888784000	0.646917000
8	-3.550040000	-3.056582000	0.353201000
7	-3.868137000	-1.354867000	1.907235000
6	-4.249956000	-0.087291000	2.122290000
7	-4.173715000	0.414058000	3.374914000
6	-4.767836000	0.749940000	1.076867000
6	-4.811155000	0.228584000	-0.170511000
1	-3.745426000	-0.174363000	4.082846000
1	-4.099049000	1.445658000	3.454815000
1	-5.103921000	1.756845000	1.249390000
1	-5.225515000	0.765118000	-1.007019000
15	-8.980188000	-2.109386000	-3.240424000
8	-9.635494000	-3.016417000	-4.231009000
8	-9.489490000	-0.770862000	-2.804416000
8	-2.689219000	3.100788000	0.477571000
6	-1.256475000	2.911337000	-2.835632000
6	-2.658795000	2.335995000	-3.145884000
6	-3.595150000	3.018915000	-2.121075000
6	-2.843336000	4.247453000	-1.597447000
6	-3.046833000	4.405432000	-0.100089000
8	-1.414582000	4.020348000	-1.889552000
1	-0.792016000	3.241225000	-3.763500000
1	-2.694820000	1.251044000	-3.037866000
8	-3.072991000	2.717184000	-4.495128000
1	-3.883622000	3.290724000	-4.319036000
1	-3.837586000	2.357608000	-1.297208000
1	-3.197687000	5.134224000	-2.130802000

1	-4.109552000	4.595288000	0.071091000
1	-2.405119000	5.194482000	0.295079000
8	-4.794163000	3.489104000	-2.821702000
7	-0.335549000	1.943064000	-2.225443000
6	0.807351000	1.585203000	-2.956709000
8	1.010975000	1.959940000	-4.122674000
7	1.684150000	0.782505000	-2.249168000
6	1.588338000	0.369109000	-0.900254000
8	2.547211000	-0.239976000	-0.384464000
6	0.359493000	0.759801000	-0.253274000
1	0.210426000	0.478992000	0.781541000
6	-0.523075000	1.540256000	-0.911740000
1	2.595239000	0.647166000	-2.692096000
1	-1.397430000	1.941856000	-0.418998000
15	-6.250339000	3.115384000	-2.088786000
8	-7.302908000	3.897496000	-2.803885000
8	-6.025832000	3.162131000	-0.603379000
8	1.675270000	1.926368000	2.880104000
6	1.802195000	5.163371000	0.797878000
6	0.289455000	4.924555000	0.688363000
6	0.041418000	3.900163000	1.802070000
6	1.037800000	4.290776000	2.891396000
6	1.478202000	3.112773000	3.737925000
8	2.196378000	4.871731000	2.168688000
1	2.049983000	6.187772000	0.522653000
1	-0.016072000	4.588693000	-0.301213000
8	-0.413027000	6.159207000	1.060829000
1	-1.057905000	5.846918000	1.763545000
1	0.211229000	2.876270000	1.485167000
1	0.596448000	5.061931000	3.529922000
1	0.707324000	2.881347000	4.474385000
1	2.414312000	3.358290000	4.250395000
8	-1.309940000	4.078380000	2.356900000
7	2.550355000	4.246356000	-0.097979000
6	2.587395000	4.602635000	-1.486421000
8	1.968385000	5.632057000	-1.835937000
7	3.286400000	3.777608000	-2.329624000
6	3.915420000	2.694774000	-1.855389000

7	4.500211000	1.850568000	-2.742312000
6	3.931348000	2.365366000	-0.460077000
6	3.208082000	3.149772000	0.378084000
1	4.502078000	2.121017000	-3.721037000
1	5.020812000	1.015140000	-2.424533000
1	4.395203000	1.462990000	-0.111899000
1	3.060468000	2.906684000	1.418496000
15	-2.357616000	2.818578000	2.057826000
8	-3.572025000	3.065086000	2.921482000
8	-1.584570000	1.536700000	2.081219000
8	3.340347000	-2.738877000	0.790588000
6	6.050449000	-0.603738000	2.317650000
6	5.031482000	0.357926000	2.938429000
6	3.702090000	-0.393792000	2.761869000
6	4.113749000	-1.862544000	2.959760000
6	3.173869000	-2.828946000	2.254117000
8	5.516216000	-1.954703000	2.466749000
1	7.020476000	-0.515434000	2.806213000
1	5.050761000	1.338662000	2.450577000
8	5.312603000	0.415239000	4.360349000
1	4.387311000	0.412852000	4.759702000
1	3.215106000	-0.239427000	1.796783000
1	4.102411000	-2.054029000	4.035563000
1	2.160822000	-2.483782000	2.484176000
1	3.320288000	-3.858665000	2.588542000
8	2.840415000	-0.039288000	3.895683000
7	9.036408000	1.809258000	-0.974794000
6	9.217895000	1.593444000	0.378296000
7	10.336868000	2.093685000	0.945012000
7	8.332846000	0.921365000	1.114704000
6	7.299241000	0.431264000	0.393650000
6	7.092670000	0.507904000	-0.981594000
6	8.008302000	1.237540000	-1.791586000
8	8.023353000	1.417088000	-3.025089000
7	5.929066000	-0.192127000	-1.331299000
6	5.436597000	-0.680376000	-0.193221000
7	6.244798000	-0.314950000	0.891249000
1	9.730403000	2.342387000	-1.494885000

1	11.152369000	2.305813000	0.378060000
1	10.476737000	1.924605000	1.935212000
1	4.530431000	-1.245327000	-0.070129000
15	1.281401000	0.448038000	3.525094000
8	0.565689000	0.638444000	4.825696000
8	0.819177000	-0.478722000	2.435864000
8	6.350407000	-4.504650000	-2.640326000
6	8.988309000	-3.691312000	0.156640000
6	7.726673000	-3.230733000	0.919305000
6	6.619800000	-3.875524000	0.084895000
6	7.221970000	-5.193944000	-0.403560000
6	6.630147000	-5.628383000	-1.753632000
8	8.674327000	-4.928378000	-0.541557000
1	9.842037000	-3.801727000	0.826968000
1	7.674586000	-2.144438000	0.885511000
8	7.720968000	-3.742494000	2.270198000
1	6.837773000	-3.406673000	2.615217000
1	6.404430000	-3.237698000	-0.766296000
1	7.065835000	-5.957438000	0.363714000
1	5.715360000	-6.199638000	-1.543066000
1	7.346636000	-6.285846000	-2.252791000
8	5.414851000	-4.171882000	0.833510000
7	11.988633000	0.352320000	-1.133366000
6	12.010486000	-0.463284000	-0.048521000
7	11.188134000	-1.498403000	0.214549000
6	10.310086000	-1.724070000	-0.785533000
6	10.224462000	-1.000213000	-1.986092000
6	11.082802000	0.108256000	-2.119928000
7	10.990809000	0.963496000	-3.162981000
7	9.221219000	-1.531582000	-2.808130000
6	8.709964000	-2.548746000	-2.118097000
7	9.332796000	-2.695082000	-0.869488000
1	12.757504000	-0.235444000	0.701195000
1	10.125696000	0.990662000	-3.700174000
1	11.635533000	1.745676000	-3.214799000
1	7.912989000	-3.216670000	-2.431221000
15	3.978175000	-4.047459000	0.033747000
8	3.181578000	-5.279432000	0.323081000

8	4.264428000	-3.588755000	-1.386726000
1	-10.001766000	-5.974243000	1.293846000
1	5.470264000	-4.088620000	-2.269232000

Figure S26. X-Y coordinates for **2** at level: B3LYP-GD3/3-21G*.

8	9.941260000	1.670525000	-2.499457000
6	9.116541000	2.658702000	0.998783000
6	10.591923000	3.052465000	1.216134000
6	11.148230000	3.030268000	-0.216339000
6	9.940595000	3.550173000	-1.020444000
6	9.877211000	3.094600000	-2.464378000
8	8.780243000	3.063112000	-0.314179000
1	8.469332000	3.152803000	1.728172000
1	11.105740000	2.369256000	1.899581000
8	10.693610000	4.407325000	1.643556000
1	10.601725000	4.440348000	2.608325000
1	11.372886000	2.003636000	-0.515912000
1	9.944539000	4.648560000	-0.996290000
1	10.721515000	3.533236000	-3.011728000
1	8.945578000	3.451574000	-2.918135000
8	12.321782000	3.792151000	-0.386932000
7	7.609380000	-0.925810000	4.210182000
6	7.646509000	0.437862000	4.370880000
7	7.275474000	0.931748000	5.593663000
7	8.079520000	1.259887000	3.436582000
6	8.451645000	0.618062000	2.304223000
6	8.446889000	-0.749131000	2.029569000
6	7.979476000	-1.648979000	3.042910000
8	7.868820000	-2.873998000	3.023485000
7	8.867025000	-0.988834000	0.732694000
6	9.124767000	0.200884000	0.237692000
7	8.886870000	1.222141000	1.149313000
1	7.263258000	-1.505059000	4.967484000
1	6.533667000	0.432673000	6.071207000
1	7.114985000	1.932227000	5.577006000
1	9.464181000	0.414329000	-0.766037000
8	6.284171000	-1.800640000	-2.073631000
6	4.890063000	1.609329000	-1.650341000
6	6.188318000	2.229365000	-2.179473000
6	6.906447000	1.006583000	-2.767284000
6	5.742553000	0.170949000	-3.309088000
6	6.010543000	-1.319973000	-3.390166000

8	4.638230000	0.443005000	-2.420583000
1	4.061438000	2.312161000	-1.751361000
1	6.756412000	2.719482000	-1.386253000
8	5.855147000	3.142666000	-3.220710000
1	6.579497000	3.069138000	-3.869002000
1	7.439195000	0.457179000	-1.988702000
1	5.494467000	0.536700000	-4.314382000
1	6.881682000	-1.474512000	-4.037366000
1	5.143210000	-1.832207000	-3.818433000
8	7.776297000	1.394905000	-3.825088000
7	4.975976000	1.260529000	-0.213694000
6	4.742968000	2.303350000	0.720702000
8	4.636756000	3.461208000	0.290475000
7	4.623765000	1.971381000	2.038341000
6	4.784209000	0.706476000	2.424471000
7	4.615988000	0.401527000	3.742558000
6	5.161432000	-0.334552000	1.520222000
6	5.224774000	-0.012483000	0.203660000
1	4.126000000	1.111780000	4.273767000
1	4.290329000	-0.555255000	3.909973000
1	5.323023000	-1.350465000	1.849491000
1	5.470418000	-0.732223000	-0.562338000
15	9.358312000	0.854321000	-3.821001000
8	9.956683000	1.398165000	-5.083687000
8	9.397038000	-0.593800000	-3.428657000
8	2.426818000	-2.364466000	1.063482000
6	1.080166000	-2.751046000	-2.288852000
6	2.509636000	-2.367399000	-2.749955000
6	3.430963000	-2.910815000	-1.623554000
6	2.540987000	-3.844619000	-0.786231000
6	2.753911000	-3.709836000	0.713737000
8	1.180276000	-3.509258000	-1.099217000
1	0.594458000	-3.324402000	-3.078648000
1	2.609546000	-1.280243000	-2.839579000
8	2.796789000	-2.970236000	-4.000587000
1	3.589485000	-3.520857000	-3.842327000
1	3.794708000	-2.084975000	-1.013455000
1	2.742823000	-4.880748000	-1.088018000

1	3.805105000	-3.923506000	0.936690000
1	2.112336000	-4.417120000	1.250346000
8	4.507203000	-3.636986000	-2.207909000
7	0.207255000	-1.592078000	-2.034685000
6	-0.754124000	-1.284642000	-2.997594000
8	-0.926757000	-1.941618000	-4.018276000
7	-1.500689000	-0.159405000	-2.708644000
6	-1.447545000	0.645488000	-1.559621000
8	-2.261785000	1.559290000	-1.421679000
6	-0.404660000	0.258851000	-0.630521000
1	-0.311614000	0.812174000	0.296738000
6	0.361753000	-0.825953000	-0.895021000
1	-2.271984000	0.009033000	-3.346068000
1	1.121378000	-1.180301000	-0.206967000
15	6.071199000	-3.384454000	-1.654784000
8	6.924001000	-4.288270000	-2.491921000
8	6.058442000	-3.392198000	-0.153566000
8	-1.848436000	-0.372786000	3.034522000
6	-2.160452000	-3.971089000	1.708754000
6	-0.626605000	-3.997942000	1.688415000
6	-0.278059000	-2.735432000	2.493661000
6	-1.403795000	-2.692831000	3.533940000
6	-1.724583000	-1.322238000	4.097643000
8	-2.554663000	-3.236293000	2.854873000
1	-2.566523000	-4.982585000	1.741390000
1	-0.237947000	-3.976805000	0.667275000
8	-0.178127000	-5.157093000	2.384695000
1	0.588832000	-4.864271000	2.911395000
1	-0.314981000	-1.844279000	1.864005000
1	-1.139914000	-3.354305000	4.370416000
1	-0.920594000	-1.022220000	4.775934000
1	-2.663707000	-1.372597000	4.664587000
8	0.989880000	-2.863036000	3.130084000
7	-2.718423000	-3.325356000	0.501700000
6	-2.917169000	-4.134314000	-0.650431000
8	-2.555675000	-5.316552000	-0.605910000
7	-3.506487000	-3.563807000	-1.742658000
6	-3.809078000	-2.267926000	-1.734355000

7	-4.358522000	-1.722461000	-2.856015000
6	-3.537944000	-1.417940000	-0.617064000
6	-2.992210000	-1.993449000	0.482996000
1	-4.781424000	-2.383196000	-3.496868000
1	-4.909184000	-0.876612000	-2.714873000
1	-3.732295000	-0.357942000	-0.651817000
1	-2.747945000	-1.432719000	1.375681000
15	2.233277000	-1.864175000	2.621481000
8	3.408988000	-2.262222000	3.477889000
8	1.742325000	-0.453162000	2.510496000
8	-4.707123000	3.744038000	0.648891000
6	-6.369323000	0.743275000	2.194498000
6	-5.028316000	0.308443000	2.812366000
6	-4.165002000	1.572224000	2.631524000
6	-5.198452000	2.694813000	2.774933000
6	-4.838005000	3.980724000	2.056699000
8	-6.429849000	2.156321000	2.255246000
1	-7.204734000	0.297566000	2.739788000
1	-4.624762000	-0.574592000	2.307430000
8	-5.227329000	0.056671000	4.193919000
1	-4.446831000	0.441566000	4.637244000
1	-3.692616000	1.603600000	1.645266000
1	-5.321157000	2.914198000	3.844076000
1	-3.877753000	4.333535000	2.451325000
1	-5.592978000	4.745336000	2.258936000
8	-3.200803000	1.695587000	3.668285000
7	-8.095100000	-2.952814000	-0.773091000
6	-8.323912000	-2.727110000	0.563917000
7	-9.068826000	-3.666498000	1.223277000
7	-7.828015000	-1.690864000	1.210789000
6	-7.136896000	-0.851986000	0.405466000
6	-6.954414000	-0.923310000	-0.975377000
6	-7.445095000	-2.072412000	-1.675315000
8	-7.367879000	-2.366043000	-2.869865000
7	-6.241032000	0.174310000	-1.427009000
6	-5.981351000	0.879960000	-0.346619000
7	-6.508200000	0.306945000	0.800039000
1	-8.452289000	-3.801615000	-1.197644000

1	-9.849849000	-4.054028000	0.702659000
1	-9.330053000	-3.378049000	2.159089000
1	-5.431378000	1.808426000	-0.316923000
15	-1.614894000	1.242237000	3.346093000
8	-0.882097000	1.424395000	4.639739000
8	-1.204131000	1.878654000	2.050930000
8	-7.853609000	4.028909000	-3.287384000
6	-10.209917000	2.607832000	-0.451083000
6	-8.984906000	2.784884000	0.464259000
6	-8.073928000	3.625029000	-0.433732000
6	-9.061955000	4.519208000	-1.185461000
6	-8.549692000	5.014810000	-2.538800000
8	-10.242081000	3.702658000	-1.347136000
1	-11.130757000	2.553541000	0.136924000
1	-8.547678000	1.816161000	0.720732000
8	-9.380045000	3.493808000	1.624914000
1	-8.547044000	3.714922000	2.078548000
1	-7.572013000	2.957053000	-1.135474000
1	-9.314659000	5.381066000	-0.553759000
1	-7.911648000	5.891482000	-2.353303000
1	-9.403176000	5.346950000	-3.139322000
8	-7.137561000	4.403205000	0.288307000
7	-11.405983000	-2.419185000	-0.776494000
6	-11.642036000	-1.502773000	0.181667000
7	-11.293213000	-0.213105000	0.209568000
6	-10.647713000	0.144818000	-0.912789000
6	-10.355532000	-0.680855000	-2.006625000
6	-10.755413000	-2.027862000	-1.892954000
7	-10.509861000	-2.940383000	-2.873655000
7	-9.677350000	0.020065000	-2.990178000
6	-9.561812000	1.234913000	-2.500113000
7	-10.132185000	1.377289000	-1.246763000
1	-12.171215000	-1.873386000	1.056928000
1	-9.697625000	-2.769528000	-3.457068000
1	-10.678830000	-3.909639000	-2.634615000
1	-9.076164000	2.073818000	-2.983717000
15	-5.627623000	4.676423000	-0.361324000
8	-5.318415000	6.128170000	-0.156347000

8	-5.545367000	4.008124000	-1.716539000
1	12.211455000	4.570108000	0.190634000
1	-6.965452000	3.946239000	-2.861453000

Figure S27. X-Y coordinates for **2** at level: B3LYP-GD3/6-31G*.

8	2.376254000	5.794506000	-3.390506000
6	4.928720000	4.364697000	-1.074043000
6	5.884359000	4.340038000	-2.264110000
6	5.135519000	5.199061000	-3.304770000
6	4.513387000	6.290027000	-2.424077000
6	3.250539000	6.900543000	-2.992761000
8	4.188328000	5.612592000	-1.141829000
1	5.470325000	4.274700000	-0.133223000
1	6.112940000	3.325469000	-2.564458000
8	7.090876000	5.085300000	-1.897073000
1	7.229883000	5.679702000	-2.695694000
1	4.383024000	4.650324000	-3.866993000
1	5.262009000	7.066310000	-2.244929000
1	3.534887000	7.515362000	-3.855747000
1	2.783274000	7.537416000	-2.232688000
8	6.088611000	5.851418000	-4.204638000
7	3.958443000	3.235144000	-1.155174000
6	4.401462000	1.974420000	-0.692255000
8	5.630660000	1.844894000	-0.427749000
7	3.477187000	0.992688000	-0.528631000
6	2.193015000	1.160308000	-0.924119000
7	1.321266000	0.186582000	-0.664557000
6	1.787315000	2.383907000	-1.558233000
6	2.682187000	3.404127000	-1.622850000
1	1.635682000	-0.686785000	-0.190464000
1	0.360218000	0.264187000	-0.979258000
1	0.782457000	2.503542000	-1.934166000
1	2.451505000	4.364439000	-2.072604000
8	4.942845000	-9.000921000	1.663550000
6	6.713098000	-5.986125000	0.148500000
6	7.622174000	-5.985089000	1.384921000
6	7.260722000	-7.312194000	2.081151000
6	7.089523000	-8.237243000	0.862304000
6	6.231584000	-9.451144000	1.098880000
8	6.439303000	-7.385096000	-0.169368000
1	7.154943000	-5.471655000	-0.705707000
1	7.489853000	-5.089860000	1.995463000

8	9.016498000	-6.217665000	1.000942000
1	9.442828000	-5.355494000	0.756975000
1	6.316782000	-7.248002000	2.621546000
1	8.082537000	-8.536860000	0.513848000
1	6.723162000	-10.125289000	1.805026000
1	6.057703000	-9.957944000	0.146562000
8	8.309463000	-7.757674000	2.965486000
7	4.375066000	-1.503173000	0.196564000
6	5.706917000	-1.799537000	-0.012202000
7	6.533898000	-0.777375000	-0.285854000
7	6.190589000	-3.052677000	0.060545000
6	5.245678000	-3.966075000	0.356949000
6	3.891821000	-3.759471000	0.648154000
6	3.376586000	-2.437950000	0.528826000
8	2.177633000	-2.058933000	0.665744000
7	3.272569000	-4.983555000	0.960332000
6	4.221024000	-5.902887000	0.839103000
7	5.446569000	-5.325805000	0.459966000
1	4.029940000	-0.518966000	-0.041021000
1	6.211230000	0.208804000	-0.349067000
1	7.478874000	-1.018650000	-0.560610000
1	4.151570000	-6.958520000	1.038426000
8	7.185565000	3.673160000	-4.823863000
6	8.511348000	0.232731000	-3.754979000
6	9.046769000	0.143526000	-5.180266000
6	8.818779000	1.570665000	-5.690109000
6	9.227555000	2.403602000	-4.469496000
6	8.595458000	3.774621000	-4.404925000
8	8.773692000	1.600548000	-3.301553000
1	8.984826000	-0.498188000	-3.097299000
1	8.589240000	-0.648150000	-5.759959000
8	10.504028000	-0.044045000	-5.114996000
1	10.840864000	0.605677000	-5.800526000
1	7.789684000	1.772166000	-5.974374000
1	10.317298000	2.490743000	-4.443816000
1	9.108370000	4.454748000	-5.088314000
1	8.622461000	4.151308000	-3.379735000
8	9.728447000	1.864794000	-6.797285000

7	4.641552000	-3.007850000	-2.793329000
6	5.970133000	-3.304267000	-3.006914000
7	6.329037000	-4.605030000	-2.933817000
7	6.891335000	-2.366980000	-3.288598000
6	6.369263000	-1.126821000	-3.404291000
6	5.031650000	-0.742671000	-3.249412000
6	4.079103000	-1.720702000	-2.869323000
8	2.856778000	-1.536579000	-2.612613000
7	4.884699000	0.630376000	-3.489080000
6	6.101750000	1.068100000	-3.769525000
7	7.054739000	0.034258000	-3.713788000
1	3.943251000	-3.794359000	-2.606336000
1	5.611333000	-5.355648000	-2.991611000
1	7.280086000	-4.818190000	-3.214822000
1	6.385363000	2.065502000	-4.055851000
15	6.476657000	4.964975000	-5.582402000
8	7.519558000	5.762125000	-6.299725000
8	5.207937000	4.451850000	-6.182613000
8	-0.044404000	-9.372201000	0.003518000
6	2.961668000	-8.696709000	-2.248235000
6	3.809958000	-9.184073000	-1.084910000
6	2.753978000	-9.773084000	-0.123908000
6	1.799253000	-10.482029000	-1.095754000
6	0.356329000	-10.624312000	-0.644119000
8	1.820688000	-9.607706000	-2.311830000
1	3.504470000	-8.684213000	-3.188938000
1	4.438167000	-8.396991000	-0.677796000
8	4.620266000	-10.319865000	-1.543435000
1	4.508206000	-10.983711000	-0.796902000
1	2.233370000	-9.032179000	0.478307000
1	2.215236000	-11.455471000	-1.363543000
1	0.287056000	-11.458771000	0.060992000
1	-0.275054000	-10.796864000	-1.518482000
8	3.387573000	-10.776409000	0.730851000
7	2.482827000	-7.323410000	-1.976781000
6	3.255075000	-6.260935000	-2.488913000
8	4.346786000	-6.545662000	-3.068215000
7	2.803884000	-4.998602000	-2.311264000

6	1.626394000	-4.742949000	-1.687543000
7	1.233542000	-3.475356000	-1.604528000
6	0.849895000	-5.816336000	-1.144334000
6	1.319875000	-7.077008000	-1.293719000
1	1.836795000	-2.715677000	-1.992197000
1	0.472146000	-3.219887000	-0.987024000
1	-0.088847000	-5.683076000	-0.630270000
1	0.796204000	-7.921198000	-0.868733000
15	3.913613000	-10.178126000	2.216607000
8	4.703051000	-11.286101000	2.837509000
8	2.774338000	-9.454243000	2.860396000
8	8.710994000	0.080178000	-8.283954000
6	7.761902000	-3.344697000	-6.865076000
6	7.776408000	-3.925169000	-8.265789000
6	8.289801000	-2.735484000	-9.090471000
6	9.434113000	-2.244174000	-8.192883000
6	9.880734000	-0.811780000	-8.325758000
8	8.889591000	-2.421478000	-6.809176000
1	7.834527000	-4.099152000	-6.082287000
1	6.829521000	-4.343316000	-8.574408000
8	8.830734000	-4.949162000	-8.326889000
1	9.259396000	-4.767689000	-9.214814000
1	7.543210000	-1.964270000	-9.261101000
1	10.293948000	-2.906089000	-8.320197000
1	10.425940000	-0.665974000	-9.261860000
1	10.534467000	-0.596215000	-7.475912000
8	8.790726000	-3.251915000	-10.366830000
7	2.863147000	-3.606239000	-5.342652000
6	3.811069000	-4.566426000	-5.417633000
7	5.076991000	-4.398708000	-5.839568000
6	5.331854000	-3.118055000	-6.197468000
6	4.425139000	-2.050077000	-6.174073000
6	3.121359000	-2.320573000	-5.712710000
7	2.152160000	-1.408973000	-5.619290000
7	5.031491000	-0.879102000	-6.635915000
6	6.280765000	-1.227678000	-6.931911000
7	6.515296000	-2.587156000	-6.671166000
1	3.496627000	-5.547741000	-5.101351000

1	2.338511000	-0.458952000	-5.918012000
1	1.232441000	-1.662675000	-5.213179000
1	7.054380000	-0.598835000	-7.343544000
15	9.042687000	1.711952000	-8.321234000
8	10.151446000	1.966025000	-9.291603000
8	7.713521000	2.399761000	-8.321644000
8	-4.388266000	-6.871521000	-2.827410000
6	-1.175575000	-7.707097000	-4.593040000
6	-0.755295000	-8.466892000	-3.333242000
6	-2.063722000	-8.426220000	-2.535336000
6	-3.094452000	-8.740784000	-3.616843000
6	-4.490867000	-8.254861000	-3.328528000
8	-2.589403000	-7.976110000	-4.801007000
1	-0.581395000	-8.005977000	-5.455240000
1	0.055180000	-7.943179000	-2.844716000
8	-0.407232000	-9.832789000	-3.668591000
1	0.555502000	-9.910918000	-3.375013000
1	-2.226938000	-7.420617000	-2.155806000
1	-3.076644000	-9.811854000	-3.836086000
1	-4.964514000	-8.875643000	-2.564711000
1	-5.076108000	-8.253997000	-4.251834000
8	-2.150135000	-9.375267000	-1.441898000
7	-0.981183000	-6.249814000	-4.387524000
6	0.328259000	-5.785913000	-4.581544000
8	1.283571000	-6.583151000	-4.701456000
7	0.449892000	-4.425168000	-4.618963000
6	-0.552737000	-3.488185000	-4.409697000
8	-0.312546000	-2.255279000	-4.521490000
6	-1.838632000	-4.051606000	-4.065631000
1	-2.656779000	-3.383068000	-3.850607000
6	-2.013473000	-5.394477000	-4.092237000
1	1.441654000	-4.062237000	-4.866829000
1	-2.952756000	-5.866079000	-3.839118000
15	-1.627660000	-8.848784000	0.041817000
8	-2.394672000	-9.606844000	1.078397000
8	-1.523840000	-7.347335000	0.023682000
8	6.682101000	-4.584042000	-11.064913000
6	4.528285000	-6.097536000	-8.589813000

6	3.900329000	-7.088220000	-9.546754000
6	4.743277000	-6.865757000	-10.821902000
6	6.153434000	-6.757994000	-10.217203000
6	7.192957000	-5.948509000	-10.961373000
8	5.937241000	-6.076292000	-8.907167000
1	4.394228000	-6.356546000	-7.542020000
1	2.836505000	-6.936293000	-9.657714000
8	4.207728000	-8.441343000	-9.071537000
1	4.457128000	-8.921094000	-9.916882000
1	4.456849000	-5.967981000	-11.368163000
1	6.525090000	-7.769733000	-10.036752000
1	7.383920000	-6.382910000	-11.947880000
1	8.102686000	-5.960640000	-10.357645000
8	4.659680000	-8.063674000	-11.663577000
7	0.177531000	-3.752119000	-7.820197000
6	0.510376000	-5.086507000	-7.746650000
7	-0.461481000	-5.977506000	-7.464124000
7	1.753562000	-5.531296000	-7.979696000
6	2.586133000	-4.573030000	-8.427940000
6	2.309215000	-3.226303000	-8.663272000
6	1.033138000	-2.729033000	-8.274525000
8	0.627446000	-1.533413000	-8.322493000
7	3.422950000	-2.608528000	-9.256922000
6	4.351876000	-3.553848000	-9.353972000
7	3.889496000	-4.780942000	-8.828479000
1	-0.817849000	-3.446556000	-7.564808000
1	-1.461924000	-5.699504000	-7.415326000
1	-0.210244000	-6.950825000	-7.617286000
1	5.297694000	-3.451292000	-9.850952000
15	7.626935000	-3.330686000	-11.583499000
8	8.367071000	-3.716536000	-12.822802000
8	6.732670000	-2.135139000	-11.431612000
8	-6.997349000	-2.206704000	-4.063891000
6	-5.610438000	-4.609158000	-6.513743000
6	-5.437964000	-5.639877000	-5.396814000
6	-6.187899000	-4.964569000	-4.230430000
6	-7.407012000	-4.380263000	-4.945670000
6	-8.050823000	-3.204176000	-4.242887000

8	-6.887466000	-3.943072000	-6.270429000
1	-5.588694000	-5.046385000	-7.509362000
1	-4.394861000	-5.885936000	-5.230594000
8	-6.207771000	-6.840645000	-5.741394000
1	-6.688921000	-7.046347000	-4.884140000
1	-5.609215000	-4.195479000	-3.722047000
1	-8.141785000	-5.176401000	-5.090879000
1	-8.445660000	-3.540118000	-3.278156000
1	-8.846551000	-2.811444000	-4.875012000
8	-6.683584000	-5.962291000	-3.283787000
7	-4.519091000	-3.593951000	-6.439875000
6	-3.269185000	-3.937683000	-6.999101000
8	-3.094761000	-5.134094000	-7.375313000
7	-2.326534000	-2.966252000	-7.083773000
6	-2.531955000	-1.715258000	-6.595969000
7	-1.603286000	-0.797455000	-6.843960000
6	-3.731207000	-1.426410000	-5.864024000
6	-4.699881000	-2.375801000	-5.840305000
1	-0.780663000	-1.034322000	-7.438199000
1	-1.712475000	0.146225000	-6.490621000
1	-3.922743000	-0.488886000	-5.364670000
1	-5.629191000	-2.218410000	-5.314255000
15	-5.667753000	-6.252867000	-1.978253000
8	-6.321116000	-7.338842000	-1.184419000
8	-5.207256000	-4.938212000	-1.433721000
8	2.129412000	-8.190408000	-11.417137000
6	-1.331186000	-7.781194000	-9.999017000
6	-1.822188000	-8.626968000	-11.180445000
6	-0.480965000	-9.104857000	-11.739801000
6	0.301766000	-9.457261000	-10.480866000
6	1.793666000	-9.439180000	-10.708344000
8	-0.091450000	-8.379068000	-9.518382000
1	-2.080784000	-7.732173000	-9.211502000
1	-2.369884000	-7.999995000	-11.872186000
8	-2.617732000	-9.740557000	-10.702066000
1	-3.508047000	-9.610517000	-11.156749000
1	0.003749000	-8.273677000	-12.244844000
1	-0.031025000	-10.426184000	-10.098992000

1	2.060229000	-10.283343000	-11.349824000
1	2.350849000	-9.457885000	-9.770964000
8	-0.508346000	-10.250348000	-12.625882000
7	-1.048722000	-6.394001000	-10.445771000
6	-2.152685000	-5.521627000	-10.473947000
8	-3.304040000	-6.039646000	-10.377042000
7	-1.910969000	-4.195225000	-10.605477000
6	-0.662571000	-3.730889000	-10.858884000
7	-0.484458000	-2.408130000	-10.890459000
6	0.423973000	-4.646288000	-11.050420000
6	0.204932000	-5.959155000	-10.779325000
1	-1.233263000	-1.782559000	-10.514212000
1	0.458451000	-2.034847000	-10.929607000
1	1.410561000	-4.292671000	-11.305341000
1	0.981361000	-6.709331000	-10.834826000
15	3.272206000	-8.165501000	-12.617046000
8	3.316869000	-9.508566000	-13.277120000
8	3.092894000	-6.857529000	-13.318724000
8	-7.372173000	3.223715000	-6.614292000
6	-8.171279000	-0.297609000	-8.079273000
6	-8.165090000	-0.966789000	-6.715433000
6	-7.929885000	0.251477000	-5.806388000
6	-8.905584000	1.269190000	-6.420358000
6	-8.656127000	2.726380000	-6.084308000
8	-8.810264000	1.010572000	-7.887518000
1	-8.696104000	-0.861753000	-8.847953000
1	-7.440654000	-1.775064000	-6.645494000
8	-9.521820000	-1.452946000	-6.425185000
1	-9.678108000	-1.144293000	-5.483821000
1	-6.898943000	0.597238000	-5.812566000
1	-9.913256000	1.013941000	-6.081652000
1	-8.631169000	2.795951000	-4.991975000
1	-9.476454000	3.344889000	-6.456207000
8	-8.354607000	-0.066101000	-4.447280000
7	-3.953841000	-2.555855000	-9.802918000
6	-5.226115000	-3.070874000	-9.656719000
7	-5.391407000	-4.379329000	-9.907747000
7	-6.273980000	-2.321832000	-9.269398000

6	-5.933278000	-1.050010000	-8.989848000
6	-4.676748000	-0.444822000	-9.094893000
6	-3.587848000	-1.220613000	-9.571780000
8	-2.410342000	-0.822467000	-9.791969000
7	-4.732624000	0.882401000	-8.645250000
6	-5.985866000	1.075588000	-8.266705000
7	-6.772774000	-0.078270000	-8.479917000
1	-3.175277000	-3.194691000	-10.155049000
1	-4.594478000	-5.010404000	-10.136281000
1	-6.335756000	-4.718712000	-10.043180000
1	-6.408741000	1.955656000	-7.822806000
15	-7.133741000	-0.675811000	-3.461528000
8	-7.687853000	-0.684766000	-2.075539000
8	-5.842516000	-0.024616000	-3.870229000
8	-2.288504000	-10.005541000	-14.412031000
6	-5.247048000	-8.098326000	-13.025258000
6	-5.977386000	-8.622098000	-14.265608000
6	-5.047993000	-9.727326000	-14.806472000
6	-4.497658000	-10.355653000	-13.510029000
6	-3.097939000	-10.936881000	-13.614998000
8	-4.449570000	-9.222764000	-12.535513000
1	-5.963123000	-7.767064000	-12.276441000
1	-6.180367000	-7.825931000	-14.988006000
8	-7.175157000	-9.287352000	-13.779209000
1	-7.250242000	-10.082063000	-14.391754000
1	-4.232845000	-9.340748000	-15.417522000
1	-5.211990000	-11.096026000	-13.143415000
1	-3.145776000	-11.916742000	-14.102491000
1	-2.670647000	-11.025989000	-12.614990000
8	-5.926747000	-10.633957000	-15.535777000
7	-4.353674000	-6.962175000	-13.311012000
6	-4.817483000	-5.678727000	-12.960024000
8	-5.977955000	-5.492142000	-12.538974000
7	-3.906475000	-4.674709000	-13.155324000
6	-2.586263000	-4.792401000	-13.586917000
8	-1.847979000	-3.774293000	-13.661534000
6	-2.189850000	-6.138487000	-13.926063000
1	-1.192419000	-6.379504000	-14.255808000

6	-3.073070000	-7.153169000	-13.787061000
1	-4.271001000	-3.687814000	-12.944124000
1	-2.787617000	-8.169598000	-14.025990000
15	-0.627570000	-9.927398000	-14.246678000
8	0.016364000	-11.059437000	-14.981095000
8	-0.283462000	-8.482515000	-14.492487000
8	-5.789894000	5.022928000	-10.901046000
6	-7.910168000	1.941366000	-12.079432000
6	-8.291571000	1.840605000	-10.595605000
6	-7.785027000	3.186641000	-10.083717000
6	-8.103227000	4.156102000	-11.220122000
6	-7.166710000	5.369394000	-11.229132000
8	-7.903150000	3.348503000	-12.452919000
1	-8.576232000	1.354164000	-12.713053000
1	-7.748631000	1.011861000	-10.153579000
8	-9.722225000	1.722361000	-10.427389000
1	-9.804322000	1.646796000	-9.428516000
1	-6.707561000	3.131191000	-9.962744000
1	-9.151840000	4.458734000	-11.148543000
1	-7.573492000	6.102392000	-10.518178000
1	-7.173615000	5.812565000	-12.228314000
8	-8.430261000	3.641742000	-8.867248000
7	-4.904875000	-2.198332000	-12.781694000
6	-6.249958000	-2.097243000	-12.667659000
7	-6.955189000	-0.965755000	-12.498125000
6	-6.156783000	0.125951000	-12.423049000
6	-4.755085000	0.143426000	-12.495573000
6	-4.105596000	-1.094031000	-12.697399000
7	-2.783056000	-1.242591000	-12.808029000
7	-4.271726000	1.446887000	-12.336701000
6	-5.356272000	2.203867000	-12.177235000
7	-6.531158000	1.441447000	-12.237617000
1	-6.770818000	-3.046400000	-12.696965000
1	-2.179436000	-0.458331000	-12.589957000
1	-2.373113000	-2.168541000	-13.031627000
1	-5.388734000	3.260603000	-11.942579000
15	-7.502615000	4.424313000	-7.752638000
8	-8.300232000	5.566030000	-7.213600000

8	-6.108058000	4.588781000	-8.325654000
1	9.133907000	-7.416877000	2.502564000
1	1.516190000	6.165289000	-3.720330000
1	-5.434385000	-11.463783000	-15.768315000
1	-5.780172000	4.886774000	-9.874094000

Figure S28. X-Y coordinates for **1:2** at level: B3LYP-GD3/3-21G*.

8	2.967438000	6.626103000	-3.631989000
6	5.401715000	4.965276000	-1.249080000
6	6.364616000	4.756038000	-2.423080000
6	5.684977000	5.594727000	-3.517212000
6	5.176121000	6.792897000	-2.707843000
6	4.006938000	7.545846000	-3.307769000
8	4.816978000	6.239720000	-1.420706000
1	5.927711000	4.914856000	-0.294148000
1	6.481225000	3.701270000	-2.669826000
8	7.620671000	5.334668000	-2.083369000
1	7.922320000	5.789373000	-2.891403000
1	4.851733000	5.049973000	-3.968270000
1	6.003518000	7.500780000	-2.568167000
1	4.372584000	8.066590000	-4.205127000
1	3.662469000	8.302151000	-2.588964000
8	6.596566000	6.038215000	-4.512780000
7	4.335264000	3.925666000	-1.207421000
6	4.673972000	2.671501000	-0.662738000
8	5.867051000	2.462217000	-0.366505000
7	3.691725000	1.758804000	-0.469867000
6	2.438904000	1.999067000	-0.888999000
7	1.510567000	1.061299000	-0.659185000
6	2.094943000	3.230735000	-1.534217000
6	3.067754000	4.172312000	-1.649202000
1	1.763920000	0.161425000	-0.234364000
1	0.576165000	1.177034000	-1.022931000
1	1.090539000	3.422033000	-1.890732000
1	2.896326000	5.143997000	-2.096631000
8	4.843811000	-8.369527000	2.529958000
6	6.647206000	-5.419433000	0.871110000
6	7.440944000	-5.202017000	2.175128000
6	7.060909000	-6.449537000	2.986975000
6	6.994977000	-7.510861000	1.876133000
6	6.177488000	-8.745027000	2.182237000
8	6.441944000	-6.814953000	0.738411000
1	7.183448000	-5.027359000	0.002039000
1	7.177360000	-4.258251000	2.661780000

8	8.843553000	-5.302284000	1.947539000
1	9.168890000	-4.442581000	1.638594000
1	6.067959000	-6.325008000	3.427876000
1	8.018675000	-7.834853000	1.639323000
1	6.653437000	-9.281602000	3.011201000
1	6.175714000	-9.396713000	1.301532000
8	7.962332000	-6.758178000	4.025971000
7	4.413731000	-0.938156000	0.339157000
6	5.742642000	-1.281580000	0.243635000
7	6.616738000	-0.283712000	-0.003044000
7	6.186759000	-2.522838000	0.411280000
6	5.194494000	-3.392760000	0.690028000
6	3.828529000	-3.149515000	0.858909000
6	3.357316000	-1.817608000	0.639315000
8	2.188661000	-1.394928000	0.683085000
7	3.164974000	-4.316916000	1.211326000
6	4.100359000	-5.238652000	1.239590000
7	5.354289000	-4.738532000	0.914279000
1	4.143782000	0.037763000	0.105744000
1	6.315687000	0.679048000	-0.192160000
1	7.553403000	-0.558196000	-0.259698000
1	3.970264000	-6.280776000	1.495091000
8	7.488090000	3.759011000	-5.241467000
6	8.522698000	0.451455000	-3.716006000
6	9.080966000	0.029357000	-5.076857000
6	8.978001000	1.347272000	-5.853903000
6	9.382712000	2.360208000	-4.776688000
6	8.892124000	3.774708000	-4.988174000
8	8.839635000	1.823121000	-3.549736000
1	8.961973000	-0.142045000	-2.908767000
1	8.516412000	-0.791927000	-5.517955000
8	10.445386000	-0.331683000	-4.899526000
1	10.886438000	-0.096814000	-5.735267000
1	7.950304000	1.533163000	-6.173802000
1	10.478072000	2.381531000	-4.703065000
1	9.425861000	4.213111000	-5.837985000
1	9.109264000	4.366793000	-4.090223000
8	9.870567000	1.403332000	-6.957768000

7	4.714921000	-2.731596000	-2.617458000
6	6.056975000	-2.994618000	-2.739879000
7	6.449256000	-4.269957000	-2.486673000
7	6.958432000	-2.068703000	-3.051067000
6	6.401452000	-0.857479000	-3.272002000
6	5.054008000	-0.493217000	-3.212714000
6	4.106605000	-1.482426000	-2.820492000
8	2.882519000	-1.342386000	-2.656390000
7	4.884643000	0.836872000	-3.562567000
6	6.098082000	1.268846000	-3.813843000
7	7.067361000	0.289533000	-3.636828000
1	4.062228000	-3.516809000	-2.410365000
1	5.755439000	-5.023798000	-2.558268000
1	7.379139000	-4.494637000	-2.814009000
1	6.369386000	2.255261000	-4.157469000
15	6.756448000	5.094137000	-5.896679000
8	7.719388000	5.841093000	-6.769159000
8	5.397796000	4.637171000	-6.335326000
8	-0.033737000	-9.386950000	0.196686000
6	3.111132000	-8.543874000	-1.713211000
6	3.969764000	-8.867795000	-0.491799000
6	2.917916000	-9.462500000	0.460439000
6	2.072349000	-10.297233000	-0.508243000
6	0.647235000	-10.604036000	-0.095893000
8	2.067519000	-9.508954000	-1.727830000
1	3.677063000	-8.593841000	-2.641761000
1	4.473704000	-7.982459000	-0.099997000
8	4.915595000	-9.871407000	-0.849129000
1	4.943789000	-10.486847000	-0.093504000
1	2.308975000	-8.680036000	0.919860000
1	2.588394000	-11.245182000	-0.704447000
1	0.672056000	-11.256139000	0.786299000
1	0.143880000	-11.134068000	-0.912149000
8	3.509174000	-10.282081000	1.456577000
7	2.556037000	-7.175081000	-1.617893000
6	3.360765000	-6.123810000	-2.097142000
8	4.501765000	-6.401410000	-2.521416000
7	2.870862000	-4.865832000	-2.062545000

6	1.659249000	-4.607342000	-1.543280000
7	1.223272000	-3.346757000	-1.573995000
6	0.851589000	-5.652958000	-0.990794000
6	1.345779000	-6.914105000	-1.040661000
1	1.831284000	-2.596663000	-1.927567000
1	0.397071000	-3.087864000	-1.056101000
1	-0.116934000	-5.458020000	-0.547692000
1	0.806432000	-7.761655000	-0.637543000
15	3.773402000	-9.565069000	2.958184000
8	4.461420000	-10.618431000	3.772767000
8	2.526308000	-8.848242000	3.381687000
8	8.883706000	-0.283225000	-8.622119000
6	7.954900000	-3.471408000	-6.800395000
6	7.878240000	-4.270258000	-8.099528000
6	8.375999000	-3.220218000	-9.105298000
6	9.524506000	-2.588425000	-8.305606000
6	9.974742000	-1.197881000	-8.695169000
8	9.044712000	-2.581305000	-6.941021000
1	8.100163000	-4.112348000	-5.927317000
1	6.876029000	-4.645633000	-8.299885000
8	8.806939000	-5.347730000	-8.024299000
1	9.226568000	-5.396374000	-8.902169000
1	7.602849000	-2.477713000	-9.321460000
1	10.397559000	-3.251371000	-8.373731000
1	10.381094000	-1.232854000	-9.713744000
1	10.781669000	-0.889469000	-8.019519000
8	8.848960000	-3.820234000	-10.302419000
7	3.080067000	-3.825090000	-5.287836000
6	4.086608000	-4.713321000	-5.270083000
7	5.352729000	-4.525886000	-5.649192000
6	5.549183000	-3.266449000	-6.084220000
6	4.601867000	-2.241578000	-6.156291000
6	3.294277000	-2.562544000	-5.727763000
7	2.271654000	-1.699075000	-5.754752000
7	5.150384000	-1.096201000	-6.703920000
6	6.399901000	-1.422004000	-6.960379000
7	6.709398000	-2.720900000	-6.589788000
1	3.823462000	-5.695566000	-4.892109000

1	2.439921000	-0.743520000	-6.029912000
1	1.373420000	-1.953160000	-5.337341000
1	7.141001000	-0.787013000	-7.423995000
15	9.237906000	1.338250000	-8.511104000
8	10.388925000	1.674116000	-9.410958000
8	7.910437000	2.036434000	-8.541902000
8	-4.368747000	-7.293541000	-2.755303000
6	-1.073156000	-8.062710000	-4.382930000
6	-0.631467000	-8.775627000	-3.094450000
6	-1.963497000	-8.824881000	-2.329902000
6	-2.962653000	-9.099901000	-3.453411000
6	-4.383466000	-8.656944000	-3.181048000
8	-2.435486000	-8.368286000	-4.587319000
1	-0.475368000	-8.392159000	-5.234281000
1	0.121838000	-8.188879000	-2.580752000
8	-0.138176000	-10.069852000	-3.387864000
1	0.765654000	-10.085624000	-3.022582000
1	-2.165471000	-7.835110000	-1.910530000
1	-2.963846000	-10.172840000	-3.688360000
1	-4.817773000	-9.293866000	-2.403468000
1	-4.974983000	-8.758606000	-4.098580000
8	-2.061143000	-9.809964000	-1.318502000
7	-0.894173000	-6.589408000	-4.284772000
6	0.399149000	-6.120421000	-4.511852000
8	1.355406000	-6.886442000	-4.633549000
7	0.517774000	-4.755677000	-4.585071000
6	-0.492786000	-3.815548000	-4.419143000
8	-0.251671000	-2.605785000	-4.544769000
6	-1.782982000	-4.380831000	-4.095166000
1	-2.617403000	-3.716140000	-3.914335000
6	-1.935240000	-5.728215000	-4.054999000
1	1.479380000	-4.399669000	-4.795902000
1	-2.880522000	-6.200564000	-3.821381000
15	-1.700159000	-9.386597000	0.250065000
8	-2.175482000	-10.532879000	1.092643000
8	-2.072558000	-7.952139000	0.497495000
8	6.666726000	-4.998519000	-11.037206000
6	4.326775000	-6.527284000	-8.552150000

6	3.732425000	-7.535068000	-9.530593000
6	4.618341000	-7.292427000	-10.765388000
6	5.989624000	-7.116577000	-10.100855000
6	7.057894000	-6.357506000	-10.861549000
8	5.702783000	-6.444589000	-8.852104000
1	4.195757000	-6.829946000	-7.509872000
1	2.670350000	-7.368350000	-9.704598000
8	3.964198000	-8.844445000	-9.020094000
1	4.204509000	-9.387233000	-9.793582000
1	4.317876000	-6.383421000	-11.294900000
1	6.388930000	-8.116111000	-9.882227000
1	7.217163000	-6.848385000	-11.829862000
1	7.991936000	-6.414708000	-10.292433000
8	4.622321000	-8.414881000	-11.638814000
7	-0.030017000	-4.079655000	-7.935877000
6	0.261149000	-5.415806000	-7.817303000
7	-0.755061000	-6.244630000	-7.471088000
7	1.476580000	-5.912989000	-7.999700000
6	2.362270000	-4.979440000	-8.402489000
6	2.156453000	-3.619620000	-8.643433000
6	0.870871000	-3.076572000	-8.336483000
8	0.494800000	-1.893164000	-8.404155000
7	3.314654000	-3.032537000	-9.132765000
6	4.194855000	-4.008103000	-9.171656000
7	3.676821000	-5.216770000	-8.724304000
1	-1.003836000	-3.761910000	-7.743378000
1	-1.729132000	-5.934185000	-7.568875000
1	-0.568113000	-7.227176000	-7.620928000
1	5.205348000	-3.940493000	-9.542693000
15	7.788835000	-3.914562000	-11.608795000
8	8.596581000	-4.537642000	-12.707023000
8	7.049343000	-2.615742000	-11.730877000
8	-7.467413000	-2.669243000	-3.965398000
6	-5.859737000	-4.946871000	-6.497969000
6	-5.571057000	-6.001761000	-5.423368000
6	-6.339986000	-5.419697000	-4.224277000
6	-7.592823000	-4.871084000	-4.911960000
6	-8.338146000	-3.778844000	-4.174939000

8	-7.122049000	-4.389826000	-6.191158000
1	-5.872281000	-5.381364000	-7.497982000
1	-4.500203000	-6.127250000	-5.256103000
8	-6.164986000	-7.231264000	-5.824582000
1	-6.572681000	-7.599316000	-5.018917000
1	-5.776515000	-4.613675000	-3.746103000
1	-8.291399000	-5.701522000	-5.079251000
1	-8.691620000	-4.180580000	-3.217825000
1	-9.206605000	-3.480142000	-4.770360000
8	-6.707733000	-6.411136000	-3.276393000
7	-4.818274000	-3.885412000	-6.507741000
6	-3.607465000	-4.191004000	-7.155542000
8	-3.458670000	-5.339119000	-7.619946000
7	-2.660792000	-3.229795000	-7.243981000
6	-2.836438000	-2.023220000	-6.678711000
7	-1.877840000	-1.113484000	-6.861011000
6	-4.016567000	-1.731995000	-5.918003000
6	-4.982754000	-2.686187000	-5.874576000
1	-1.052310000	-1.338513000	-7.425864000
1	-1.958584000	-0.194949000	-6.451940000
1	-4.163663000	-0.776388000	-5.431322000
1	-5.914064000	-2.550665000	-5.340374000
15	-5.677991000	-6.652325000	-1.968310000
8	-6.345122000	-7.700987000	-1.131147000
8	-5.224475000	-5.319037000	-1.453805000
8	2.062985000	-8.529977000	-11.804652000
6	-1.459157000	-7.989080000	-10.567581000
6	-1.964988000	-8.752461000	-11.805014000
6	-0.644994000	-9.327882000	-12.337412000
6	0.098532000	-9.679988000	-11.051721000
6	1.605078000	-9.738213000	-11.194167000
8	-0.283456000	-8.635739000	-10.121641000
1	-2.216363000	-7.985870000	-9.782252000
1	-2.431674000	-8.066163000	-12.504066000
8	-2.873467000	-9.768899000	-11.420281000
1	-3.700623000	-9.567361000	-11.894380000
1	-0.100609000	-8.531538000	-12.853052000
1	-0.259257000	-10.645751000	-10.670195000

1	1.865034000	-10.600300000	-11.816956000
1	2.066670000	-9.852420000	-10.207306000
8	-0.745105000	-10.466001000	-13.171197000
7	-1.160867000	-6.566311000	-10.874534000
6	-2.257990000	-5.688099000	-10.934993000
8	-3.404945000	-6.175870000	-10.894131000
7	-2.015631000	-4.358574000	-11.022428000
6	-0.763330000	-3.897678000	-11.160654000
7	-0.586971000	-2.563806000	-11.176865000
6	0.346122000	-4.791223000	-11.295851000
6	0.105545000	-6.115631000	-11.105826000
1	-1.349082000	-1.983268000	-10.803708000
1	0.344919000	-2.211898000	-11.002137000
1	1.351369000	-4.427290000	-11.464072000
1	0.883285000	-6.866728000	-11.131353000
15	3.394038000	-8.491402000	-12.791194000
8	3.575702000	-9.813238000	-13.474560000
8	3.319757000	-7.174256000	-13.504079000
8	-7.824898000	2.689997000	-6.169908000
6	-8.324507000	-0.617747000	-8.043782000
6	-8.481446000	-1.432725000	-6.763078000
6	-8.449491000	-0.312041000	-5.712992000
6	-9.303463000	0.755112000	-6.409817000
6	-9.143637000	2.184660000	-5.930164000
8	-8.961108000	0.630345000	-7.809859000
1	-8.780166000	-1.115161000	-8.903252000
1	-7.697056000	-2.181572000	-6.654119000
8	-9.764997000	-2.050758000	-6.774906000
1	-10.122363000	-1.941205000	-5.874965000
1	-7.430620000	0.049815000	-5.547425000
1	-10.359448000	0.483835000	-6.275395000
1	-9.339107000	2.195132000	-4.850841000
1	-9.893892000	2.817346000	-6.412706000
8	-9.051799000	-0.708758000	-4.490483000
7	-4.192885000	-2.665861000	-10.148930000
6	-5.448297000	-3.201866000	-9.977642000
7	-5.631504000	-4.462733000	-10.414726000
7	-6.460879000	-2.532198000	-9.431135000

6	-6.100177000	-1.298432000	-9.021602000
6	-4.856859000	-0.669739000	-9.121541000
6	-3.797225000	-1.373142000	-9.768782000
8	-2.647495000	-0.968781000	-10.007379000
7	-4.883052000	0.574132000	-8.509482000
6	-6.107370000	0.695785000	-8.053230000
7	-6.905904000	-0.402218000	-8.356570000
1	-3.444519000	-3.262981000	-10.552457000
1	-4.838361000	-5.072927000	-10.644034000
1	-6.527751000	-4.885424000	-10.223839000
1	-6.503992000	1.536083000	-7.507164000
15	-8.044421000	-1.276710000	-3.268007000
8	-8.965703000	-1.607796000	-2.134344000
8	-6.849132000	-0.377328000	-3.161895000
8	-2.392997000	-9.853249000	-15.031880000
6	-5.306541000	-7.782176000	-13.898555000
6	-6.042284000	-8.136213000	-15.198340000
6	-5.159750000	-9.250506000	-15.778546000
6	-4.720232000	-9.994654000	-14.504992000
6	-3.406779000	-10.748406000	-14.582748000
8	-4.612730000	-8.953333000	-13.499629000
1	-6.013151000	-7.479353000	-13.126635000
1	-6.133228000	-7.268186000	-15.862473000
8	-7.313082000	-8.653330000	-14.836051000
1	-7.557751000	-9.286009000	-15.534980000
1	-4.288480000	-8.822473000	-16.287515000
1	-5.519248000	-10.686246000	-14.212497000
1	-3.518470000	-11.590936000	-15.278528000
1	-3.154553000	-11.143406000	-13.593157000
8	-5.944834000	-10.032735000	-16.661008000
7	-4.354960000	-6.661687000	-14.059770000
6	-4.847286000	-5.380498000	-13.789221000
8	-6.031253000	-5.178175000	-13.532236000
7	-3.911586000	-4.375795000	-13.852719000
6	-2.563719000	-4.499906000	-14.180027000
8	-1.824489000	-3.506765000	-14.190267000
6	-2.152376000	-5.845511000	-14.508507000
1	-1.126278000	-6.035516000	-14.793055000

6	-3.049466000	-6.858102000	-14.442294000
1	-4.271823000	-3.419396000	-13.646287000
1	-2.773363000	-7.880542000	-14.670851000
15	-0.788403000	-10.258216000	-14.819145000
8	-0.531239000	-11.615469000	-15.403061000
8	-0.030160000	-9.020640000	-15.209669000
8	-5.534953000	5.204985000	-9.911196000
6	-7.575596000	2.414275000	-11.818470000
6	-8.166059000	2.076885000	-10.440224000
6	-7.680753000	3.279956000	-9.628115000
6	-7.769423000	4.427828000	-10.633470000
6	-6.835279000	5.597766000	-10.324196000
8	-7.443188000	3.820314000	-11.903143000
1	-8.209747000	2.032113000	-12.623768000
1	-7.759963000	1.130246000	-10.080676000
8	-9.578487000	2.025408000	-10.527180000
1	-9.872394000	1.873779000	-9.610353000
1	-6.635996000	3.112045000	-9.361353000
1	-8.805141000	4.791050000	-10.672711000
1	-7.323653000	6.216431000	-9.556398000
1	-6.725425000	6.211774000	-11.224370000
8	-8.463746000	3.552989000	-8.480648000
7	-4.891521000	-1.731015000	-13.298204000
6	-6.214304000	-1.527785000	-13.167958000
7	-6.844862000	-0.425620000	-12.758583000
6	-5.969448000	0.546873000	-12.440278000
6	-4.573386000	0.470654000	-12.492160000
6	-4.025341000	-0.741397000	-12.969245000
7	-2.705260000	-0.936955000	-13.139611000
7	-3.995736000	1.654548000	-12.067945000
6	-5.019243000	2.427245000	-11.772759000
7	-6.243011000	1.818915000	-11.989362000
1	-6.832820000	-2.385341000	-13.423334000
1	-2.077050000	-0.327984000	-12.634866000
1	-2.361636000	-1.865785000	-13.398942000
1	-4.966807000	3.434458000	-11.380149000
15	-7.715968000	4.068098000	-7.086235000
8	-8.580625000	5.144891000	-6.504091000

8	-6.240548000	4.260296000	-7.359042000
1	8.844303000	-6.524825000	3.682044000
1	2.190411000	7.133032000	-3.913241000
1	-5.379548000	-10.697232000	-17.084829000
1	-5.628809000	4.887495000	-8.980682000

Figure S29. X-Y coordinates for **1:2** at level: B3LYP-GD3/6-31G*.

8	1.730584000	5.345614000	-4.761877000
6	4.214662000	4.567376000	-2.036073000
6	5.250027000	4.441289000	-3.156549000
6	4.521948000	5.077789000	-4.365846000
6	3.722422000	6.213036000	-3.705715000
6	2.450548000	6.591560000	-4.442078000
8	3.372702000	5.720898000	-2.337209000
1	4.695713000	4.672322000	-1.059978000
1	5.557156000	3.406431000	-3.289619000
8	6.384257000	5.324985000	-2.842186000
1	6.496048000	5.808734000	-3.729723000
1	3.888367000	4.382366000	-4.918454000
1	4.375375000	7.090873000	-3.613692000
1	2.743636000	7.126678000	-5.360259000
1	1.850763000	7.260841000	-3.806600000
8	5.503095000	5.718932000	-5.259423000
7	3.340199000	3.351971000	-1.976103000
6	3.827449000	2.230429000	-1.246475000
8	5.040292000	2.250374000	-0.867250000
7	2.952914000	1.220695000	-0.969757000
6	1.691937000	1.213705000	-1.486985000
7	0.861560000	0.234589000	-1.108625000
6	1.267096000	2.263368000	-2.373870000
6	2.101061000	3.328670000	-2.565107000
1	1.195951000	-0.526312000	-0.464518000
1	-0.069011000	0.176619000	-1.515763000
1	0.289614000	2.232417000	-2.841344000
1	1.847100000	4.173599000	-3.205262000
8	4.801941000	-8.307318000	2.474119000
6	6.564458000	-5.397156000	0.733818000
6	7.359106000	-5.182800000	2.031266000
6	7.006217000	-6.434422000	2.867193000
6	6.991297000	-7.521933000	1.769444000
6	6.166878000	-8.745934000	2.086420000
8	6.418304000	-6.846554000	0.557564000
1	7.034516000	-4.946101000	-0.146310000
1	7.124488000	-4.225475000	2.509324000

8	8.804171000	-5.368538000	1.798557000
1	9.200119000	-4.487043000	1.554961000
1	6.014729000	-6.359369000	3.321253000
1	8.028799000	-7.815578000	1.557892000
1	6.624881000	-9.295026000	2.919615000
1	6.106257000	-9.382007000	1.194640000
8	8.002994000	-6.688307000	3.888668000
7	3.944197000	-1.079834000	0.132452000
6	5.304499000	-1.314575000	0.017974000
7	6.086227000	-0.276811000	-0.341342000
7	5.866625000	-2.523357000	0.266168000
6	4.957382000	-3.459991000	0.615550000
6	3.569952000	-3.309406000	0.817297000
6	2.982426000	-2.041950000	0.526335000
8	1.748202000	-1.730662000	0.570383000
7	2.998423000	-4.536279000	1.230169000
6	4.012587000	-5.409311000	1.256901000
7	5.229533000	-4.796198000	0.878765000
1	3.552770000	-0.149446000	-0.253690000
1	5.703224000	0.674971000	-0.538007000
1	7.052205000	-0.493855000	-0.571273000
1	3.990262000	-6.444220000	1.565354000
8	6.827747000	3.566234000	-5.568724000
6	8.352611000	0.423187000	-3.967068000
6	8.991429000	0.202954000	-5.342543000
6	8.719295000	1.546748000	-6.038017000
6	8.951887000	2.552658000	-4.899806000
6	8.190919000	3.854174000	-5.057887000
8	8.502218000	1.853267000	-3.654969000
1	8.823880000	-0.196310000	-3.196008000
1	8.603335000	-0.675410000	-5.855482000
8	10.451716000	0.115784000	-5.169651000
1	10.774007000	0.696171000	-5.933013000
1	7.713836000	1.638576000	-6.448703000
1	10.028347000	2.755717000	-4.821908000
1	8.699287000	4.494167000	-5.789180000
1	8.090056000	4.360262000	-4.090049000
8	9.734796000	1.793116000	-7.075946000

7	4.638992000	-2.924297000	-2.695067000
6	5.995267000	-3.152183000	-2.812636000
7	6.436791000	-4.409072000	-2.558182000
7	6.879421000	-2.191587000	-3.175810000
6	6.278366000	-1.022740000	-3.500277000
6	4.903003000	-0.714360000	-3.458088000
6	3.997359000	-1.694816000	-2.969020000
8	2.747187000	-1.562394000	-2.786045000
7	4.676069000	0.598027000	-3.923096000
6	5.885789000	1.075167000	-4.231199000
7	6.904695000	0.128109000	-3.973470000
1	3.978405000	-3.743320000	-2.456009000
1	5.767204000	-5.214262000	-2.558027000
1	7.410376000	-4.586583000	-2.796242000
1	6.119677000	2.036990000	-4.666586000
15	6.080933000	4.719463000	-6.517547000
8	7.110389000	5.557314000	-7.226896000
8	4.901176000	4.039444000	-7.154808000
8	0.057325000	-9.229792000	0.352493000
6	3.286011000	-8.656249000	-1.674420000
6	4.013727000	-8.931667000	-0.364803000
6	2.879700000	-9.466391000	0.541511000
6	2.077010000	-10.352790000	-0.425259000
6	0.596677000	-10.519899000	-0.118733000
8	2.213007000	-9.654611000	-1.755763000
1	3.932955000	-8.707428000	-2.550166000
1	4.538016000	-8.050244000	0.005221000
8	4.943016000	-10.063116000	-0.558459000
1	4.740976000	-10.617587000	0.268415000
1	2.257693000	-8.692093000	0.991512000
1	2.562036000	-11.332370000	-0.508619000
1	0.484438000	-11.285327000	0.662788000
1	0.072145000	-10.815321000	-1.035060000
8	3.467071000	-10.325253000	1.582861000
7	2.693276000	-7.294622000	-1.624280000
6	3.466317000	-6.226620000	-2.152749000
8	4.631733000	-6.499268000	-2.592405000
7	2.929188000	-4.980827000	-2.133854000

6	1.673215000	-4.747541000	-1.648633000
7	1.210732000	-3.498796000	-1.711646000
6	0.898829000	-5.822105000	-1.097986000
6	1.448337000	-7.067119000	-1.088693000
1	1.799508000	-2.732995000	-2.135842000
1	0.346168000	-3.253483000	-1.237906000
1	-0.100703000	-5.705240000	-0.697337000
1	0.925855000	-7.908870000	-0.642914000
15	3.770621000	-9.493387000	3.044254000
8	4.529740000	-10.473993000	3.896085000
8	2.512836000	-8.767759000	3.439535000
8	8.879440000	-0.035558000	-8.656119000
6	8.176718000	-3.465761000	-7.013085000
6	8.105513000	-4.069072000	-8.407029000
6	8.558239000	-2.885125000	-9.286095000
6	9.727846000	-2.330084000	-8.451263000
6	10.097410000	-0.875588000	-8.629643000
8	9.291823000	-2.518279000	-7.021892000
1	8.297369000	-4.209167000	-6.219817000
1	7.129039000	-4.487029000	-8.638092000
8	9.161389000	-5.096327000	-8.541057000
1	9.529201000	-4.866984000	-9.458013000
1	7.783660000	-2.139230000	-9.470381000
1	10.613149000	-2.954294000	-8.629108000
1	10.658185000	-0.739615000	-9.562909000
1	10.724775000	-0.585056000	-7.775228000
8	9.051333000	-3.429874000	-10.563756000
7	3.310930000	-3.824178000	-5.349207000
6	4.317917000	-4.732727000	-5.330287000
7	5.590462000	-4.531004000	-5.751074000
6	5.770469000	-3.268521000	-6.222015000
6	4.805807000	-2.242386000	-6.283275000
6	3.510292000	-2.546106000	-5.809063000
7	2.494082000	-1.679526000	-5.780191000
7	5.348238000	-1.083230000	-6.862969000
6	6.617240000	-1.401038000	-7.159978000
7	6.923907000	-2.723500000	-6.770782000
1	4.054399000	-5.702770000	-4.926490000

1	2.657300000	-0.725905000	-6.091126000
1	1.581304000	-1.955815000	-5.353145000
1	7.355094000	-0.773969000	-7.646677000
15	9.177668000	1.618570000	-8.666793000
8	10.373041000	1.903814000	-9.534416000
8	7.828301000	2.273761000	-8.786893000
8	-3.850641000	-7.075077000	-3.028492000
6	-0.614714000	-8.092006000	-4.586605000
6	-0.257779000	-8.726239000	-3.230509000
6	-1.625459000	-8.662295000	-2.532279000
6	-2.599170000	-9.049221000	-3.643634000
6	-3.990963000	-8.493158000	-3.428865000
8	-2.007630000	-8.421411000	-4.876698000
1	0.050765000	-8.441830000	-5.380516000
1	0.481034000	-8.104244000	-2.731253000
8	0.198216000	-10.095761000	-3.403323000
1	1.093869000	-10.095816000	-2.920110000
1	-1.822742000	-7.634722000	-2.223047000
1	-2.619147000	-10.140659000	-3.764699000
1	-4.481016000	-9.039260000	-2.613349000
1	-4.582415000	-8.523476000	-4.351231000
8	-1.807385000	-9.550964000	-1.390412000
7	-0.470878000	-6.606463000	-4.496826000
6	0.834371000	-6.100610000	-4.673759000
8	1.823233000	-6.873807000	-4.748258000
7	0.904843000	-4.731120000	-4.743281000
6	-0.145243000	-3.817475000	-4.607383000
8	0.058928000	-2.569877000	-4.726699000
6	-1.425124000	-4.421805000	-4.319359000
1	-2.285010000	-3.784415000	-4.159976000
6	-1.546658000	-5.778454000	-4.301649000
1	1.904300000	-4.329401000	-4.944267000
1	-2.482994000	-6.275797000	-4.074845000
15	-1.574958000	-8.862869000	0.116122000
8	-2.419616000	-9.643407000	1.086462000
8	-1.611160000	-7.354475000	-0.003358000
8	6.784179000	-4.642770000	-11.078989000
6	4.542675000	-6.203370000	-8.542927000

6	3.904001000	-7.160515000	-9.533319000
6	4.751964000	-6.908797000	-10.802704000
6	6.164470000	-6.820533000	-10.199312000
6	7.227660000	-6.044293000	-10.946963000
8	5.960966000	-6.150835000	-8.867758000
1	4.412112000	-6.496470000	-7.498726000
1	2.838861000	-6.983733000	-9.647448000
8	4.188685000	-8.542811000	-9.107563000
1	4.428587000	-8.970379000	-9.994972000
1	4.464155000	-6.003507000	-11.342171000
1	6.520414000	-7.844687000	-10.026082000
1	7.399728000	-6.494090000	-11.934726000
1	8.143488000	-6.082596000	-10.344422000
8	4.669839000	-8.102223000	-11.666522000
7	0.152975000	-3.776515000	-7.904913000
6	0.451360000	-5.124355000	-7.830057000
7	-0.548284000	-5.989331000	-7.567496000
7	1.702005000	-5.604280000	-8.020884000
6	2.575297000	-4.656753000	-8.422855000
6	2.334072000	-3.293834000	-8.675972000
6	1.051940000	-2.769364000	-8.329690000
8	0.674365000	-1.553272000	-8.379828000
7	3.495954000	-2.686739000	-9.209566000
6	4.420381000	-3.656675000	-9.247628000
7	3.906241000	-4.878460000	-8.751308000
1	-0.844511000	-3.451102000	-7.649131000
1	-1.545447000	-5.683140000	-7.521526000
1	-0.321700000	-6.974536000	-7.691700000
1	5.404604000	-3.597442000	-9.683463000
15	7.839252000	-3.544783000	-11.766062000
8	8.536098000	-4.168515000	-12.944398000
8	7.073012000	-2.247547000	-11.768848000
8	-6.709635000	-2.250246000	-3.671386000
6	-5.559808000	-4.644120000	-6.268509000
6	-5.202649000	-5.656292000	-5.178751000
6	-5.835218000	-5.014901000	-3.919019000
6	-7.153516000	-4.467564000	-4.473996000
6	-7.744049000	-3.297584000	-3.711776000

8	-6.824601000	-4.023844000	-5.872255000
1	-5.639376000	-5.085909000	-7.262878000
1	-4.129050000	-5.817882000	-5.127648000
8	-5.940330000	-6.904887000	-5.421556000
1	-6.273761000	-7.112728000	-4.486233000
1	-5.216101000	-4.238945000	-3.465862000
1	-7.881193000	-5.287650000	-4.524431000
1	-8.007706000	-3.623240000	-2.695268000
1	-8.625287000	-2.935346000	-4.251883000
8	-6.169983000	-6.057488000	-2.931046000
7	-4.484406000	-3.599423000	-6.326105000
6	-3.287210000	-3.938188000	-7.015931000
8	-3.168812000	-5.126984000	-7.453674000
7	-2.333602000	-2.974547000	-7.140198000
6	-2.479174000	-1.736932000	-6.581735000
7	-1.530655000	-0.831750000	-6.840284000
6	-3.622600000	-1.452188000	-5.760223000
6	-4.604883000	-2.396812000	-5.679940000
1	-0.718797000	-1.080058000	-7.456799000
1	-1.589075000	0.097144000	-6.430551000
1	-3.756336000	-0.518713000	-5.226839000
1	-5.488296000	-2.254772000	-5.065010000
15	-4.872443000	-6.427839000	-1.883213000
8	-5.372346000	-7.517705000	-0.972746000
8	-4.249732000	-5.129398000	-1.447023000
8	2.092749000	-8.143677000	-11.477853000
6	-1.466295000	-7.838908000	-10.182591000
6	-1.879870000	-8.665347000	-11.411796000
6	-0.499974000	-9.110387000	-11.913842000
6	0.239397000	-9.466489000	-10.627111000
6	1.741826000	-9.412047000	-10.791043000
8	-0.229833000	-8.417712000	-9.650107000
1	-2.255585000	-7.826393000	-9.427652000
1	-2.389248000	-8.024406000	-12.127637000
8	-2.697036000	-9.800224000	-11.004313000
1	-3.555823000	-9.662669000	-11.530894000
1	-0.006423000	-8.261838000	-12.389378000
1	-0.081046000	-10.455990000	-10.274370000

1	2.045081000	-10.246665000	-11.436762000
1	2.273516000	-9.435439000	-9.833625000
8	-0.467378000	-10.252197000	-12.818449000
7	-1.205863000	-6.426292000	-10.582906000
6	-2.333968000	-5.566413000	-10.610560000
8	-3.483841000	-6.106427000	-10.526538000
7	-2.111263000	-4.228223000	-10.711327000
6	-0.852449000	-3.737573000	-10.903585000
7	-0.697892000	-2.406351000	-10.909384000
6	0.261386000	-4.627953000	-11.065075000
6	0.056697000	-5.958740000	-10.843793000
1	-1.489249000	-1.797537000	-10.571226000
1	0.242494000	-2.018993000	-10.868253000
1	1.255996000	-4.244760000	-11.255421000
1	0.852291000	-6.695944000	-10.875043000
15	3.278624000	-8.143447000	-12.657824000
8	3.318049000	-9.487716000	-13.337390000
8	3.151930000	-6.812326000	-13.346392000
8	-7.298918000	3.087614000	-6.164892000
6	-8.244818000	-0.491334000	-7.555372000
6	-8.144603000	-1.113882000	-6.172300000
6	-7.856810000	0.133205000	-5.314042000
6	-8.866213000	1.139322000	-5.899587000
6	-8.593790000	2.607717000	-5.617120000
8	-8.881350000	0.827607000	-7.370915000
1	-8.810727000	-1.079791000	-8.281019000
1	-7.404131000	-1.912087000	-6.130471000
8	-9.476075000	-1.603052000	-5.755761000
1	-9.529151000	-1.245873000	-4.809250000
1	-6.823202000	0.477778000	-5.372794000
1	-9.855102000	0.900817000	-5.485987000
1	-8.555212000	2.703737000	-4.522395000
1	-9.417061000	3.224193000	-5.997716000
8	-8.221742000	-0.148972000	-3.919226000
7	-4.164950000	-2.644132000	-9.828071000
6	-5.406727000	-3.195043000	-9.557692000
7	-5.583843000	-4.497254000	-9.853721000
7	-6.426242000	-2.489467000	-9.006413000

6	-6.075986000	-1.222287000	-8.698470000
6	-4.841228000	-0.580755000	-8.917726000
6	-3.797240000	-1.307839000	-9.553543000
8	-2.648862000	-0.865029000	-9.867139000
7	-4.861201000	0.731105000	-8.398461000
6	-6.076412000	0.882984000	-7.868607000
7	-6.869789000	-0.279829000	-8.049050000
1	-3.389640000	-3.267982000	-10.240965000
1	-4.799747000	-5.113607000	-10.174653000
1	-6.518450000	-4.876462000	-9.731428000
1	-6.471708000	1.746750000	-7.360017000
15	-6.919500000	-0.743946000	-2.989712000
8	-7.456664000	-0.857453000	-1.591569000
8	-5.674790000	0.004247000	-3.402170000
8	-2.171624000	-9.939501000	-14.712055000
6	-5.243590000	-8.140752000	-13.411733000
6	-5.896546000	-8.631975000	-14.711529000
6	-4.918601000	-9.711724000	-15.233344000
6	-4.423586000	-10.375816000	-13.929470000
6	-3.001499000	-10.916455000	-13.979593000
8	-4.463858000	-9.276341000	-12.901987000
1	-6.001429000	-7.827658000	-12.691080000
1	-6.056589000	-7.807752000	-15.421131000
8	-7.121558000	-9.327064000	-14.329550000
1	-7.107353000	-10.117555000	-14.967283000
1	-4.075756000	-9.298395000	-15.794279000
1	-5.134957000	-11.151951000	-13.621522000
1	-2.998867000	-11.887332000	-14.498266000
1	-2.618546000	-11.022727000	-12.958447000
8	-5.750143000	-10.611584000	-16.045634000
7	-4.345934000	-6.984654000	-13.621690000
6	-4.852034000	-5.708479000	-13.258425000
8	-6.032944000	-5.558810000	-12.863238000
7	-3.952224000	-4.679415000	-13.416386000
6	-2.606912000	-4.769890000	-13.803477000
8	-1.883299000	-3.728707000	-13.863838000
6	-2.168704000	-6.109034000	-14.124178000
1	-1.149121000	-6.327472000	-14.412649000

6	-3.040633000	-7.150077000	-14.037018000
1	-4.341665000	-3.692455000	-13.178885000
1	-2.726638000	-8.163846000	-14.278686000
15	-0.503530000	-9.882260000	-14.449761000
8	0.164789000	-11.020972000	-15.170888000
8	-0.135937000	-8.428380000	-14.655695000
8	-5.867574000	4.893369000	-10.526819000
6	-8.015920000	1.782335000	-11.658145000
6	-8.322897000	1.664832000	-10.154942000
6	-7.820298000	3.023392000	-9.661479000
6	-8.198528000	3.998017000	-10.776094000
6	-7.265201000	5.220788000	-10.810253000
8	-8.069136000	3.196503000	-12.035010000
1	-8.695738000	1.175716000	-12.265675000
1	-7.735908000	0.848554000	-9.733613000
8	-9.748869000	1.505083000	-9.923070000
1	-9.772567000	1.429750000	-8.913153000
1	-6.734599000	2.984525000	-9.576060000
1	-9.246790000	4.301033000	-10.649877000
1	-7.661866000	5.944709000	-10.075886000
1	-7.307480000	5.674441000	-11.808863000
8	-8.429012000	3.469563000	-8.413531000
7	-4.984861000	-2.251722000	-12.886938000
6	-6.325332000	-2.184356000	-12.671014000
7	-7.041083000	-1.081353000	-12.344611000
6	-6.248150000	0.017315000	-12.222003000
6	-4.846682000	0.071054000	-12.391689000
6	-4.194507000	-1.134152000	-12.754200000
7	-2.879046000	-1.246587000	-12.980730000
7	-4.368685000	1.375482000	-12.161752000
6	-5.461897000	2.100448000	-11.865630000
7	-6.630575000	1.313300000	-11.900095000
1	-6.840242000	-3.137632000	-12.754051000
1	-2.275519000	-0.464468000	-12.741180000
1	-2.465597000	-2.164748000	-13.259322000
1	-5.496577000	3.146123000	-11.564553000
15	-7.441646000	4.271061000	-7.345555000
8	-8.201997000	5.455268000	-6.818524000

8	-6.045168000	4.385922000	-7.953008000
1	8.835774000	-6.338224000	3.429367000
1	0.817189000	5.592394000	-5.077828000
1	-5.260033000	-11.470695000	-16.172682000
1	-5.836315000	4.728313000	-9.490955000

Figure S30. X-Y coordinates for **1:2** at level: B97D3/3-21G*.

8	2.779823000	6.543133000	-3.714771000
6	5.246763000	4.981097000	-1.261962000
6	6.220266000	4.772594000	-2.430766000
6	5.536686000	5.589870000	-3.542679000
6	4.979024000	6.783898000	-2.753369000
6	3.792470000	7.495386000	-3.376787000
8	4.628825000	6.241986000	-1.450483000
1	5.765627000	4.954353000	-0.297416000
1	6.347386000	3.712283000	-2.668406000
8	7.473870000	5.371526000	-2.097407000
1	7.748917000	5.823486000	-2.923170000
1	4.728783000	5.017870000	-4.013652000
1	5.783363000	7.525007000	-2.617242000
1	4.160937000	8.022125000	-4.275407000
1	3.412698000	8.250862000	-2.668435000
8	6.463825000	6.054804000	-4.522136000
7	4.203001000	3.911210000	-1.208239000
6	4.565709000	2.672088000	-0.623744000
8	5.765034000	2.495442000	-0.309102000
7	3.594829000	1.744899000	-0.415527000
6	2.334996000	1.952673000	-0.853379000
7	1.418076000	1.006016000	-0.589466000
6	1.976504000	3.156265000	-1.544786000
6	2.936262000	4.119595000	-1.675696000
1	1.687709000	0.123306000	-0.126825000
1	0.484924000	1.089745000	-0.971794000
1	0.969796000	3.319102000	-1.920407000
1	2.752746000	5.079708000	-2.153233000
8	4.904685000	-8.302512000	2.672465000
6	6.669642000	-5.385270000	0.909908000
6	7.460709000	-5.109333000	2.207646000
6	7.107812000	-6.340826000	3.061451000
6	7.055058000	-7.444111000	1.984335000
6	6.245170000	-8.677078000	2.330813000
8	6.507024000	-6.792899000	0.807891000
1	7.186948000	-4.997271000	0.022663000
1	7.172534000	-4.154840000	2.666514000

8	8.872405000	-5.180427000	1.985273000
1	9.171455000	-4.302342000	1.691810000
1	6.112827000	-6.218808000	3.506940000
1	8.085512000	-7.772735000	1.763506000
1	6.731133000	-9.182519000	3.179161000
1	6.246548000	-9.362275000	1.470882000
8	8.025147000	-6.593438000	4.108786000
7	4.351899000	-0.927595000	0.376076000
6	5.684272000	-1.258401000	0.242472000
7	6.544897000	-0.249912000	-0.024276000
7	6.150924000	-2.501813000	0.402407000
6	5.173686000	-3.382193000	0.710273000
6	3.799855000	-3.151813000	0.913714000
6	3.307263000	-1.821299000	0.710160000
8	2.130704000	-1.406210000	0.798708000
7	3.157354000	-4.328046000	1.297661000
6	4.109769000	-5.246919000	1.314221000
7	5.354969000	-4.731912000	0.949099000
1	4.066624000	0.052994000	0.150094000
1	6.226348000	0.715400000	-0.194187000
1	7.476066000	-0.516588000	-0.316638000
1	3.996976000	-6.289474000	1.588017000
8	7.386158000	3.769247000	-5.286573000
6	8.480229000	0.475194000	-3.753496000
6	9.044621000	0.059582000	-5.116044000
6	8.926382000	1.378651000	-5.893100000
6	9.312752000	2.402711000	-4.815472000
6	8.794495000	3.809174000	-5.034794000
8	8.789403000	1.852590000	-3.576348000
1	8.916941000	-0.118053000	-2.939005000
1	8.483642000	-0.768288000	-5.560154000
8	10.419580000	-0.289074000	-4.949728000
1	10.843936000	-0.001443000	-5.783460000
1	7.896212000	1.550575000	-6.224467000
1	10.411828000	2.450946000	-4.743918000
1	9.321305000	4.246630000	-5.894995000
1	9.004967000	4.420709000	-4.143657000
8	9.828546000	1.444777000	-6.995854000

7	4.682950000	-2.753267000	-2.632468000
6	6.029188000	-3.007229000	-2.764116000
7	6.436577000	-4.279896000	-2.505687000
7	6.929914000	-2.071135000	-3.086359000
6	6.362418000	-0.863164000	-3.310190000
6	5.002603000	-0.507767000	-3.246482000
6	4.062298000	-1.502610000	-2.838273000
8	2.832615000	-1.364654000	-2.663678000
7	4.819685000	0.825041000	-3.602455000
6	6.036670000	1.273776000	-3.861744000
7	7.019430000	0.297598000	-3.682695000
1	4.037365000	-3.549445000	-2.411736000
1	5.741897000	-5.040637000	-2.560358000
1	7.360854000	-4.500527000	-2.859482000
1	6.297285000	2.263815000	-4.215936000
15	6.636877000	5.115676000	-5.929381000
8	7.595908000	5.896190000	-6.789722000
8	5.277608000	4.642203000	-6.374666000
8	0.011799000	-9.364536000	0.386414000
6	3.141750000	-8.594425000	-1.606464000
6	4.010175000	-8.878948000	-0.379525000
6	2.969057000	-9.455512000	0.598468000
6	2.105227000	-10.313114000	-0.337845000
6	0.681350000	-10.595695000	0.105156000
8	2.097587000	-9.565967000	-1.591779000
1	3.699857000	-8.662822000	-2.543697000
1	4.505565000	-7.973289000	-0.014183000
8	4.969543000	-9.887595000	-0.705027000
1	4.982161000	-10.472986000	0.081608000
1	2.367182000	-8.662256000	1.056582000
1	2.610502000	-11.276201000	-0.510948000
1	0.721121000	-11.229253000	1.005915000
1	0.155510000	-11.146017000	-0.688320000
8	3.580799000	-10.262312000	1.600604000
7	2.581413000	-7.219975000	-1.542498000
6	3.391620000	-6.168050000	-2.039828000
8	4.539207000	-6.455112000	-2.455210000
7	2.891001000	-4.909716000	-2.032180000

6	1.665230000	-4.651575000	-1.527819000
7	1.217415000	-3.392003000	-1.594544000
6	0.860662000	-5.691296000	-0.956962000
6	1.364092000	-6.957321000	-0.976771000
1	1.825311000	-2.639484000	-1.960220000
1	0.368836000	-3.135658000	-1.107684000
1	-0.116326000	-5.494726000	-0.523843000
1	0.829131000	-7.805159000	-0.556225000
15	3.836994000	-9.514675000	3.108314000
8	4.530850000	-10.566038000	3.934633000
8	2.577645000	-8.795672000	3.518925000
8	8.824132000	-0.292326000	-8.640272000
6	7.938193000	-3.505089000	-6.812930000
6	7.851561000	-4.300791000	-8.115730000
6	8.342950000	-3.244982000	-9.122896000
6	9.493283000	-2.601803000	-8.327878000
6	9.926334000	-1.201354000	-8.714070000
8	9.036723000	-2.619301000	-6.947581000
1	8.077699000	-4.144385000	-5.932604000
1	6.841436000	-4.671292000	-8.310080000
8	8.781880000	-5.384749000	-8.062197000
1	9.184825000	-5.403400000	-8.955007000
1	7.561082000	-2.508999000	-9.346169000
1	10.378848000	-3.253425000	-8.413565000
1	10.330763000	-1.233522000	-9.738233000
1	10.735757000	-0.883444000	-8.039491000
8	8.824449000	-3.848525000	-10.321567000
7	3.037082000	-3.873253000	-5.321657000
6	4.048239000	-4.762386000	-5.306379000
7	5.325929000	-4.569183000	-5.674033000
6	5.521563000	-3.302764000	-6.101393000
6	4.566670000	-2.271970000	-6.173622000
6	3.254729000	-2.599017000	-5.748348000
7	2.226982000	-1.736199000	-5.766171000
7	5.117309000	-1.120625000	-6.721064000
6	6.378800000	-1.443342000	-6.977426000
7	6.687766000	-2.749380000	-6.604979000
1	3.782261000	-5.754555000	-4.945546000

1	2.402782000	-0.769250000	-6.003737000
1	1.331046000	-1.998276000	-5.336865000
1	7.122034000	-0.806350000	-7.443915000
15	9.174563000	1.345367000	-8.557258000
8	10.326198000	1.679765000	-9.469498000
8	7.832001000	2.031181000	-8.588741000
8	-4.333785000	-7.286860000	-2.567556000
6	-1.100902000	-8.111878000	-4.313990000
6	-0.613929000	-8.797300000	-3.022848000
6	-1.924916000	-8.838361000	-2.213373000
6	-2.968453000	-9.121033000	-3.297603000
6	-4.375762000	-8.659988000	-2.974629000
8	-2.473286000	-8.418528000	-4.473997000
1	-0.529191000	-8.453960000	-5.183184000
1	0.146779000	-8.186068000	-2.539733000
8	-0.105522000	-10.093349000	-3.307828000
1	0.769962000	-10.114924000	-2.868986000
1	-2.110207000	-7.843143000	-1.789850000
1	-2.992583000	-10.201849000	-3.515122000
1	-4.778791000	-9.285112000	-2.165359000
1	-5.014324000	-8.771842000	-3.863567000
8	-1.992568000	-9.819878000	-1.188770000
7	-0.914851000	-6.631799000	-4.248840000
6	0.377825000	-6.166391000	-4.532605000
8	1.327460000	-6.941834000	-4.693242000
7	0.492067000	-4.797315000	-4.610830000
6	-0.512957000	-3.850473000	-4.396190000
8	-0.273491000	-2.632313000	-4.519998000
6	-1.791059000	-4.415748000	-4.024693000
1	-2.622013000	-3.750959000	-3.808870000
6	-1.945844000	-5.770114000	-3.977865000
1	1.456797000	-4.437966000	-4.847615000
1	-2.884099000	-6.246129000	-3.707448000
15	-1.669627000	-9.347880000	0.389328000
8	-2.185494000	-10.474145000	1.248744000
8	-2.028676000	-7.894790000	0.589662000
8	6.605017000	-5.003766000	-11.085778000
6	4.254333000	-6.569073000	-8.607134000

6	3.656544000	-7.562092000	-9.601842000
6	4.551358000	-7.310335000	-10.831552000
6	5.924144000	-7.138026000	-10.162954000
6	6.992899000	-6.369955000	-10.919979000
8	5.638092000	-6.488474000	-8.893934000
1	4.115822000	-6.877103000	-7.563185000
1	2.593383000	-7.378901000	-9.778891000
8	3.873863000	-8.888653000	-9.115319000
1	4.123003000	-9.399107000	-9.914807000
1	4.248630000	-6.399439000	-11.363160000
1	6.329537000	-8.143149000	-9.958911000
1	7.143266000	-6.856744000	-11.896830000
1	7.935340000	-6.435308000	-10.358204000
8	4.564116000	-8.435377000	-11.711135000
7	-0.117652000	-4.097024000	-7.971828000
6	0.167697000	-5.438878000	-7.860952000
7	-0.850692000	-6.261644000	-7.500418000
7	1.386399000	-5.948086000	-8.058264000
6	2.278917000	-5.014007000	-8.452408000
6	2.077747000	-3.640959000	-8.683070000
6	0.791670000	-3.091384000	-8.372877000
8	0.421253000	-1.898687000	-8.435004000
7	3.245601000	-3.050173000	-9.162213000
6	4.132554000	-4.032931000	-9.204737000
7	3.603606000	-5.250589000	-8.772488000
1	-1.094486000	-3.778146000	-7.763083000
1	-1.828524000	-5.942532000	-7.576119000
1	-0.671392000	-7.248883000	-7.641462000
1	5.148598000	-3.964592000	-9.570533000
15	7.752964000	-3.919706000	-11.642837000
8	8.571079000	-4.539879000	-12.745592000
8	7.019404000	-2.607476000	-11.751801000
8	-7.382460000	-2.586803000	-3.721205000
6	-5.927436000	-4.943021000	-6.300743000
6	-5.616274000	-5.988719000	-5.221118000
6	-6.336262000	-5.383934000	-3.999213000
6	-7.600847000	-4.803030000	-4.646542000
6	-8.289194000	-3.679994000	-3.893945000

8	-7.172835000	-4.356881000	-5.961652000
1	-5.982072000	-5.387797000	-7.299461000
1	-4.537974000	-6.122062000	-5.086095000
8	-6.239333000	-7.223001000	-5.579306000
1	-6.626437000	-7.549467000	-4.739185000
1	-5.734402000	-4.595058000	-3.531869000
1	-8.334307000	-5.616238000	-4.773205000
1	-8.618206000	-4.068585000	-2.917936000
1	-9.175535000	-3.360798000	-4.458621000
8	-6.701528000	-6.375874000	-3.041797000
7	-4.864205000	-3.897754000	-6.364295000
6	-3.681927000	-4.225043000	-7.071012000
8	-3.568335000	-5.386219000	-7.528446000
7	-2.733826000	-3.267489000	-7.221218000
6	-2.879572000	-2.045999000	-6.661835000
7	-1.923216000	-1.140688000	-6.900140000
6	-4.018815000	-1.737079000	-5.847008000
6	-4.992071000	-2.688054000	-5.739947000
1	-1.115973000	-1.375970000	-7.496186000
1	-2.002829000	-0.206997000	-6.520061000
1	-4.136442000	-0.771574000	-5.363586000
1	-5.898161000	-2.541410000	-5.158653000
15	-5.627764000	-6.626406000	-1.747395000
8	-6.297561000	-7.668897000	-0.891138000
8	-5.141980000	-5.289853000	-1.248979000
8	1.983545000	-8.539959000	-11.897703000
6	-1.560202000	-8.029428000	-10.701177000
6	-2.044630000	-8.761302000	-11.970354000
6	-0.714806000	-9.340889000	-12.486243000
6	0.010126000	-9.715790000	-11.193166000
6	1.521447000	-9.765432000	-11.316029000
8	-0.395045000	-8.692592000	-10.237661000
1	-2.335872000	-8.032600000	-9.928311000
1	-2.480558000	-8.048499000	-12.669753000
8	-2.986013000	-9.771793000	-11.631597000
1	-3.759296000	-9.592464000	-12.204444000
1	-0.155814000	-8.542249000	-12.989599000
1	-0.348273000	-10.694874000	-10.834192000

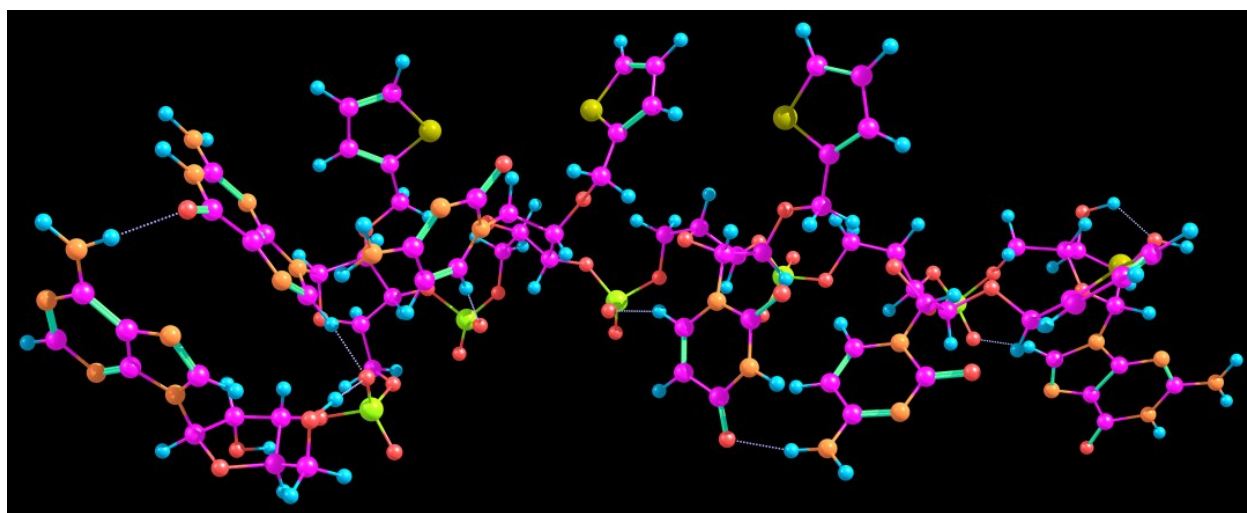
1	1.790878000	-10.616139000	-11.957460000
1	1.978088000	-9.899513000	-10.324940000
8	-0.807976000	-10.473756000	-13.337024000
7	-1.247334000	-6.596683000	-10.972563000
6	-2.339505000	-5.697939000	-11.016816000
8	-3.497177000	-6.175473000	-10.975878000
7	-2.076345000	-4.367519000	-11.087503000
6	-0.809352000	-3.922211000	-11.219065000
7	-0.617015000	-2.586761000	-11.242387000
6	0.290319000	-4.829518000	-11.349513000
6	0.029562000	-6.159756000	-11.181682000
1	-1.374313000	-1.993195000	-10.865379000
1	0.323165000	-2.250474000	-11.066788000
1	1.306446000	-4.477925000	-11.502337000
1	0.797934000	-6.925997000	-11.209547000
15	3.328685000	-8.488804000	-12.882856000
8	3.522505000	-9.806405000	-13.587981000
8	3.255423000	-7.151700000	-13.574612000
8	-7.613874000	2.763061000	-6.076000000
6	-8.249869000	-0.582186000	-7.878905000
6	-8.410488000	-1.372374000	-6.581982000
6	-8.339924000	-0.234768000	-5.547871000
6	-9.166060000	0.854982000	-6.252333000
6	-8.945598000	2.291996000	-5.805934000
8	-8.872262000	0.682079000	-7.665799000
1	-8.714254000	-1.083156000	-8.736424000
1	-7.635879000	-2.136527000	-6.471457000
8	-9.710552000	-1.966524000	-6.557099000
1	-10.032594000	-1.815231000	-5.644115000
1	-7.306602000	0.093155000	-5.381666000
1	-10.232716000	0.629554000	-6.085574000
1	-9.117123000	2.323933000	-4.718420000
1	-9.691085000	2.942341000	-6.281367000
8	-8.958264000	-0.599859000	-4.316691000
7	-4.206367000	-2.638482000	-10.195500000
6	-5.461817000	-3.166835000	-9.986899000
7	-5.689867000	-4.407026000	-10.480324000
7	-6.447311000	-2.505913000	-9.365190000

6	-6.053406000	-1.288562000	-8.929759000
6	-4.797672000	-0.667855000	-9.060871000
6	-3.773109000	-1.359585000	-9.781441000
8	-2.622699000	-0.959177000	-10.052770000
7	-4.783445000	0.562260000	-8.408018000
6	-5.996497000	0.689949000	-7.897025000
7	-6.824065000	-0.394987000	-8.203647000
1	-3.473584000	-3.244441000	-10.630009000
1	-4.898675000	-5.026096000	-10.717093000
1	-6.555064000	-4.843844000	-10.186043000
1	-6.366086000	1.527185000	-7.319774000
15	-7.942414000	-1.150161000	-3.069235000
8	-8.876433000	-1.423973000	-1.920695000
8	-6.724479000	-0.264980000	-3.000088000
8	-2.340047000	-9.856175000	-15.328683000
6	-5.264475000	-7.775799000	-14.239943000
6	-5.941955000	-8.072006000	-15.588198000
6	-5.062414000	-9.199257000	-16.155875000
6	-4.690598000	-9.989051000	-14.883268000
6	-3.377252000	-10.751980000	-14.925975000
8	-4.625303000	-8.979266000	-13.832501000
1	-6.001079000	-7.466061000	-13.493537000
1	-5.967153000	-7.180046000	-16.233767000
8	-7.252795000	-8.556863000	-15.313328000
1	-7.447603000	-9.194249000	-16.029418000
1	-4.157670000	-8.782801000	-16.621674000
1	-5.508667000	-10.686295000	-14.646158000
1	-3.472790000	-11.585317000	-15.642422000
1	-3.161920000	-11.169246000	-13.932324000
8	-5.833258000	-9.940554000	-17.094403000
7	-4.274582000	-6.673256000	-14.323256000
6	-4.750985000	-5.382202000	-14.029706000
8	-5.943861000	-5.164094000	-13.799258000
7	-3.786142000	-4.397422000	-14.041658000
6	-2.425389000	-4.544037000	-14.340960000
8	-1.662469000	-3.559445000	-14.324357000
6	-2.034528000	-5.895449000	-14.675402000
1	-1.001345000	-6.114617000	-14.926158000

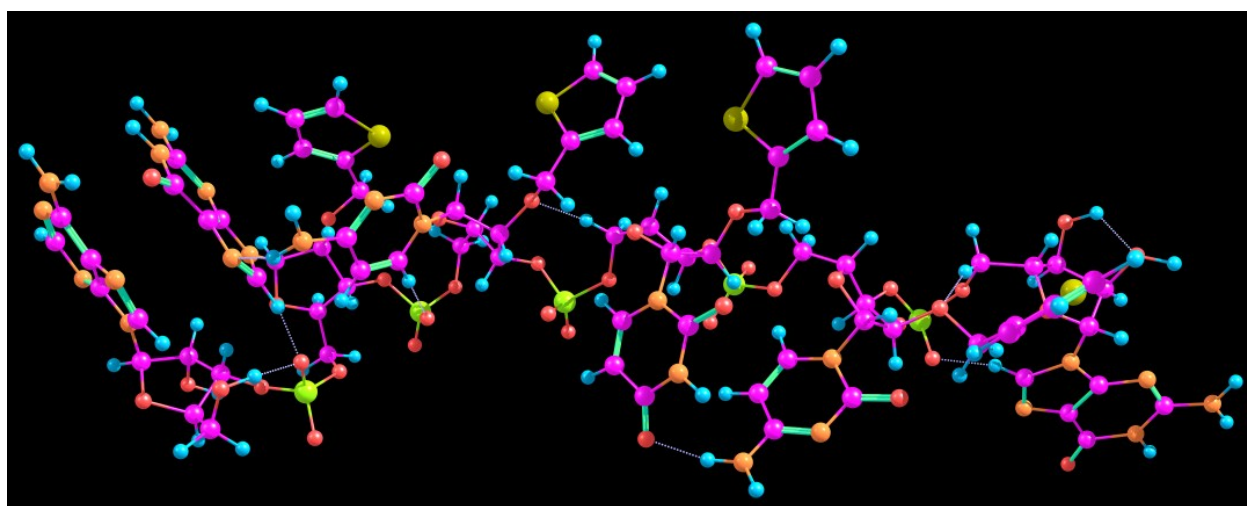
6	-2.960017000	-6.894651000	-14.661188000
1	-4.129612000	-3.433115000	-13.801749000
1	-2.698641000	-7.923813000	-14.898306000
15	-0.735796000	-10.240676000	-14.994676000
8	-0.409297000	-11.594579000	-15.571453000
8	0.019340000	-8.974305000	-15.324430000
8	-5.369238000	5.217824000	-9.913030000
6	-7.406074000	2.347152000	-11.767458000
6	-7.938795000	2.016993000	-10.361388000
6	-7.478784000	3.258992000	-9.585323000
6	-7.603796000	4.385277000	-10.613928000
6	-6.680263000	5.577333000	-10.336611000
8	-7.298438000	3.757562000	-11.887192000
1	-8.060859000	1.937788000	-12.548316000
1	-7.467946000	1.097933000	-9.996003000
8	-9.353752000	1.888365000	-10.395443000
1	-9.591278000	1.731585000	-9.457714000
1	-6.425663000	3.122530000	-9.317321000
1	-8.648883000	4.736505000	-10.640600000
1	-7.182709000	6.206144000	-9.579213000
1	-6.578129000	6.175982000	-11.252963000
8	-8.261512000	3.544677000	-8.435064000
7	-4.728545000	-1.780491000	-13.371808000
6	-6.050023000	-1.595416000	-13.173552000
7	-6.680043000	-0.495894000	-12.727939000
6	-5.798629000	0.488391000	-12.446229000
6	-4.395969000	0.429887000	-12.561066000
6	-3.856329000	-0.774837000	-13.080432000
7	-2.545132000	-0.954220000	-13.340395000
7	-3.813255000	1.624770000	-12.155930000
6	-4.838928000	2.392614000	-11.812356000
7	-6.067572000	1.764244000	-11.979449000
1	-6.671465000	-2.463376000	-13.401327000
1	-1.889989000	-0.321725000	-12.897445000
1	-2.207572000	-1.891726000	-13.596235000
1	-4.781918000	3.402095000	-11.416940000
15	-7.492134000	4.112794000	-7.059770000
8	-8.345652000	5.229520000	-6.517181000

8	-6.005265000	4.270740000	-7.337076000
1	8.893923000	-6.330147000	3.740365000
1	1.986459000	7.041311000	-3.977221000
1	-5.258424000	-10.614302000	-17.498072000
1	-5.472088000	4.898703000	-8.976911000

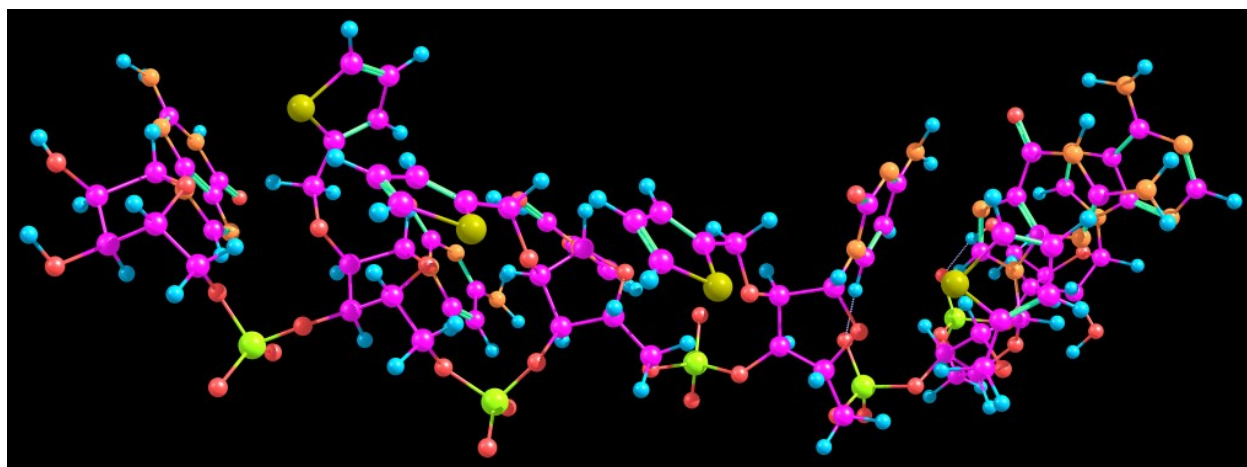
Figure S31. X-Y coordinates for **1:2** at level: B97D3/6-31G*.



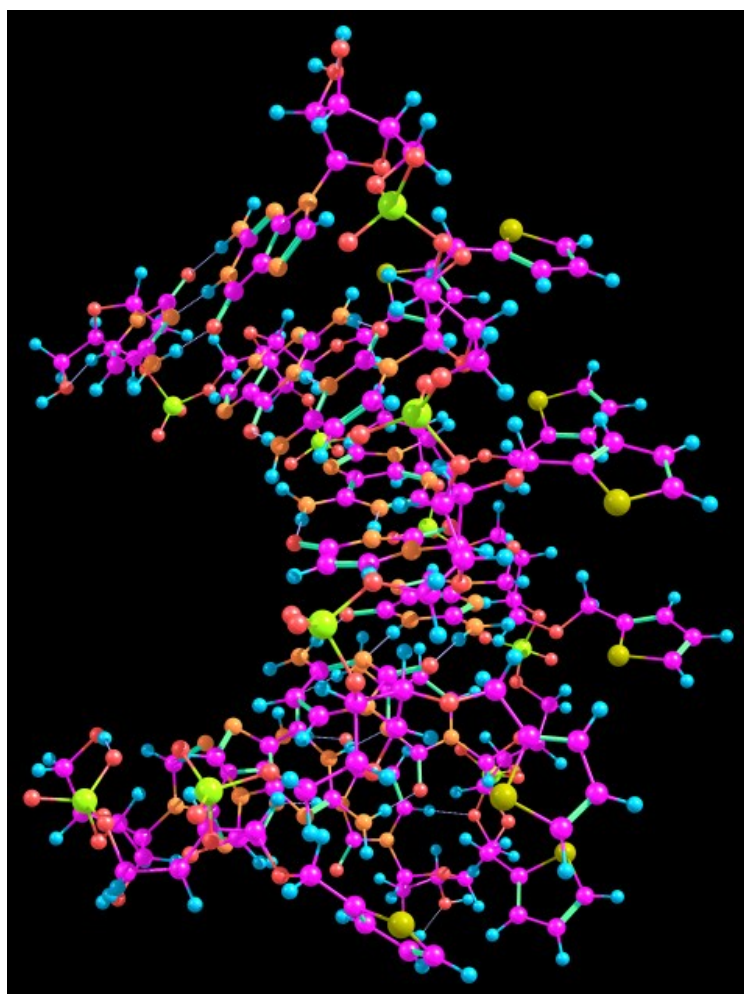
3 at level: B3LYP/3-21G*.



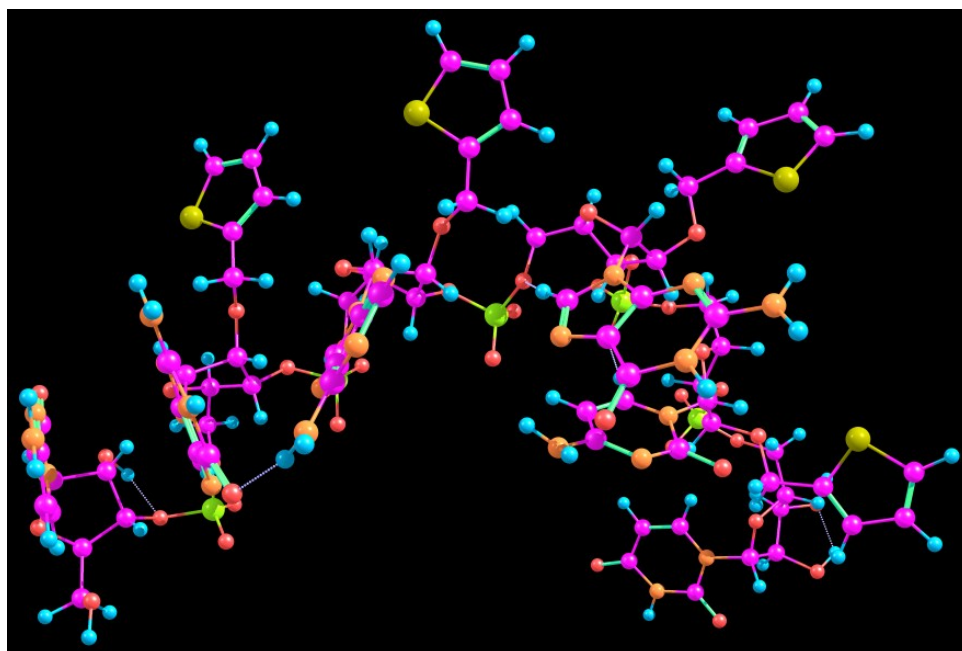
3 at level: B3LYP-GD3/3-21G*.



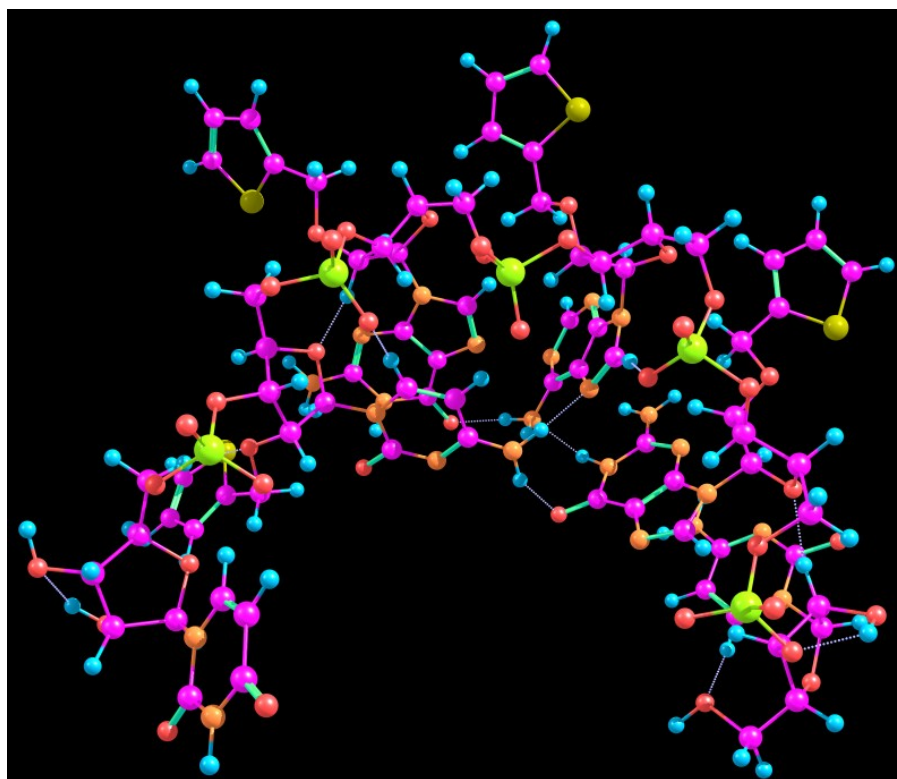
3 at level: B3LYP-GD3/6-31G*.



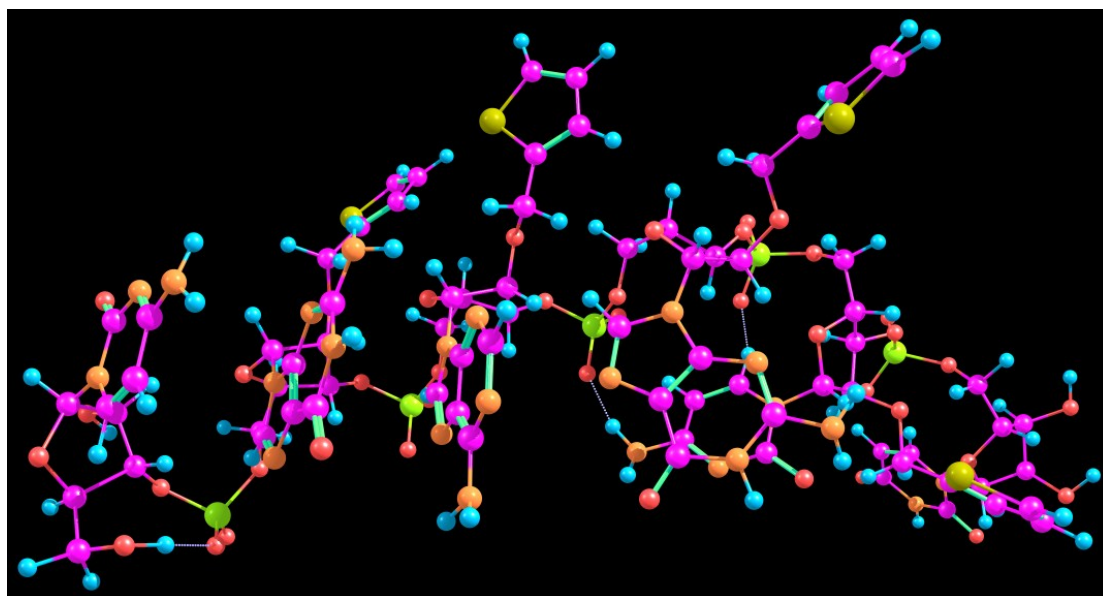
3:4 at level: B3LYP /6-31G*.



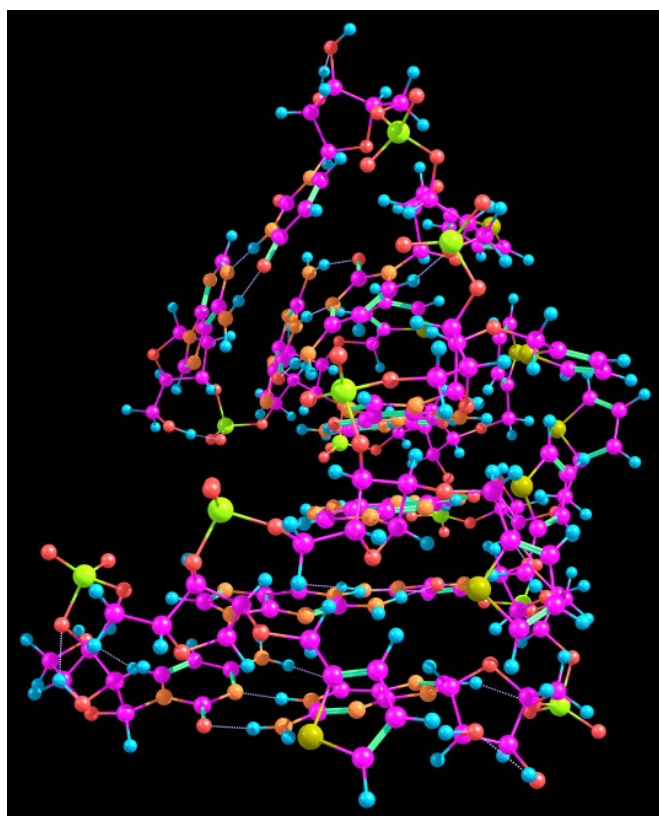
4 at level: B3LYP /3-21G*.



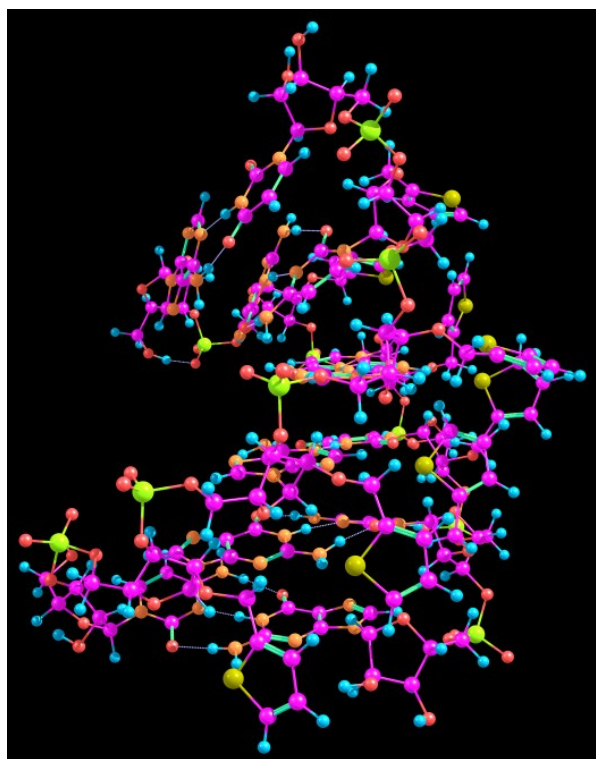
4 at level: B3LYP-GD3/3-21G*.



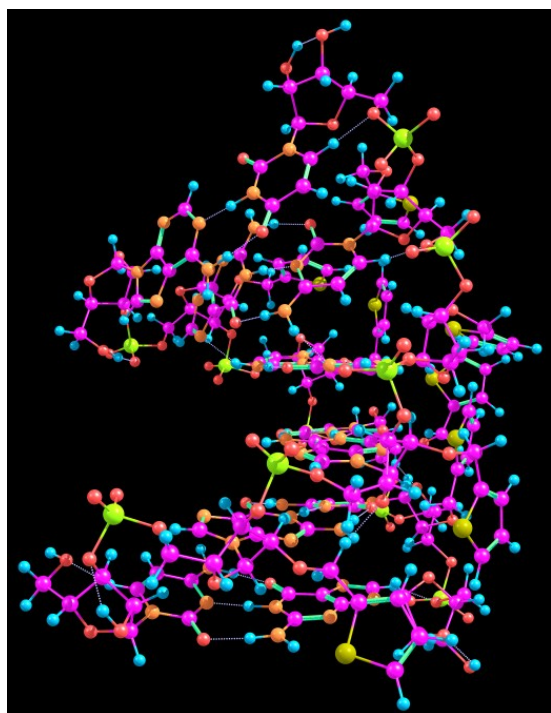
4 at level: B3LYP-GD3/6-31G*.



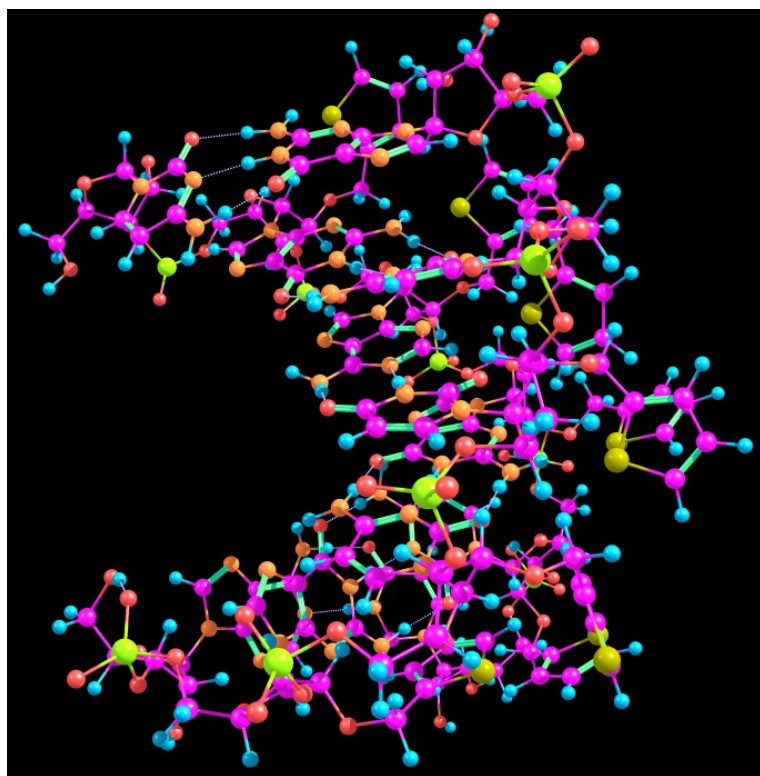
3:4 at level: B3LYP-GD3/3-21G*.



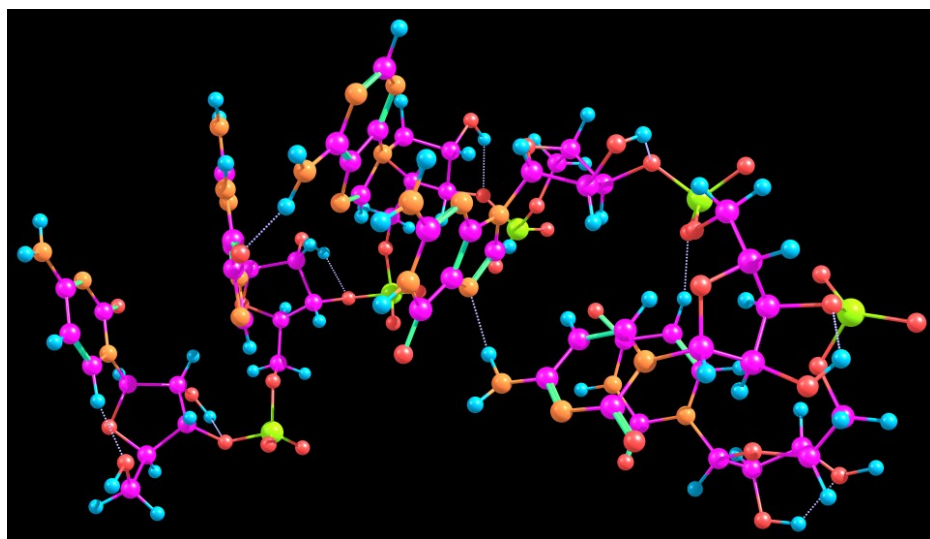
3:4 at level: B3LYP-GD3/6-31G*



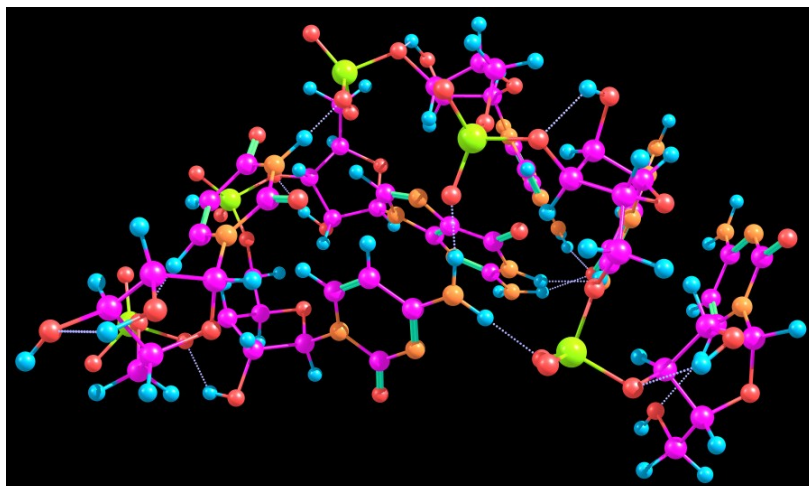
3:4 at level: B97D3/3-21G*



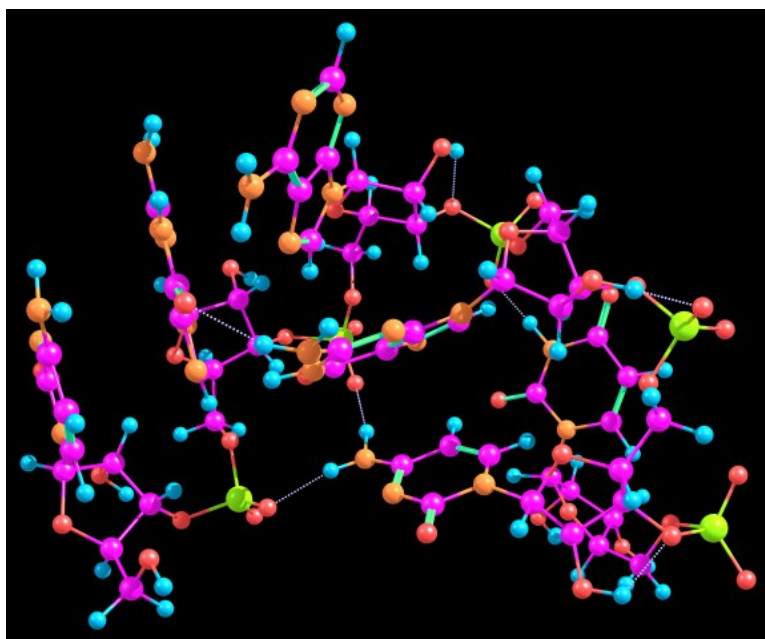
3:4 at level: B97D3/6-31G*.



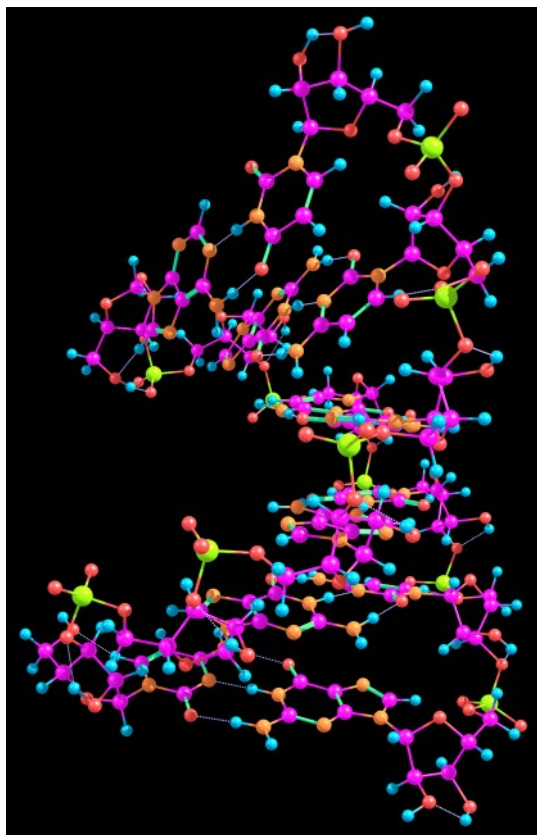
1 at level: B3LYP/3-21G*.



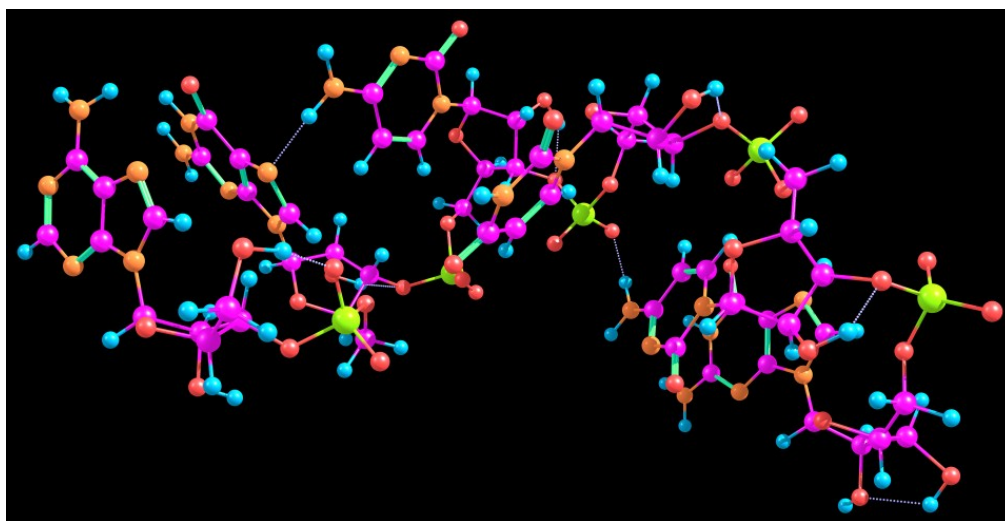
1 at level: B3LYP-GD3/3-21G*.



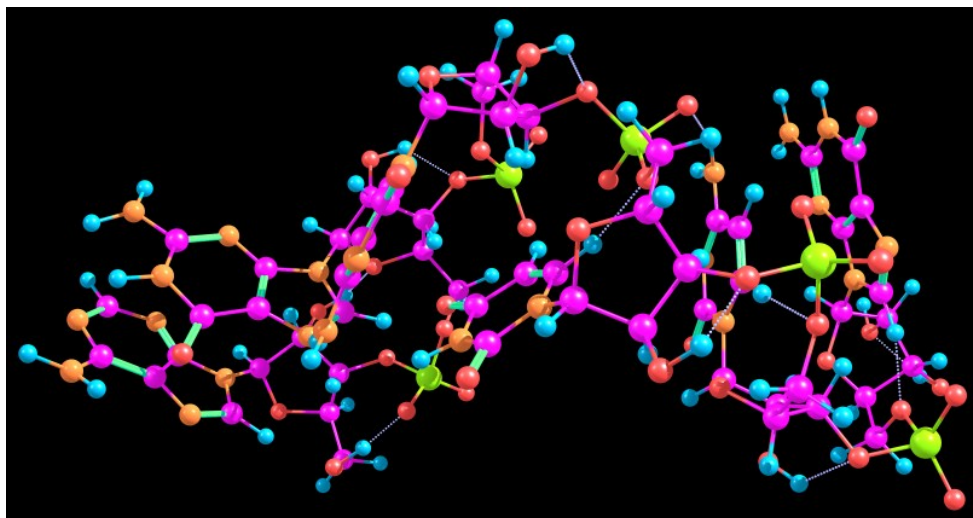
1 at level: B3LYP-GD3/6-31G*.



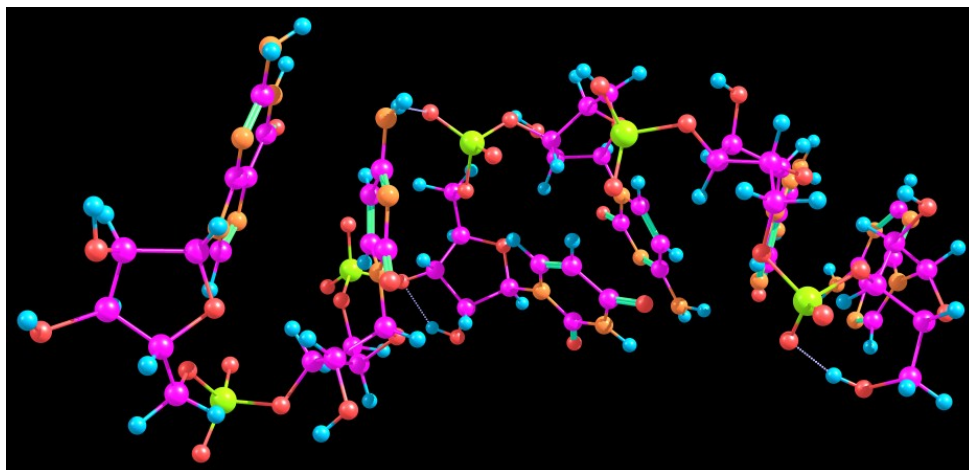
1:2 at level: B3LYP/3-21G*



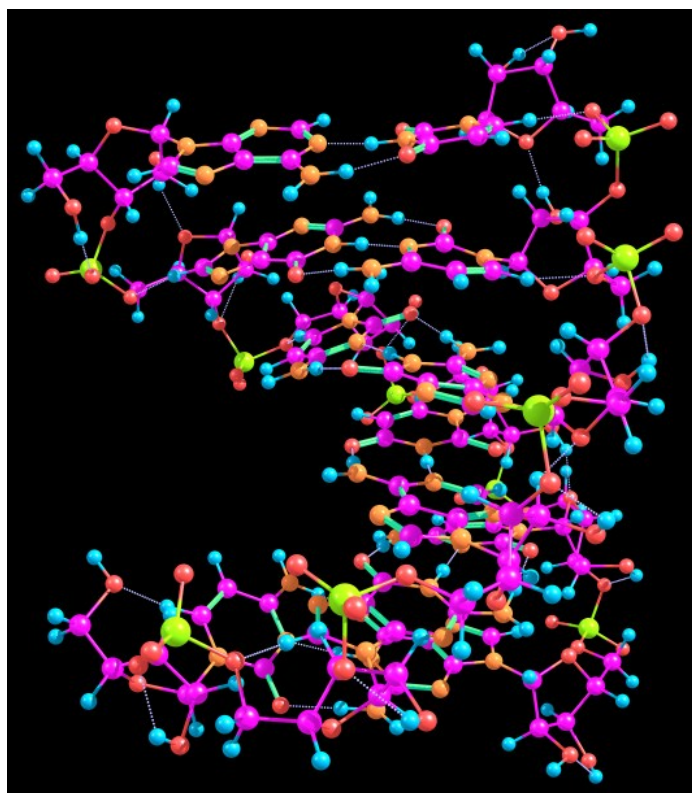
2 at level: B3LYP/3-21G*.



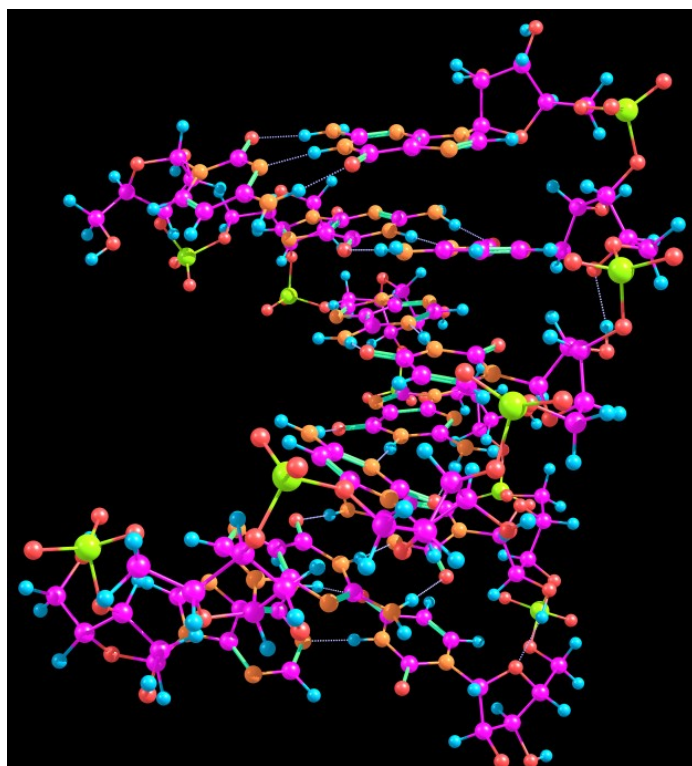
2 at level: B3LYP-GD3/3-21G*.



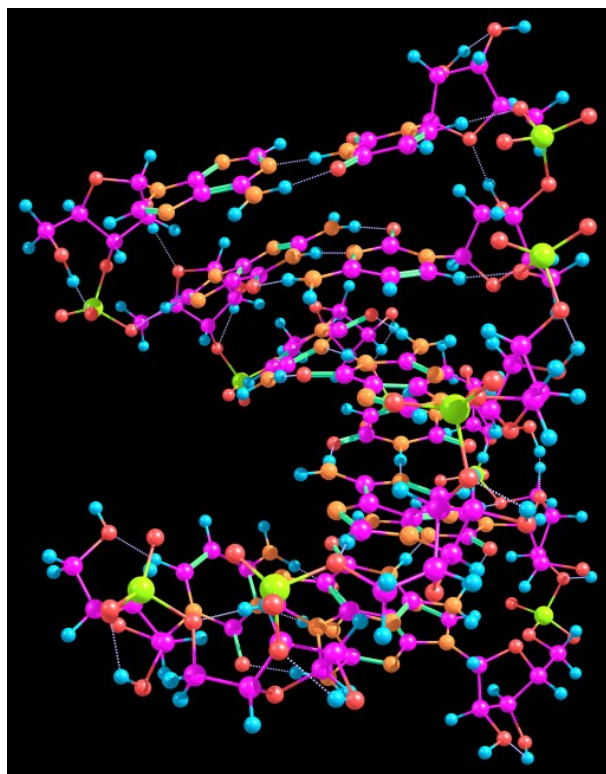
2 at level: B3LYP-GD3/6-31G*.



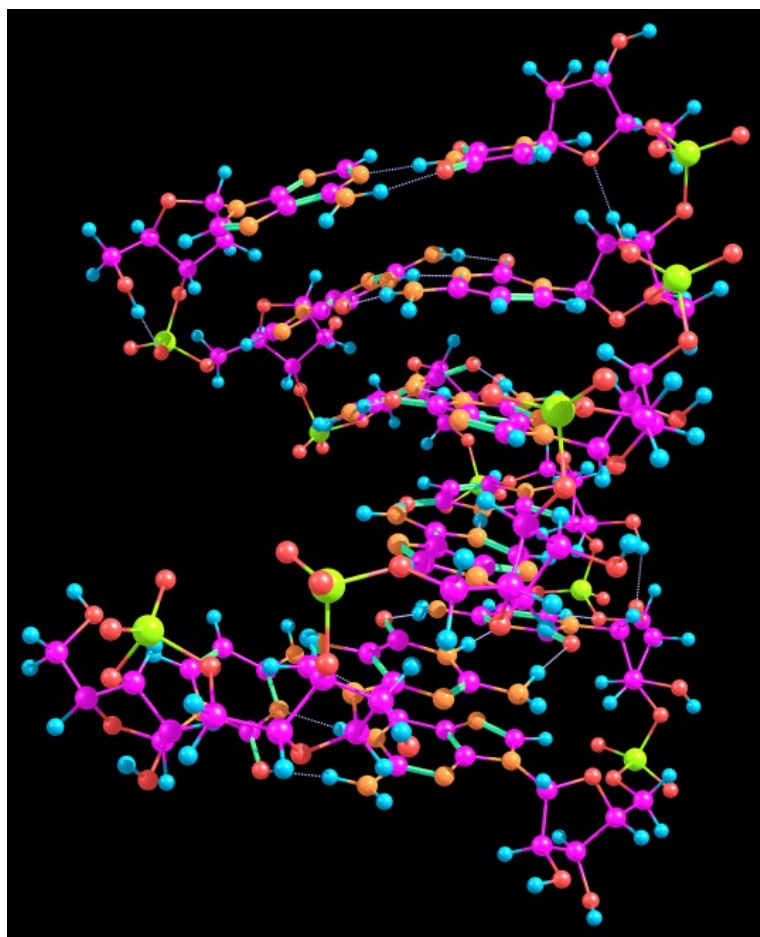
1:2 at level: B3LYP-GD3/3-21G*.



1:2 at level: B3LYP-GD3/6-31G*.



1:2 at level: B97D3/3-21G*.



1:2 at level: B97D3/6-31G*.

Figure S32. Images of all the structures and levels of theory.

8	25.776431000	5.207953000	-4.055128000
6	25.111914000	8.769877000	-3.132024000
6	26.628968000	8.993666000	-3.054978000
6	27.139555000	7.668625000	-3.636446000
6	26.177596000	7.450799000	-4.805263000
6	26.053370000	6.010370000	-5.248770000
8	24.864167000	7.909391000	-4.276113000
1	24.566276000	9.708308000	-3.218697000
1	26.970126000	9.239714000	-2.056486000
8	26.999119000	10.046819000	-4.007083000
1	26.885798000	10.907338000	-3.517336000
1	27.010832000	6.869904000	-2.904124000
1	26.488682000	8.089901000	-5.635992000
1	27.009164000	5.728489000	-5.708452000
1	25.252515000	5.923346000	-5.992742000
8	28.500386000	7.655280000	-4.128362000
7	24.652995000	8.087974000	-1.893553000
6	24.445094000	8.918665000	-0.770772000
8	24.701693000	10.150990000	-0.904648000
7	23.981097000	8.353932000	0.370183000
6	23.836085000	7.009808000	0.478259000
7	23.419629000	6.519637000	1.644011000
6	24.101248000	6.157240000	-0.647786000
6	24.486671000	6.731512000	-1.817076000
1	23.207397000	7.155991000	2.439211000
1	23.362237000	5.517742000	1.787625000
1	23.984715000	5.087075000	-0.566813000
1	24.726031000	6.163600000	-2.711025000
8	20.842820000	13.436802000	8.535118000
6	23.566703000	13.633206000	6.079422000
6	22.850552000	14.818200000	5.425724000
6	21.759651000	15.163092000	6.455752000
6	22.523964000	14.958224000	7.782067000
6	21.637694000	14.605556000	8.949242000
8	23.451439000	13.815037000	7.521929000
1	24.617092000	13.575320000	5.787251000
1	22.494051000	14.578398000	4.422393000
8	23.693313000	16.016912000	5.468750000
1	24.297737000	16.027832000	4.679771000
1	20.925474000	14.464340000	6.412161000
1	23.113809000	15.854593000	7.990726000

1	20.976498000	15.448391000	9.176927000
1	22.234497000	14.333737000	9.822030000
8	21.285681000	16.517893000	6.300916000
7	23.597362000	10.066532000	2.509578000
6	24.034873000	11.375555000	2.441248000
7	24.593399000	11.780280000	1.288434000
7	23.892174000	12.239530000	3.461841000
6	23.224949000	11.714556000	4.509901000
6	22.660189000	10.441853000	4.630548000
6	22.899923000	9.498490000	3.594566000
8	22.563821000	8.282687000	3.572324000
7	21.957708000	10.334052000	5.841961000
6	22.116720000	11.501171000	6.449567000
7	22.923204000	12.372698000	5.686573000
1	23.788375000	9.408707000	1.694238000
1	24.661853000	11.167976000	0.448698000
1	24.939297000	12.731778000	1.256771000
1	21.631601000	11.836458000	7.347309000
8	29.458915000	8.504938000	-1.966564000
6	27.983007000	10.836466000	0.444794000
6	29.395706000	11.135936000	0.972636000
6	30.259811000	10.494887000	-0.123167000
6	29.505058000	10.828927000	-1.404721000
6	29.751200000	9.842255000	-2.518609000
8	28.068652000	10.742561000	-1.009738000
1	27.289320000	11.622365000	0.743585000
1	29.537316000	10.661048000	1.937275000
8	29.597140000	12.569681000	1.066891000
1	29.705619000	12.713146000	2.057371000
1	30.259510000	9.414406000	0.016659000
1	29.747561000	11.851799000	-1.708976000
1	30.799596000	9.894767000	-2.829858000
1	29.083805000	10.029468000	-3.361687000
8	31.622296000	10.978309000	-0.233708000
7	25.815768000	8.964042000	4.553933000
6	26.342418000	10.215944000	4.311526000
7	26.252432000	11.135351000	5.286891000
7	26.928556000	10.537636000	3.147511000
6	26.967947000	9.512056000	2.273910000
6	26.533456000	8.194375000	2.449054000
6	25.849821000	7.876321000	3.658595000

8	25.291401000	6.786607000	3.969041000
7	26.848485000	7.434940000	1.307207000
6	27.437338000	8.278514000	0.463955000
7	27.503563000	9.572889000	1.007950000
1	25.318351000	8.786612000	5.480794000
1	25.985257000	10.888938000	6.260765000
1	26.659876000	12.040712000	5.087347000
1	27.890527000	8.053644000	-0.486181000
15	29.640389000	7.221490000	-2.993673000
8	30.966112000	7.298129000	-3.684452000
8	29.142075000	6.033268000	-2.227553000
8	20.760494000	8.881707000	11.282399000
6	23.941980000	10.513576000	10.008730000
6	23.094460000	11.773804000	9.810913000
6	21.789267000	11.362641000	10.507289000
6	22.295546000	10.676496000	11.776397000
6	21.361744000	9.642470000	12.382540000
8	23.527438000	9.967833000	11.299928000
1	25.008563000	10.719508000	10.005651000
1	22.998107000	12.048052000	8.770124000
8	23.673381000	12.878795000	10.578462000
1	24.317164000	13.324730000	9.961302000
1	21.263880000	10.633839000	9.891689000
1	22.587054000	11.433105000	12.507637000
1	20.586409000	10.162550000	12.953323000
1	21.934638000	8.964336000	13.018950000
8	20.881116000	12.436166000	10.844689000
7	23.683255000	9.525881000	8.936471000
6	24.570328000	9.541055000	7.839597000
8	25.422173000	10.479666000	7.790353000
7	24.451133000	8.573976000	6.902001000
6	23.503235000	7.608089000	6.990407000
7	23.482631000	6.669930000	6.045848000
6	22.572246000	7.611537000	8.081060000
6	22.688893000	8.587891000	9.014024000
1	24.161458000	6.695848000	5.251427000
1	22.775716000	5.943270000	6.070919000
1	21.790620000	6.879956000	8.212648000
1	21.998038000	8.654932000	9.842822000
15	19.784681000	12.810412000	9.646501000
8	18.916752000	13.894936000	10.202177000

8	19.284617000	11.546017000	9.014304000
8	32.516581000	10.964839000	2.154767000
6	30.145786000	11.532342000	4.802527000
6	31.305919000	11.862731000	5.743835000
6	32.475594000	11.965944000	4.756949000
6	31.857678000	12.734018000	3.590670000
6	32.476033000	12.426735000	2.243907000
8	30.443499000	12.229249000	3.553820000
1	29.202406000	11.883352000	5.219328000
1	31.437639000	11.071157000	6.472373000
8	31.053541000	13.147273000	6.369582000
1	30.928585000	12.909330000	7.345154000
1	32.757644000	10.968235000	4.424914000
1	31.853189000	13.802961000	3.813852000
1	33.483781000	12.854286000	2.204760000
1	31.847594000	12.811963000	1.439564000
8	33.638832000	12.676172000	5.253101000
7	27.720624000	7.468026000	6.613247000
6	27.860740000	8.722527000	7.099886000
7	28.594058000	9.705132000	6.550558000
6	29.222723000	9.308698000	5.423040000
6	29.191113000	8.030995000	4.851702000
6	28.356150000	7.074256000	5.470633000
7	28.123711000	5.847608000	4.997477000
7	29.999026000	7.994103000	3.708999000
6	30.491727000	9.225972000	3.580835000
7	30.022526000	10.078628000	4.596663000
1	27.302811000	8.927856000	7.999040000
1	28.559877000	5.564247000	4.127417000
1	27.389449000	5.257275000	5.430485000
1	31.195704000	9.542451000	2.832593000
15	32.749499000	10.202563000	0.704633000
8	34.089392000	10.553356000	0.138445000
8	32.284918000	8.798153000	0.970658000
8	22.406353000	3.302447000	11.350224000
6	24.856410000	6.012255000	11.468613000
6	23.718902000	7.016095000	11.630925000
6	22.526748000	6.077699000	11.872226000
6	23.122108000	5.037868000	12.817798000
6	22.454937000	3.681885000	12.771084000
8	24.522611000	4.870919000	12.309843000

1	25.808085000	6.441046000	11.767722000
1	23.614461000	7.594413000	10.724464000
8	23.962428000	7.851098000	12.790383000
1	24.038229000	8.776492000	12.388580000
1	22.239227000	5.604194000	10.935785000
1	23.149072000	5.443815000	13.832438000
1	21.443572000	3.744260000	13.184439000
1	23.055173000	2.944727000	13.311044000
8	21.366315000	6.705208000	12.476890000
7	24.966368000	5.600681000	10.043632000
6	25.702346000	6.463993000	9.214343000
8	26.028184000	7.609317000	9.599458000
7	26.015344000	5.941783000	7.990158000
6	25.558358000	4.744817000	7.445329000
8	25.958919000	4.366866000	6.312080000
6	24.624523000	4.027602000	8.283892000
1	24.144736000	3.130314000	7.926195000
6	24.389791000	4.457098000	9.546501000
1	26.691089000	6.536980000	7.387869000
1	23.710392000	3.937570000	10.212187000
15	20.222602000	7.315859000	11.442680000
8	18.915278000	7.294304000	12.169338000
8	20.422126000	6.712938000	10.077427000
8	34.001079000	11.747672000	7.589491000
6	31.007145000	10.854388000	9.513880000
6	31.851930000	10.884179000	10.785350000
6	33.152459000	11.466067000	10.239482000
6	32.655642000	12.615848000	9.360322000
6	33.581512000	12.996567000	8.225910000
8	31.408821000	12.038681000	8.751314000
1	29.939224000	10.887980000	9.729738000
1	31.936012000	9.905004000	11.228903000
8	31.279983000	11.830989000	11.742818000
1	30.646471000	11.290239000	12.291366000
1	33.627163000	10.721619000	9.604305000
1	32.386629000	13.472510000	9.980826000
1	34.444620000	13.530593000	8.636708000
1	33.050498000	13.605204000	7.491222000
8	34.110551000	11.930750000	11.222774000
7	29.463191000	6.088829000	8.998444000
6	29.139613000	7.029865000	9.948832000

7	28.352406000	6.636013000	10.968517000
7	29.610683000	8.288349000	9.918374000
6	30.539987000	8.475779000	8.958420000
6	31.013101000	7.552813000	8.026190000
6	30.396509000	6.277002000	7.966553000
8	30.609803000	5.373090000	7.112679000
7	32.071775000	8.102930000	7.291678000
6	32.229686000	9.334665000	7.756033000
7	31.277174000	9.624956000	8.763707000
1	28.963296000	5.143059000	8.996581000
1	28.016784000	5.655877000	11.055258000
1	27.923681000	7.370847000	11.516423000
1	32.983640000	10.039072000	7.451267000
15	34.730657000	11.757909000	6.104888000
8	36.002606000	12.543945000	6.156072000
8	34.628077000	10.329667000	5.651909000
8	24.811906000	-0.908022000	9.169047000
6	26.596732000	1.492179000	11.413371000
6	25.213813000	1.998171000	11.837585000
6	24.301699000	0.946338000	11.199690000
6	25.039903000	-0.360108000	11.489928000
6	24.747193000	-1.484012000	10.512987000
8	26.481546000	0.030296000	11.349100000
1	27.380921000	1.785894000	12.110698000
1	25.051145000	3.016906000	11.518008000
8	25.066893000	1.887948000	13.289597000
1	25.414946000	2.746539000	13.656673000
1	24.267067000	1.099586000	10.121496000
1	24.853520000	-0.661843000	12.522253000
1	23.743692000	-1.872688000	10.718697000
1	25.500576000	-2.267494000	10.603752000
8	22.954748000	0.865163000	11.723785000
7	26.963433000	2.015495000	10.080149000
6	27.545130000	3.300068000	10.044216000
8	27.447594000	4.020759000	11.078390000
7	28.168835000	3.674727000	8.899492000
6	28.141918000	2.901379000	7.783002000
7	28.886988000	3.275340000	6.745847000
6	27.326552000	1.723401000	7.754639000
6	26.783467000	1.304891000	8.923274000
1	29.529135000	4.098242000	6.822353000

1	28.888376000	2.715365000	5.900850000
1	27.150990000	1.131100000	6.870783000
1	26.164572000	0.422847000	8.976725000
15	21.834880000	1.802723000	10.930992000
8	20.524943000	1.546473000	11.605217000
8	22.077861000	1.724425000	9.452880000
8	33.919421000	9.910418000	12.734700000
6	31.144897000	7.556232000	12.982319000
6	31.659614000	7.052073000	14.331514000
6	32.770498000	8.077297000	14.615633000
6	32.117695000	9.390647000	14.195542000
6	33.114181000	10.470804000	13.818044000
8	31.300354000	9.011888000	13.001670000
1	30.106139000	7.286224000	12.807294000
1	32.028161000	6.039395000	14.227853000
8	30.606653000	7.154709000	15.323988000
1	30.502636000	6.210259000	15.665646000
1	33.633939000	7.868409000	13.985627000
1	31.453635000	9.726521000	14.996073000
1	33.726335000	10.695653000	14.698665000
1	32.602803000	11.361508000	13.447291000
8	33.185854000	8.188592000	16.000949000
7	31.953778000	6.952163000	11.883673000
6	31.602495000	5.638344000	11.499820000
8	30.795199000	5.004005000	12.242783000
7	32.143390000	5.140012000	10.359323000
6	33.069098000	5.837942000	9.654470000
7	33.450385000	5.349720000	8.471072000
6	33.597034000	7.064484000	10.177527000
6	32.992069000	7.596073000	11.269036000
1	32.975857000	4.511110000	8.074620000
1	33.957053000	5.961191000	7.838666000
1	34.413853000	7.612048000	9.733534000
1	33.330493000	8.524104000	11.707393000
15	35.062727000	10.729469000	11.867038000
8	36.050454000	11.398963000	12.765616000
8	35.416977000	9.747629000	10.781595000
8	28.872693000	-4.139814000	6.044063000
6	29.649935000	-2.067458000	9.215104000
6	28.147679000	-1.732047000	9.351996000
6	27.552467000	-2.593216000	8.217814000

6	28.350773000	-3.876095000	8.384943000
6	28.301088000	-4.823466000	7.214576000
8	29.735837000	-3.369045000	8.554201000
1	30.128317000	-2.100354000	10.194476000
1	27.984756000	-0.668604000	9.217487000
8	27.678001000	-2.197837000	10.637465000
1	27.360018000	-1.367707000	11.117081000
1	27.768741000	-2.135034000	7.252847000
1	28.001518000	-4.367958000	9.299109000
1	27.251577000	-5.061639000	7.019554000
1	28.868434000	-5.725325000	7.443396000
8	26.148165000	-2.914814000	8.353022000
7	31.166690000	2.670136000	9.456211000
6	30.456053000	1.901249000	10.356048000
7	30.090305000	2.464773000	11.521925000
7	30.128450000	0.624430000	10.109974000
6	30.527365000	0.203980000	8.893164000
6	31.187890000	0.913549000	7.890382000
6	31.597649000	2.250211000	8.180415000
8	32.310136000	3.008237000	7.468285000
7	31.377744000	0.084468000	6.769635000
6	30.849988000	-1.094356000	7.096607000
7	30.325377000	-1.063552000	8.399822000
1	31.497992000	3.626991000	9.766677000
1	30.335608000	3.447077000	11.761474000
1	29.924174000	1.826362000	12.294227000
1	30.807704000	-1.969753000	6.466007000
15	25.050242000	-1.805842000	7.794838000
8	23.807062000	-2.555273000	7.435068000
8	25.755214000	-0.861974000	6.858730000
8	33.614097000	5.953127000	17.135910000
6	31.258652000	3.337994000	15.747453000
6	31.595819000	2.509947000	17.001752000
6	32.381709000	3.521145000	17.845082000
6	31.554088000	4.806960000	17.646112000
6	32.309926000	6.114228000	17.793562000
8	31.097047000	4.706877000	16.221854000
1	30.344453000	2.983261000	15.272663000
1	32.153681000	1.604302000	16.749333000
8	30.367977000	2.267125000	17.740317000
1	29.843548000	1.577596000	17.250496000

1	33.367997000	3.675798000	17.400724000
1	30.682342000	4.763467000	18.300016000
1	32.443178000	6.330270000	18.858984000
1	31.753298000	6.912013000	17.298823000
8	32.442932000	3.106782000	19.226486000
7	32.327914000	3.303534000	14.725429000
6	32.207926000	2.319440000	13.734665000
8	31.379301000	1.385482000	13.848852000
7	33.055838000	2.469548000	12.672631000
6	33.989444000	3.492238000	12.474338000
8	34.635052000	3.564123000	11.396886000
6	34.141804000	4.379824000	13.600329000
1	34.879424000	5.164629000	13.619344000
6	33.317412000	4.261114000	14.665159000
1	33.038516000	1.674103000	11.951559000
1	33.415528000	4.912486000	15.520807000
15	34.451973000	7.240802000	16.489939000
8	35.179188000	7.975709000	17.570804000
8	35.135083000	6.685240000	15.269293000
8	33.687402000	-3.796517000	5.068275000
6	33.618395000	-4.377468000	8.878209000
6	32.183294000	-4.923944000	8.758709000
6	32.073557000	-4.890755000	7.243222000
6	33.383869000	-5.550323000	6.810039000
6	33.785900000	-5.212577000	5.376414000
8	34.369821000	-4.985732000	7.779663000
1	34.086401000	-4.623077000	9.833223000
1	31.429638000	-4.311816000	9.245445000
8	32.170924000	-6.322332000	9.165280000
1	32.173950000	-6.348477000	10.159719000
1	32.120839000	-3.845890000	6.951718000
1	33.315599000	-6.631391000	6.952434000
1	33.144245000	-5.818879000	4.718404000
1	34.824663000	-5.515705000	5.217179000
8	30.937362000	-5.526345000	6.614589000
7	33.191895000	0.354971000	11.007074000
6	32.703365000	-0.830509000	11.443264000
7	32.778606000	-2.015725000	10.810053000
6	33.386636000	-1.914248000	9.599535000
6	33.864316000	-0.728836000	9.019670000
6	33.789562000	0.452251000	9.784110000

7	34.294990000	1.625332000	9.392347000
7	34.388617000	-0.971781000	7.749519000
6	34.259778000	-2.281224000	7.566552000
7	33.669583000	-2.910040000	8.678567000
1	32.193897000	-0.780867000	12.397590000
1	34.570722000	1.749683000	8.424646000
1	34.339485000	2.421387000	10.054623000
1	34.413624000	-2.827930000	6.647074000
15	30.233655000	-4.722204000	5.348746000
8	29.930000000	-5.720792000	4.278601000
8	31.095686000	-3.498954000	5.034994000
1	22.110019000	16.996399000	5.981019000
1	25.661348000	4.259960000	-4.325582000
1	33.177256000	3.621860000	19.654836000
1	32.674892000	-3.583381000	4.987150000

Figure S33. X-Y coordinates for **1:2** at level: B97D3/3-21G*. Adjustment of all C3'-C2'-O2'-H2' to 180°

8	3.300281000	-5.681598000	-15.470009000
6	2.167309000	-3.259653000	-18.067621000
6	2.252466000	-4.392035000	-19.110515000
6	2.496502000	-5.597937000	-18.191684000
6	1.529400000	-5.311083000	-17.042444000
6	1.895923000	-5.992891000	-15.744553000
8	1.605959000	-3.836656000	-16.860169000
1	1.562150000	-2.427420000	-18.424006000
1	2.991323000	-4.210078000	-19.884776000
8	0.919786000	-4.591533000	-19.694599000
1	0.818853000	-3.912449000	-20.416060000
1	3.522666000	-5.575040000	-17.821383000
1	0.522068000	-5.591360000	-17.360751000
1	1.742856000	-7.069567000	-15.891089000
1	1.236701000	-5.637650000	-14.943241000
8	2.194276000	-6.907160000	-18.728059000
7	3.524157000	-2.726846000	-17.759653000
6	4.030858000	-1.765438000	-18.658495000
8	3.331763000	-1.511807000	-19.682365000
7	5.215173000	-1.170741000	-18.375202000
6	5.957211000	-1.563406000	-17.312238000
7	7.128958000	-0.961440000	-17.112265000
6	5.469418000	-2.583402000	-16.424352000
6	4.246510000	-3.125041000	-16.666672000
1	7.465550000	-0.218320000	-17.759173000
1	7.724901000	-1.249208000	-16.343822000
1	6.058429000	-2.902198000	-15.577667000
1	3.810357000	-3.909291000	-16.054946000
8	9.758121000	6.225568000	-24.121936000
6	7.490306000	3.185175000	-24.358041000
6	6.314263000	4.152858000	-24.550447000
6	7.018343000	5.510907000	-24.737978000
6	8.224579000	5.089130000	-25.596708000
6	9.408182000	6.013970000	-25.540224000
8	8.633525000	3.767409000	-25.046958000
1	7.272600000	2.183991000	-24.734652000
1	5.601307000	4.104928000	-23.725603000
8	5.689793000	3.954961000	-25.860176000
1	5.007441000	3.237151000	-25.798416000
1	7.374307000	5.921549000	-23.793524000
1	7.888396000	4.964301000	-26.630263000

1	9.160841000	6.972042000	-26.005052000
1	10.244322000	5.542588000	-26.060470000
8	6.172204000	6.466389000	-25.409593000
7	6.206575000	0.649716000	-20.218841000
6	5.591577000	0.707000000	-21.454507000
7	4.483650000	-0.024953000	-21.641902000
7	6.053506000	1.479092000	-22.452380000
6	7.137108000	2.196862000	-22.104387000
6	7.794119000	2.260454000	-20.871486000
6	7.349359000	1.385422000	-19.836141000
8	7.854768000	1.211216000	-18.692954000
7	8.842756000	3.198228000	-20.936685000
6	8.825502000	3.668499000	-22.177970000
7	7.804844000	3.066704000	-22.935708000
1	5.838269000	-0.048699000	-19.507201000
1	4.048179000	-0.610858000	-20.898478000
1	4.108598000	-0.041449000	-22.583176000
1	9.435862000	4.446858000	-22.602078000
8	3.689785000	-6.603073000	-20.711135000
6	4.456139000	-3.672987000	-22.866935000
6	4.952979000	-4.684372000	-23.919622000
6	4.403054000	-6.001625000	-23.353449000
6	3.039739000	-5.603480000	-22.792116000
6	2.570191000	-6.493014000	-21.667416000
8	3.265527000	-4.238696000	-22.233706000
1	4.234864000	-2.716417000	-23.345671000
1	6.036958000	-4.681569000	-23.943246000
8	4.398435000	-4.384903000	-25.217097000
1	5.213560000	-4.126872000	-25.750942000
1	5.036839000	-6.333134000	-22.533171000
1	2.306056000	-5.558983000	-23.603091000
1	2.333224000	-7.488362000	-22.056177000
1	1.708270000	-6.061631000	-21.152644000
8	4.250302000	-7.066353000	-24.328329000
7	8.560151000	-0.944333000	-21.757839000
6	7.855483000	-1.031242000	-22.940431000
7	8.286307000	-0.285176000	-23.975886000
7	6.782310000	-1.825163000	-23.084526000
6	6.505967000	-2.550211000	-21.979588000
6	7.198074000	-2.582681000	-20.765180000
6	8.286522000	-1.685885000	-20.592103000

8	8.968402000	-1.502614000	-19.545550000
7	6.624463000	-3.534914000	-19.905424000
6	5.601459000	-4.049487000	-20.578606000
7	5.477078000	-3.455364000	-21.846514000
1	9.405948000	-0.297552000	-21.702850000
1	9.230384000	0.149306000	-23.977953000
1	7.801663000	-0.419908000	-24.855591000
1	4.958879000	-4.861250000	-20.285320000
15	3.473673000	-7.674080000	-19.469530000
8	2.932970000	-8.965919000	-19.999138000
8	4.695430000	-7.549594000	-18.611260000
8	14.235850000	5.242346000	-21.428673000
6	12.628851000	2.877546000	-23.963364000
6	11.827621000	4.082176000	-24.431369000
6	12.505292000	5.245265000	-23.677740000
6	13.990149000	4.879749000	-23.806595000
6	14.912802000	5.399514000	-22.718939000
8	13.984979000	3.382279000	-23.749046000
1	12.626977000	2.062325000	-24.680726000
1	10.761089000	3.962077000	-24.270017000
8	12.119158000	4.301789000	-25.855946000
1	12.262232000	5.294769000	-25.900948000
1	12.204168000	5.340018000	-22.637178000
1	14.353032000	5.184490000	-24.790061000
1	15.123332000	6.456085000	-22.913323000
1	15.831355000	4.809237000	-22.717453000
8	12.262955000	6.497505000	-24.391050000
7	12.084685000	2.362038000	-22.685157000
6	11.169090000	1.289084000	-22.751239000
8	10.787384000	0.907673000	-23.899488000
7	10.733869000	0.743018000	-21.592004000
6	11.169479000	1.185979000	-20.386382000
7	10.720600000	0.573392000	-19.294764000
6	12.093762000	2.278292000	-20.312137000
6	12.506921000	2.841173000	-21.471782000
1	10.031552000	-0.208749000	-19.365211000
1	10.970978000	0.927697000	-18.378705000
1	12.493097000	2.671567000	-19.390386000
1	13.178736000	3.688358000	-21.468103000
15	10.931802000	7.356106000	-23.815766000
8	10.771705000	8.517426000	-24.743849000

8	11.037194000	7.441168000	-22.325905000
8	6.495739000	-7.141458000	-25.508038000
6	8.187640000	-3.968800000	-25.816295000
6	9.101792000	-4.582686000	-26.870372000
6	8.396352000	-5.910831000	-27.158072000
6	6.920752000	-5.510831000	-27.190987000
6	5.955942000	-6.596207000	-26.753497000
8	6.843906000	-4.423869000	-26.152158000
1	8.239538000	-2.880566000	-25.837351000
1	10.098541000	-4.723529000	-26.483811000
8	9.111057000	-3.739324000	-28.049869000
1	10.032458000	-3.337583000	-28.010952000
1	8.556788000	-6.593577000	-26.325390000
1	6.666831000	-5.092306000	-28.166932000
1	5.885615000	-7.367062000	-27.529027000
1	4.975599000	-6.159398000	-26.549493000
8	8.815556000	-6.531022000	-28.400914000
7	11.244271000	-2.594580000	-22.034100000
6	11.109309000	-2.129780000	-23.294543000
7	10.272583000	-2.615483000	-24.228526000
6	9.560080000	-3.673593000	-23.776762000
6	9.661291000	-4.278230000	-22.519670000
6	10.533352000	-3.670427000	-21.588187000
7	10.691439000	-4.068195000	-20.324777000
7	8.819049000	-5.393034000	-22.450764000
6	8.214586000	-5.458361000	-23.637191000
7	8.604064000	-4.395514000	-24.470309000
1	11.728145000	-1.283153000	-23.542122000
1	10.238272000	-4.919289000	-20.014756000
1	11.304177000	-3.535780000	-19.680355000
1	7.526802000	-6.225560000	-23.945900000
15	5.548838000	-8.077152000	-24.523492000
8	5.050480000	-9.278351000	-25.263518000
8	6.332408000	-8.135279000	-23.241217000
8	17.289396000	1.632443000	-18.030590000
6	16.049961000	0.605099000	-21.434929000
6	15.638487000	2.057356000	-21.664580000
6	16.249263000	2.727709000	-20.428829000
6	17.621137000	2.060990000	-20.376303000
6	18.291464000	2.048660000	-19.029784000
8	17.318799000	0.636382000	-20.725698000

1	16.132681000	0.069184000	-22.377738000
1	14.560591000	2.137247000	-21.704653000
8	16.279433000	2.551287000	-22.867164000
1	15.501963000	2.763066000	-23.475908000
1	15.674613000	2.462264000	-19.544614000
1	18.263893000	2.498668000	-21.144777000
1	18.668180000	3.040806000	-18.771316000
1	19.104320000	1.317534000	-19.046441000
8	16.369753000	4.170501000	-20.517142000
7	15.038049000	-0.089123000	-20.603838000
6	13.913709000	-0.564189000	-21.297952000
8	13.701086000	-0.234681000	-22.483704000
7	13.108219000	-1.393682000	-20.568065000
6	13.226743000	-1.704158000	-19.219799000
8	12.427349000	-2.514930000	-18.678406000
6	14.313504000	-1.033824000	-18.541625000
1	14.443833000	-1.193640000	-17.483804000
6	15.186441000	-0.280529000	-19.251958000
1	12.305233000	-1.857506000	-21.126058000
1	16.019535000	0.235875000	-18.793992000
15	15.068457000	5.058577000	-19.995575000
8	15.591396000	6.381033000	-19.531478000
8	14.177216000	4.182374000	-19.156837000
8	11.359942000	-6.349454000	-28.262995000
6	12.687593000	-3.481674000	-26.578834000
6	14.040696000	-3.586364000	-27.284684000
6	13.734784000	-4.713614000	-28.291622000
6	12.370733000	-4.271874000	-28.831393000
6	11.458830000	-5.365764000	-29.341268000
8	11.705289000	-3.667987000	-27.629687000
1	12.515880000	-2.518589000	-26.098375000
1	14.854347000	-3.766740000	-26.590870000
8	14.263908000	-2.384435000	-28.093957000
1	14.419752000	-1.628774000	-27.464123000
1	13.630997000	-5.661776000	-27.760891000
1	12.527539000	-3.490433000	-29.576394000
1	11.886083000	-5.805602000	-30.248400000
1	10.465168000	-4.954448000	-29.533461000
8	14.663799000	-4.836857000	-29.395088000
7	14.246503000	-4.246588000	-21.897127000
6	14.688296000	-3.372435000	-22.864963000

7	15.756014000	-2.603933000	-22.577287000
7	14.126605000	-3.294583000	-24.082419000
6	13.227144000	-4.271513000	-24.307583000
6	12.818025000	-5.282351000	-23.441196000
6	13.268764000	-5.239613000	-22.093396000
8	12.897885000	-5.976999000	-21.139359000
7	12.002164000	-6.196184000	-24.123787000
6	11.896889000	-5.734369000	-25.364467000
7	12.607948000	-4.515391000	-25.518409000
1	14.686769000	-4.210638000	-20.920917000
1	16.313620000	-2.720702000	-21.703719000
1	16.088234000	-2.020203000	-23.336384000
1	11.416955000	-6.248115000	-26.176058000
15	10.165162000	-7.496388000	-28.287176000
8	10.233673000	-8.283314000	-29.557212000
8	10.223894000	-8.087036000	-26.905023000
8	17.149462000	-2.390550000	-14.386375000
6	18.382832000	-2.768858000	-17.841528000
6	18.418430000	-1.247156000	-17.992966000
6	18.165242000	-0.782563000	-16.545063000
6	19.003403000	-1.785570000	-15.750195000
6	18.554398000	-1.992902000	-14.320971000
8	18.873052000	-3.063747000	-16.498759000
1	18.980465000	-3.282946000	-18.590992000
1	17.732966000	-0.893298000	-18.755611000
8	19.795105000	-0.847231000	-18.315757000
1	19.953852000	-0.079350000	-17.688418000
1	17.117995000	-0.807824000	-16.249213000
1	20.046517000	-1.459483000	-15.770472000
1	18.677986000	-1.055279000	-13.768831000
1	19.156817000	-2.787216000	-13.881926000
8	18.751180000	0.536208000	-16.307561000
7	16.983564000	-3.274280000	-17.956487000
6	16.461262000	-3.448976000	-19.253149000
8	17.121310000	-2.980566000	-20.225987000
7	15.283586000	-4.112099000	-19.380312000
6	14.582200000	-4.544748000	-18.300979000
7	13.521195000	-5.313418000	-18.527221000
6	15.016187000	-4.185721000	-16.982242000
6	16.225720000	-3.584580000	-16.857958000
1	13.286078000	-5.610653000	-19.499006000

1	12.970897000	-5.659798000	-17.749623000
1	14.451397000	-4.391096000	-16.086156000
1	16.614650000	-3.293387000	-15.894359000
15	17.677295000	1.820342000	-16.430977000
8	18.496179000	3.058651000	-16.251508000
8	16.441068000	1.480190000	-15.661453000
8	16.652202000	-4.786044000	-27.850899000
6	18.161786000	-3.593558000	-24.693710000
6	19.531739000	-4.000330000	-25.253199000
6	19.161616000	-4.281273000	-26.713368000
6	18.199244000	-3.146070000	-27.043297000
6	17.277029000	-3.494399000	-28.187195000
8	17.409380000	-2.977400000	-25.782082000
1	18.274196000	-2.913228000	-23.852043000
1	19.887787000	-4.880265000	-24.733423000
8	20.461448000	-2.894078000	-25.148747000
1	21.215072000	-3.266410000	-24.594770000
1	18.635531000	-5.230062000	-26.773036000
1	18.768665000	-2.234813000	-27.246491000
1	17.869563000	-3.615902000	-29.098635000
1	16.483126000	-2.759340000	-28.331823000
8	20.253342000	-4.272889000	-27.668174000
7	17.421799000	-4.789200000	-24.209628000
6	17.734582000	-5.236356000	-22.909722000
8	18.764151000	-4.749399000	-22.355084000
7	16.918866000	-6.158940000	-22.338426000
6	15.903243000	-6.725043000	-23.035749000
7	15.084806000	-7.559852000	-22.388982000
6	15.709486000	-6.407331000	-24.419256000
6	16.456151000	-5.407819000	-24.954366000
1	15.127477000	-7.620182000	-21.345614000
1	14.233009000	-7.867184000	-22.849286000
1	14.939666000	-6.892228000	-24.999667000
1	16.357287000	-5.085003000	-25.981894000
15	16.034733000	-5.723272000	-29.069737000
8	16.911688000	-5.603082000	-30.277864000
8	15.644299000	-7.014010000	-28.417897000
8	15.430742000	-7.782121000	-12.479024000
6	18.522414000	-6.797881000	-14.666170000
6	18.359793000	-5.320437000	-14.344949000
6	17.180996000	-5.370364000	-13.358668000

6	17.591582000	-6.550424000	-12.467229000
6	16.483371000	-7.172950000	-11.643532000
8	18.203090000	-7.518866000	-13.422748000
1	19.520917000	-7.064766000	-15.007769000
1	18.231814000	-4.704231000	-15.231716000
8	19.534734000	-4.885795000	-13.573534000
1	19.131395000	-4.372661000	-12.812333000
1	16.220536000	-5.524114000	-13.845034000
1	18.364740000	-6.198935000	-11.779015000
1	16.037793000	-6.360749000	-11.060355000
1	16.896883000	-7.914943000	-10.956714000
8	17.162363000	-4.157956000	-12.547269000
7	17.239573000	-6.553527000	-19.612513000
6	18.388712000	-6.111366000	-18.989359000
7	19.270691000	-5.439035000	-19.749385000
7	18.635011000	-6.317038000	-17.682193000
6	17.612752000	-6.919105000	-17.041933000
6	16.401828000	-7.366437000	-17.583086000
6	16.189077000	-7.235575000	-18.980792000
8	15.208058000	-7.670076000	-19.644767000
7	15.566891000	-7.866890000	-16.574600000
6	16.247842000	-7.724868000	-15.449304000
7	17.525551000	-7.171176000	-15.682639000
1	17.139409000	-6.420974000	-20.664433000
1	19.070848000	-5.191647000	-20.741347000
1	20.227555000	-5.380167000	-19.422842000
1	15.919931000	-7.951304000	-14.454168000
15	16.192870000	-2.924138000	-13.151811000
8	16.091445000	-1.905853000	-12.065071000
8	15.026501000	-3.557226000	-13.856360000
8	22.211929000	-5.704368000	-26.923032000
6	22.454461000	-5.527971000	-23.139965000
6	23.876418000	-6.094613000	-23.331122000
6	24.066257000	-5.992773000	-24.847420000
6	23.443295000	-4.617659000	-25.152741000
6	22.887242000	-4.450361000	-26.555432000
8	22.299073000	-4.523444000	-24.188938000
1	22.339117000	-5.082231000	-22.152811000
1	23.965062000	-7.112022000	-22.940374000
8	24.828738000	-5.153383000	-22.762092000
1	24.773785000	-5.222046000	-21.770736000

1	23.469128000	-6.761239000	-25.343354000
1	24.172996000	-3.843604000	-24.910844000
1	23.713700000	-4.245506000	-27.243555000
1	22.162182000	-3.634719000	-26.564677000
8	25.465294000	-6.055590000	-25.197389000
7	21.388723000	-6.541521000	-23.278864000
6	20.879311000	-7.084953000	-22.085908000
8	21.435686000	-6.875499000	-20.986661000
7	19.766999000	-7.866799000	-22.246566000
6	19.094456000	-8.155894000	-23.434527000
8	18.040801000	-8.846152000	-23.418008000
6	19.718735000	-7.616071000	-24.616753000
1	19.317600000	-7.773779000	-25.604218000
6	20.821694000	-6.842624000	-24.499347000
1	19.400862000	-8.333398000	-21.350834000
1	21.291259000	-6.418651000	-25.376588000
15	20.951617000	-5.733020000	-28.017174000
8	21.485355000	-5.660672000	-29.412611000
8	20.047176000	-6.838386000	-27.540992000
8	14.918513000	-12.217846000	-14.546600000
6	18.650354000	-11.378690000	-15.383229000
6	18.411583000	-10.150558000	-14.493647000
6	17.085485000	-10.536204000	-13.844874000
6	17.215562000	-12.037032000	-13.601253000
6	15.851301000	-12.733710000	-13.553168000
8	18.002431000	-12.525788000	-14.764574000
1	19.712262000	-11.555358000	-15.559445000
1	18.312008000	-9.275150000	-15.128463000
8	19.456628000	-10.006958000	-13.507547000
1	19.192159000	-9.148095000	-13.057803000
1	16.285878000	-10.367470000	-14.559584000
1	17.783656000	-12.202319000	-12.681237000
1	15.458881000	-12.610942000	-12.533540000
1	15.991847000	-13.800453000	-13.746007000
8	16.816421000	-9.871722000	-12.585571000
7	18.980280000	-9.162453000	-20.023220000
6	19.855737000	-9.179532000	-18.991251000
7	19.690763000	-9.806601000	-17.814598000
6	18.488954000	-10.426367000	-17.733538000
6	17.486323000	-10.443923000	-18.714966000
6	17.770339000	-9.791000000	-19.933908000

7	16.945612000	-9.759873000	-20.982499000
7	16.361076000	-11.136511000	-18.254747000
6	16.677967000	-11.535729000	-17.023649000
7	17.976644000	-11.143477000	-16.673066000
1	20.757719000	-8.604305000	-19.162059000
1	15.985257000	-10.060258000	-20.863756000
1	17.255395000	-9.346038000	-21.881719000
1	16.028674000	-12.017767000	-16.304365000
15	15.260059000	-9.420031000	-12.281750000
8	14.954469000	-9.748520000	-10.857309000
8	14.395059000	-9.887515000	-13.437187000
1	5.628672000	5.877485000	-26.015965000
1	3.560131000	-6.096369000	-14.606591000
1	25.517123000	-6.299000000	-26.159479000
1	14.596484000	-11.304747000	-14.179659000

Figure S34. X-Y coordinates for **1:2** at level: B97D3/3-21G*. Adjustment of one strand C3'-C2'-O2'-H2' to 180° and another randomized.

8	4.406672000	5.254696000	17.138440000
6	2.138284000	2.361074000	16.219776000
6	2.166855000	1.901569000	17.693015000
6	2.878327000	3.098279000	18.337546000
6	2.260804000	4.272921000	17.575015000
6	3.076606000	5.548452000	17.560058000
8	2.090894000	3.772298000	16.228613000
1	1.264905000	1.957416000	15.703546000
1	2.691067000	0.954836000	17.816688000
8	0.844394000	1.822753000	18.208694000
1	0.458893000	0.995283000	17.877472000
1	3.945301000	3.036976000	18.097806000
1	1.273821000	4.495063000	18.001229000
1	3.064674000	5.963361000	18.578622000
1	2.595297000	6.273067000	16.888550000
8	2.694392000	3.265224000	19.726921000
7	3.326104000	1.900506000	15.452953000
6	3.304852000	0.570039000	14.997301000
8	2.369710000	-0.161496000	15.381750000
7	4.278978000	0.153065000	14.155351000
6	5.313170000	0.955753000	13.854563000
7	6.241389000	0.488430000	13.009605000
6	5.408838000	2.279391000	14.395877000
6	4.380219000	2.718877000	15.168399000
1	6.194383000	-0.474276000	12.655041000
1	7.071821000	1.030886000	12.822336000
1	6.250155000	2.922984000	14.171477000
1	4.341100000	3.714963000	15.594726000
8	5.627814000	-9.586949000	10.378550000
6	4.150451000	-7.679471000	13.314822000
6	2.741365000	-7.924085000	12.736396000
6	3.062077000	-8.901978000	11.603725000
6	4.145979000	-9.775868000	12.252470000
6	5.038271000	-10.522171000	11.284104000
8	4.909051000	-8.848894000	13.050315000
1	4.091699000	-7.495430000	14.390830000
1	2.278319000	-7.000817000	12.385209000
8	1.900913000	-8.474719000	13.739470000
1	1.811945000	-9.431564000	13.618722000
1	3.522098000	-8.329400000	10.795358000
1	3.678673000	-10.521995000	12.914890000

1	4.419934000	-11.246115000	10.739535000
1	5.818103000	-11.060402000	11.833215000
8	1.985512000	-9.605546000	11.020436000
7	4.376353000	-2.652457000	13.415552000
6	3.577515000	-3.517808000	14.127742000
7	2.682971000	-2.969799000	14.975825000
7	3.631322000	-4.837528000	13.989579000
6	4.544786000	-5.224954000	13.077492000
6	5.369113000	-4.439801000	12.267118000
6	5.326547000	-3.022143000	12.446205000
8	5.997890000	-2.150495000	11.867361000
7	6.112414000	-5.237423000	11.407720000
6	5.752278000	-6.467113000	11.696201000
7	4.812687000	-6.523304000	12.718710000
1	4.323355000	-1.639764000	13.640255000
1	2.635859000	-1.960385000	15.151541000
1	2.239747000	-3.598112000	15.629462000
1	6.107927000	-7.368155000	11.217627000
8	3.487855000	0.947293000	20.441152000
6	3.152389000	-2.555072000	19.084404000
6	3.641243000	-3.084756000	20.442891000
6	3.594579000	-1.800961000	21.275601000
6	2.322429000	-1.125856000	20.758172000
6	2.272942000	0.376262000	20.933608000
8	2.291298000	-1.460757000	19.348344000
1	2.622075000	-3.329507000	18.522045000
1	4.638973000	-3.508030000	20.372291000
8	2.738185000	-4.035345000	20.987030000
1	3.018596000	-4.901224000	20.648990000
1	4.454033000	-1.179179000	21.009131000
1	1.448094000	-1.570151000	21.252702000
1	2.155185000	0.602277000	21.999709000
1	1.422135000	0.791642000	20.381870000
8	3.541283000	-1.996020000	22.674089000
7	6.598999000	-3.998824000	15.668817000
6	5.726179000	-4.763587000	16.405290000
7	5.729607000	-6.096865000	16.157689000
7	4.880169000	-4.251422000	17.293663000
6	4.999378000	-2.909948000	17.410666000
6	5.877358000	-2.048143000	16.749648000
6	6.749439000	-2.604890000	15.769289000

8	7.566243000	-2.004105000	15.050042000
7	5.713731000	-0.743083000	17.189711000
6	4.753942000	-0.813113000	18.082864000
7	4.268925000	-2.102796000	18.250301000
1	7.253297000	-4.473609000	15.011945000
1	6.550719000	-6.523234000	15.710592000
1	5.254804000	-6.656792000	16.852302000
1	4.372350000	0.000090000	18.681879000
15	3.802748000	2.543990000	20.747357000
8	3.353856000	2.907232000	22.132371000
8	5.192686000	2.780976000	20.231796000
8	10.937449000	-8.442631000	9.626780000
6	9.315794000	-8.746185000	12.994046000
6	8.101416000	-9.465840000	12.382196000
6	8.600367000	-9.674305000	10.945221000
6	10.066035000	-10.050044000	11.175218000
6	11.008970000	-9.815100000	10.014192000
8	10.457597000	-9.232164000	12.308236000
1	9.413725000	-8.945618000	14.060306000
1	7.196659000	-8.862130000	12.447803000
8	7.911513000	-10.738507000	12.987335000
1	7.495150000	-10.581597000	13.850711000
1	8.554145000	-8.717093000	10.415676000
1	10.120760000	-11.107869000	11.462281000
1	10.712562000	-10.469155000	9.184570000
1	12.029534000	-10.062207000	10.320065000
8	7.934214000	-10.673038000	10.201506000
7	9.195581000	-7.274620000	12.854635000
6	8.467825000	-6.606086000	13.855477000
8	7.905050000	-7.294562000	14.733427000
7	8.409061000	-5.257585000	13.825131000
6	8.985665000	-4.563878000	12.830749000
7	8.925433000	-3.231309000	12.890007000
6	9.657547000	-5.228333000	11.755436000
6	9.732200000	-6.581910000	11.809592000
1	8.401908000	-2.770886000	13.645503000
1	9.255178000	-2.674640000	12.115988000
1	10.098243000	-4.683743000	10.929862000
1	10.213276000	-7.167026000	11.036836000
15	6.671907000	-10.178323000	9.227192000
8	6.122443000	-11.437454000	8.623481000

8	7.087479000	-8.982420000	8.420363000
8	5.668324000	-3.367944000	23.086071000
6	6.535561000	-5.866907000	20.441453000
6	7.464113000	-6.608325000	21.411366000
6	7.122482000	-5.907864000	22.731183000
6	5.607060000	-5.720526000	22.604539000
6	4.994552000	-4.586755000	23.402629000
8	5.399537000	-5.480095000	21.187396000
1	6.238232000	-6.505209000	19.605793000
1	8.506830000	-6.502923000	21.133891000
8	7.111237000	-7.980247000	21.488747000
1	7.648351000	-8.427291000	20.813493000
1	7.602894000	-4.924307000	22.741913000
1	5.104947000	-6.656817000	22.881762000
1	5.097372000	-4.815807000	24.471020000
1	3.931917000	-4.507295000	23.149908000
8	7.457724000	-6.638539000	23.895337000
7	9.810804000	-4.425955000	16.817011000
6	9.303331000	-5.622982000	17.150446000
7	8.428546000	-5.902083000	18.118637000
6	8.073584000	-4.790097000	18.790376000
6	8.534395000	-3.488185000	18.574026000
6	9.448296000	-3.317535000	17.506456000
7	9.983501000	-2.138500000	17.158153000
7	7.984098000	-2.613618000	19.495338000
6	7.210097000	-3.370071000	20.247689000
7	7.200044000	-4.696653000	19.851459000
1	9.651440000	-6.453612000	16.545946000
1	9.662243000	-1.297608000	17.613371000
1	10.545846000	-2.066674000	16.306207000
1	6.629146000	-3.036782000	21.096609000
15	4.962004000	-1.931662000	23.540137000
8	4.547312000	-1.996221000	24.981342000
8	5.860642000	-0.865813000	22.980483000
8	15.245585000	-4.749060000	10.037519000
6	13.837362000	-6.732306000	12.908165000
6	13.037581000	-7.578437000	11.906810000
6	13.643955000	-7.109058000	10.580646000
6	15.120905000	-6.963781000	10.947300000
6	15.915410000	-6.012795000	10.080634000
8	15.100594000	-6.489455000	12.321563000

1	13.951412000	-7.261799000	13.855262000
1	11.975807000	-7.380141000	11.981888000
8	13.296501000	-8.959933000	12.110292000
1	12.526518000	-9.295544000	12.601236000
1	13.243116000	-6.118695000	10.343214000
1	15.602298000	-7.950414000	10.920096000
1	15.993429000	-6.436700000	9.072891000
1	16.920920000	-5.881797000	10.495163000
8	13.464108000	-7.980619000	9.478718000
7	13.152919000	-5.450646000	13.229970000
6	12.128322000	-5.537135000	14.174360000
8	11.706360000	-6.621194000	14.574512000
7	11.629342000	-4.331622000	14.602624000
6	12.006740000	-3.066446000	14.166730000
8	11.496950000	-2.052085000	14.665410000
6	12.996368000	-3.069946000	13.112795000
1	13.314395000	-2.127763000	12.686934000
6	13.535965000	-4.244242000	12.700943000
1	10.898874000	-4.384071000	15.349476000
1	14.282861000	-4.298400000	11.919803000
15	12.066555000	-7.818021000	8.580966000
8	12.232701000	-8.737643000	7.407504000
8	11.704900000	-6.364688000	8.459021000
8	9.943613000	-7.206173000	23.422572000
6	10.991997000	-7.752967000	19.921869000
6	12.206454000	-8.621240000	20.286045000
6	11.992190000	-8.752526000	21.803372000
6	10.477024000	-8.965203000	21.875492000
6	9.784342000	-8.602106000	23.175119000
8	9.954746000	-8.155601000	20.790218000
1	10.667254000	-7.896964000	18.888068000
1	13.153133000	-8.158239000	20.007643000
8	12.072460000	-9.912338000	19.705795000
1	12.246604000	-9.821400000	18.754555000
1	12.255104000	-7.801062000	22.280078000
1	10.266340000	-10.019305000	21.655022000
1	10.230000000	-9.194651000	23.984938000
1	8.722057000	-8.847464000	23.092970000
8	12.669206000	-9.828838000	22.417532000
7	13.430444000	-3.958214000	17.715295000
6	13.474767000	-5.307414000	17.466435000

7	14.286535000	-5.716859000	16.462409000
7	12.761089000	-6.197774000	18.145047000
6	12.073100000	-5.636308000	19.160453000
6	12.027631000	-4.297576000	19.556188000
6	12.704696000	-3.335905000	18.745406000
8	12.726999000	-2.099521000	18.868481000
7	11.267951000	-4.157368000	20.707351000
6	10.852080000	-5.372445000	20.987104000
7	11.292401000	-6.316407000	20.065193000
1	13.995199000	-3.328447000	17.107041000
1	15.020863000	-5.101935000	16.089517000
1	14.433531000	-6.714608000	16.408399000
1	10.275699000	-5.659920000	21.851657000
15	8.983842000	-6.461360000	24.554341000
8	8.955056000	-7.273255000	25.816148000
8	9.392454000	-5.016354000	24.500503000
8	17.199261000	0.337164000	11.271896000
6	17.646788000	-2.628036000	13.462819000
6	17.209067000	-3.591078000	12.340232000
6	17.168151000	-2.625219000	11.148231000
6	18.384575000	-1.737994000	11.413118000
6	18.340002000	-0.364373000	10.773374000
8	18.439966000	-1.627663000	12.856105000
1	18.228914000	-3.146547000	14.226665000
1	16.253445000	-4.065678000	12.560133000
8	18.219928000	-4.562654000	12.106688000
1	18.160982000	-5.210888000	12.827696000
1	16.258715000	-2.018751000	11.220047000
1	19.284941000	-2.259061000	11.063464000
1	18.270997000	-0.492583000	9.685574000
1	19.250143000	0.189987000	11.016106000
8	17.276611000	-3.209145000	9.866652000
7	16.492376000	-2.016833000	14.174510000
6	15.861201000	-2.812672000	15.146447000
8	16.201805000	-4.010067000	15.240155000
7	14.929789000	-2.243195000	15.943842000
6	14.552616000	-0.964600000	15.769361000
7	13.696360000	-0.447104000	16.652281000
6	15.065222000	-0.191105000	14.677433000
6	16.044988000	-0.751335000	13.921524000
1	13.405344000	-0.986718000	17.476310000

1	13.414037000	0.518569000	16.576644000
1	14.733377000	0.821397000	14.486266000
1	16.510011000	-0.233551000	13.092863000
15	15.862663000	-3.560610000	9.055176000
8	16.295616000	-4.144506000	7.742637000
8	14.906203000	-2.409965000	9.181103000
8	14.952834000	-9.226887000	21.439371000
6	16.635997000	-7.557661000	18.564650000
6	17.987643000	-8.140718000	19.017697000
6	17.519613000	-9.128538000	20.091440000
6	16.237523000	-9.688721000	19.478798000
6	15.243577000	-10.241623000	20.478056000
8	15.662626000	-8.562405000	18.767765000
1	16.665369000	-7.271833000	17.511693000
1	18.644413000	-7.368838000	19.403225000
8	18.612077000	-8.836346000	17.948431000
1	19.264322000	-8.220220000	17.574811000
1	17.261614000	-8.564291000	20.992570000
1	16.491625000	-10.473425000	18.754049000
1	15.685730000	-11.117970000	20.966053000
1	14.318184000	-10.540842000	19.974789000
8	18.411318000	-10.177482000	20.411438000
7	16.272487000	-6.328157000	19.319380000
6	16.882501000	-5.132172000	18.902965000
8	17.793450000	-5.203067000	18.054300000
7	16.438234000	-3.963362000	19.424713000
6	15.507763000	-3.951364000	20.391244000
7	15.076364000	-2.754519000	20.829829000
6	14.994211000	-5.168142000	20.940134000
6	15.376480000	-6.330341000	20.346903000
1	15.242545000	-1.929060000	20.239207000
1	14.216615000	-2.735571000	21.361843000
1	14.275987000	-5.169565000	21.750269000
1	15.007988000	-7.298899000	20.655505000
15	14.250684000	-9.589943000	22.895995000
8	14.720716000	-10.927835000	23.385405000
8	14.348655000	-8.321801000	23.694065000
8	17.640188000	5.219457000	14.459579000
6	19.409290000	1.947784000	15.137233000
6	19.032694000	1.374598000	13.759654000
6	18.400769000	2.611601000	13.106509000

6	19.334189000	3.718593000	13.602404000
6	18.771485000	5.126189000	13.588330000
8	19.658889000	3.327588000	14.953570000
1	20.298357000	1.452467000	15.538684000
1	18.357105000	0.528110000	13.844071000
8	20.203367000	1.012149000	13.039768000
1	20.429166000	0.109655000	13.319234000
1	17.401505000	2.761668000	13.530290000
1	20.245005000	3.705404000	12.987610000
1	18.463789000	5.361482000	12.562105000
1	19.551821000	5.833501000	13.884078000
8	18.347458000	2.604602000	11.694031000
7	17.303294000	-1.511753000	18.107723000
6	18.378443000	-1.604564000	17.256430000
7	18.971980000	-2.809577000	17.162303000
7	18.849843000	-0.573241000	16.562399000
6	18.118037000	0.545356000	16.745619000
6	16.984019000	0.737831000	17.538503000
6	16.528120000	-0.361855000	18.329068000
8	15.587004000	-0.391122000	19.142628000
7	16.497141000	2.027946000	17.381005000
6	17.315487000	2.596015000	16.522911000
7	18.336767000	1.746366000	16.116534000
1	17.000207000	-2.374115000	18.600764000
1	18.518973000	-3.670040000	17.494105000
1	19.732531000	-2.890997000	16.504339000
1	17.238353000	3.600976000	16.138534000
15	17.007041000	1.952119000	10.941399000
8	17.219452000	2.205520000	9.478362000
8	15.765619000	2.348532000	11.689351000
8	20.621309000	-8.972040000	20.880964000
6	21.546261000	-5.958237000	18.867297000
6	23.017853000	-6.117423000	19.312109000
6	22.970427000	-7.491119000	19.985588000
6	22.004970000	-8.260455000	19.066085000
6	21.276032000	-9.430751000	19.697578000
8	21.042987000	-7.260185000	18.642642000
1	21.479342000	-5.368297000	17.951698000
1	23.317967000	-5.313950000	19.994294000
8	23.871695000	-6.199191000	18.184067000
1	23.904780000	-5.317329000	17.778413000

1	22.502786000	-7.370984000	20.970964000
1	22.564196000	-8.613737000	18.190977000
1	22.003896000	-10.217213000	19.939044000
1	20.541595000	-9.828446000	18.990986000
8	24.251293000	-8.075675000	20.095946000
7	20.712229000	-5.253603000	19.870890000
6	20.702020000	-3.859819000	19.792446000
8	21.461648000	-3.248503000	19.044662000
7	19.790919000	-3.240895000	20.616881000
6	18.953077000	-3.854789000	21.544993000
8	18.165202000	-3.181110000	22.223480000
6	19.110196000	-5.286349000	21.640957000
1	18.524810000	-5.838387000	22.363821000
6	19.970344000	-5.923565000	20.811897000
1	19.760960000	-2.201134000	20.553006000
1	20.114428000	-6.996064000	20.849148000
15	19.503500000	-9.942510000	21.642135000
8	20.100810000	-11.292085000	21.910917000
8	18.899394000	-9.066589000	22.703498000
8	16.833544000	6.530370000	19.193810000
6	20.218854000	4.586420000	19.305899000
6	20.280213000	4.707846000	17.767504000
6	19.100612000	5.648217000	17.547079000
6	19.254734000	6.639917000	18.704268000
6	17.972855000	7.368834000	19.098898000
8	19.740757000	5.823640000	19.797478000
1	21.205725000	4.365470000	19.725050000
1	20.157779000	3.742892000	17.271922000
8	21.474361000	5.360366000	17.365000000
1	22.203231000	4.725121000	17.452361000
1	18.192555000	5.064478000	17.713043000
1	20.025172000	7.378610000	18.447866000
1	17.814053000	8.175244000	18.366632000
1	18.121617000	7.836920000	20.078105000
8	19.059418000	6.296664000	16.293238000
7	19.715508000	-0.422495000	20.409304000
6	20.701515000	0.259148000	19.798975000
7	20.749194000	1.559205000	19.502437000
6	19.619116000	2.187781000	19.879497000
6	18.501040000	1.608490000	20.487410000
6	18.583999000	0.228447000	20.778880000

7	17.614582000	-0.438866000	21.430254000
7	17.517309000	2.552371000	20.722446000
6	18.032099000	3.675525000	20.270691000
7	19.308683000	3.524284000	19.756947000
1	21.559685000	-0.343495000	19.509548000
1	16.683352000	-0.047958000	21.396356000
1	17.704780000	-1.448541000	21.573190000
1	17.544995000	4.641520000	20.253189000
15	17.595649000	6.481826000	15.525166000
8	17.656232000	7.790715000	14.798388000
8	16.476162000	6.135192000	16.484052000
1	1.500598000	-10.078362000	11.717175000
1	4.882344000	6.092663000	17.031888000
1	24.172061000	-8.838289000	20.690504000
1	16.567328000	6.329976000	18.262116000

Figure S35. X-Y coordinates for **1:2** at level: B3LYP-GD3/6-31G*. Adjustment of all C3'-C2'-O2'-H2' to 180°

8	-10.057808000	-7.560098000	5.540473000
6	-13.087668000	-5.310965000	5.309017000
6	-12.745143000	-5.039130000	3.826860000
6	-11.626498000	-6.066068000	3.611401000
6	-12.149858000	-7.264403000	4.407008000
6	-11.102764000	-8.257008000	4.865901000
8	-12.804732000	-6.672177000	5.553214000
1	-14.140159000	-5.102085000	5.511941000
1	-12.437078000	-4.007620000	3.660002000
8	-13.852137000	-5.381386000	3.002341000
1	-14.482684000	-4.646658000	3.057176000
1	-10.714765000	-5.690488000	4.088438000
1	-12.896541000	-7.796779000	3.803432000
1	-10.725282000	-8.779440000	3.974820000
1	-11.576779000	-8.998995000	5.523813000
8	-11.368310000	-6.435943000	2.276176000
7	-12.301736000	-4.463114000	6.243075000
6	-12.756813000	-3.145587000	6.430412000
8	-13.691467000	-2.743849000	5.706989000
7	-12.178850000	-2.386476000	7.389748000
6	-11.116560000	-2.841494000	8.073721000
7	-10.594385000	-2.046760000	9.016405000
6	-10.573839000	-4.145021000	7.826149000
6	-11.213244000	-4.930122000	6.919640000
1	-10.957159000	-1.097696000	9.164163000
1	-9.750614000	-2.321305000	9.497427000
1	-9.705374000	-4.506965000	8.362049000
1	-10.899220000	-5.940176000	6.681781000
8	-14.166611000	7.843480000	9.419381000
6	-14.291811000	5.162884000	6.692968000
6	-15.820409000	5.083730000	6.882538000
6	-16.088754000	6.285518000	7.800299000
6	-15.070538000	7.302128000	7.257962000
6	-14.670721000	8.408435000	8.207295000
8	-13.916414000	6.511631000	6.903975000
1	-13.997365000	4.833641000	5.692197000
1	-16.130578000	4.124241000	7.306946000
8	-16.503881000	5.366753000	5.664919000
1	-16.554776000	4.551247000	5.142294000
1	-15.833698000	6.035668000	8.833747000
1	-15.484589000	7.764752000	6.350514000

1	-15.550219000	9.030071000	8.411394000
1	-13.908986000	9.030036000	7.724706000
8	-17.423291000	6.739987000	7.780169000
7	-12.937956000	0.405882000	7.605509000
6	-13.678534000	0.935211000	6.573512000
7	-14.152521000	0.071040000	5.652989000
7	-13.962306000	2.228964000	6.470255000
6	-13.450099000	2.950994000	7.487027000
6	-12.732127000	2.517981000	8.605058000
6	-12.404916000	1.128471000	8.689350000
8	-11.746370000	0.541444000	9.565111000
7	-12.452366000	3.585477000	9.447440000
6	-12.977770000	4.630749000	8.850393000
7	-13.586179000	4.308159000	7.644933000
1	-12.695772000	-0.604093000	7.565756000
1	-13.919242000	-0.928079000	5.661803000
1	-14.533620000	0.474487000	4.810172000
1	-12.984313000	5.646581000	9.218993000
8	-10.905383000	-4.081455000	1.393089000
6	-12.290916000	-0.599048000	1.942573000
6	-11.517613000	-0.153852000	0.683200000
6	-11.081574000	-1.507318000	0.121390000
6	-12.299833000	-2.387543000	0.413600000
6	-12.015382000	-3.871696000	0.516773000
8	-12.809390000	-1.890958000	1.676261000
1	-13.104616000	0.095806000	2.170644000
1	-10.679987000	0.487158000	0.937129000
8	-12.370935000	0.498433000	-0.246483000
1	-12.273626000	1.447655000	-0.075454000
1	-10.234200000	-1.872571000	0.705766000
1	-13.057682000	-2.229420000	-0.365605000
1	-11.779903000	-4.254020000	-0.482916000
1	-12.895342000	-4.397736000	0.903946000
8	-10.770762000	-1.513879000	-1.255611000
7	-10.483593000	2.046840000	5.865516000
6	-11.200217000	2.478616000	4.775456000
7	-11.538643000	3.792902000	4.753878000
7	-11.593652000	1.672834000	3.794632000
6	-11.187843000	0.396386000	3.977462000
6	-10.429324000	-0.138658000	5.021384000
6	-10.046756000	0.728749000	6.086196000

8	-9.409480000	0.439309000	7.113406000
7	-10.190019000	-1.488682000	4.814846000
6	-10.794210000	-1.762249000	3.681692000
7	-11.432282000	-0.658732000	3.130823000
1	-10.169977000	2.748202000	6.568987000
1	-10.991437000	4.458208000	5.311223000
1	-11.860074000	4.128587000	3.856393000
1	-10.791960000	-2.710769000	3.166123000
15	-10.198679000	-5.577326000	1.448923000
8	-10.162380000	-6.186379000	0.077829000
8	-8.988952000	-5.407847000	2.321354000
8	-9.183229000	8.119019000	11.882410000
6	-9.732076000	7.652181000	8.190181000
6	-11.183642000	8.113322000	8.303755000
6	-11.232120000	8.587008000	9.767481000
6	-9.873218000	9.283797000	9.902212000
6	-9.286960000	9.411874000	11.294542000
8	-8.991105000	8.480030000	9.076091000
1	-9.345843000	7.754289000	7.177452000
1	-11.888155000	7.313635000	8.069514000
8	-11.373970000	9.225296000	7.433455000
1	-11.923113000	9.858414000	7.931432000
1	-11.299229000	7.741641000	10.457619000
1	-9.946659000	10.287043000	9.464725000
1	-9.942671000	10.058874000	11.891181000
1	-8.298533000	9.878641000	11.225022000
8	-12.292031000	9.502944000	9.994688000
7	-9.586887000	6.226250000	8.563663000
6	-9.783265000	5.276367000	7.542681000
8	-10.143387000	5.688626000	6.420713000
7	-9.584142000	3.969903000	7.822975000
6	-9.241283000	3.571882000	9.059465000
7	-9.006523000	2.271860000	9.255577000
6	-9.109437000	4.513612000	10.130708000
6	-9.302398000	5.823444000	9.837106000
1	-9.161196000	1.593216000	8.498425000
1	-8.863391000	1.922613000	10.191406000
1	-8.864761000	4.210626000	11.141152000
1	-9.230525000	6.598521000	10.589563000
15	-13.713617000	8.872388000	10.641114000
8	-14.652237000	10.038143000	10.719904000

8	-13.369439000	7.986410000	11.800661000
8	-8.916389000	0.253929000	-1.425379000
6	-9.385047000	3.179380000	0.855022000
6	-8.348970000	3.983342000	0.057392000
6	-8.141132000	3.065300000	-1.148800000
6	-9.566333000	2.564765000	-1.414281000
6	-9.699260000	1.228296000	-2.119399000
8	-10.155067000	2.463406000	-0.089985000
1	-10.028780000	3.832270000	1.448365000
1	-7.441173000	4.136519000	0.627253000
8	-8.890992000	5.228467000	-0.350717000
1	-8.557326000	5.873619000	0.293414000
1	-7.522159000	2.218223000	-0.838027000
1	-10.114850000	3.321569000	-1.990211000
1	-9.351672000	1.340131000	-3.154187000
1	-10.754219000	0.932666000	-2.122551000
8	-7.574719000	3.695116000	-2.279515000
7	-7.289295000	2.906885000	5.481788000
6	-7.883216000	3.912288000	4.820981000
7	-8.420727000	3.882177000	3.599972000
6	-8.295538000	2.662261000	3.042386000
6	-7.679760000	1.536562000	3.595558000
6	-7.164314000	1.687782000	4.904223000
7	-6.556053000	0.710058000	5.588082000
7	-7.697172000	0.477120000	2.704296000
6	-8.313277000	0.952313000	1.640863000
7	-8.730284000	2.263540000	1.798315000
1	-7.935812000	4.850438000	5.362901000
1	-6.517347000	-0.218198000	5.195592000
1	-6.311052000	0.854381000	6.571043000
1	-8.491123000	0.414628000	0.719695000
15	-9.180314000	-1.361881000	-1.722169000
8	-9.181310000	-1.614268000	-3.202153000
8	-8.288007000	-2.082826000	-0.750731000
8	-4.265855000	5.491130000	13.138637000
6	-5.120198000	6.640124000	9.661487000
6	-6.326134000	7.404702000	10.225660000
6	-6.058666000	7.284945000	11.732310000
6	-4.538719000	7.444630000	11.787235000
6	-3.854482000	6.852326000	12.998833000
8	-4.067245000	6.775380000	10.591258000

1	-4.829305000	7.040605000	8.689350000
1	-7.250124000	6.925106000	9.924407000
8	-6.298413000	8.752496000	9.793037000
1	-7.140337000	8.881134000	9.318093000
1	-6.323737000	6.276280000	12.062420000
1	-4.283700000	8.511004000	11.723174000
1	-4.131536000	7.427382000	13.888645000
1	-2.769237000	6.911574000	12.859449000
8	-6.697511000	8.248080000	12.547754000
7	-5.427728000	5.200499000	9.451942000
6	-6.128013000	4.892662000	8.284868000
8	-6.607041000	5.769553000	7.565963000
7	-6.244150000	3.552202000	8.016602000
6	-5.794555000	2.497280000	8.801929000
8	-5.945703000	1.325206000	8.425971000
6	-5.177205000	2.900837000	10.045201000
1	-4.834076000	2.140870000	10.734371000
6	-5.007661000	4.219382000	10.312442000
1	-6.720356000	3.310076000	7.114678000
1	-4.549187000	4.574021000	11.225882000
15	-8.185994000	7.876657000	13.195494000
8	-8.447203000	8.932119000	14.228420000
8	-8.274540000	6.400310000	13.461351000
8	-5.530526000	4.884655000	-1.213434000
6	-5.780774000	6.075944000	2.263918000
6	-4.689197000	7.148053000	2.113977000
6	-4.422465000	7.047438000	0.602181000
6	-5.847019000	6.897809000	0.054524000
6	-6.011469000	6.225109000	-1.295984000
8	-6.539533000	6.127438000	1.074355000
1	-6.438710000	6.261298000	3.117276000
1	-3.818356000	6.936265000	2.735140000
8	-5.224587000	8.436517000	2.391080000
1	-5.343357000	8.497731000	3.351680000
1	-3.856761000	6.129495000	0.406840000
1	-6.299658000	7.896071000	0.001852000
1	-5.445167000	6.799468000	-2.040446000
1	-7.068941000	6.223862000	-1.575660000
8	-3.785508000	8.165319000	0.019811000
7	-3.551556000	3.191387000	5.722594000
6	-3.845993000	4.532464000	5.738612000

7	-3.501193000	5.221428000	6.853598000
7	-4.450114000	5.158560000	4.736269000
6	-4.648772000	4.353045000	3.672891000
6	-4.307459000	3.009355000	3.515330000
6	-3.765398000	2.318207000	4.641882000
8	-3.470596000	1.115579000	4.737615000
7	-4.574892000	2.587805000	2.222857000
6	-5.092725000	3.638598000	1.626050000
7	-5.185410000	4.742437000	2.468956000
1	-3.103428000	2.768951000	6.564459000
1	-2.820064000	4.834488000	7.518756000
1	-3.561183000	6.226670000	6.772621000
1	-5.367352000	3.700985000	0.584929000
15	-5.909163000	3.781399000	-2.394327000
8	-5.649427000	4.374266000	-3.748496000
8	-5.302965000	2.494812000	-1.907740000
8	-1.287661000	0.666841000	13.594212000
6	-0.641977000	3.365206000	11.059164000
6	-1.559311000	4.342691000	11.800935000
6	-1.849469000	3.556938000	13.089491000
6	-0.485279000	2.915268000	13.360568000
6	-0.488901000	1.668633000	14.218258000
8	0.050549000	2.628584000	12.048151000
1	0.065225000	3.893868000	10.418688000
1	-2.442383000	4.599726000	11.215307000
8	-0.807757000	5.512100000	12.110404000
1	-1.048955000	5.744029000	13.025964000
1	-2.612987000	2.791178000	12.925394000
1	0.156096000	3.658306000	13.852213000
1	-0.884052000	1.923817000	15.208679000
1	0.541688000	1.318896000	14.332213000
8	-2.201952000	4.402686000	14.173529000
7	-1.402213000	2.444558000	10.172635000
6	-1.808900000	2.952774000	8.925668000
8	-1.640799000	4.168245000	8.702117000
7	-2.357362000	2.102902000	8.027754000
6	-2.575287000	0.811425000	8.333404000
7	-3.046341000	0.019394000	7.369585000
6	-2.299453000	0.312059000	9.648427000
6	-1.696761000	1.157413000	10.523718000
1	-3.170766000	0.380850000	6.416194000

1	-3.159359000	-0.968929000	7.537541000
1	-2.514660000	-0.711145000	9.928457000
1	-1.427199000	0.860552000	11.528673000
15	-3.833661000	4.647037000	14.498873000
8	-3.854923000	5.545300000	15.698379000
8	-4.556734000	3.336969000	14.409177000
8	-1.862027000	8.224646000	1.711675000
6	-0.767058000	7.415779000	5.193235000
6	0.529638000	8.208880000	4.945252000
6	0.191908000	8.904082000	3.625767000
6	-1.288913000	9.238249000	3.798340000
6	-2.043798000	9.403497000	2.495459000
8	-1.818232000	8.133049000	4.574574000
1	-0.956316000	7.307433000	6.262436000
1	1.378788000	7.540255000	4.872911000
8	0.749225000	9.162334000	5.977906000
1	1.437331000	8.777136000	6.543139000
1	0.291265000	8.176280000	2.814812000
1	-1.392064000	10.161114000	4.384311000
1	-1.635844000	10.274820000	1.970838000
1	-3.111142000	9.564682000	2.679857000
8	0.925897000	10.072923000	3.323910000
7	-0.692280000	6.033675000	4.643671000
6	0.011453000	5.078933000	5.401050000
8	0.675547000	5.477420000	6.380326000
7	-0.062231000	3.776536000	5.031859000
6	-0.708805000	3.417089000	3.909770000
7	-0.801219000	2.108302000	3.625269000
6	-1.278120000	4.396781000	3.037267000
6	-1.279811000	5.686014000	3.463515000
1	-0.618994000	1.430362000	4.376484000
1	-1.484597000	1.825712000	2.935596000
1	-1.753552000	4.119882000	2.104909000
1	-1.727315000	6.490705000	2.896359000
15	-2.115698000	8.229753000	0.074078000
8	-1.746584000	9.565975000	-0.499582000
8	-1.552990000	6.924334000	-0.410317000
8	0.444392000	-4.394604000	11.421248000
6	2.207295000	-1.006358000	10.979431000
6	1.420776000	-0.356069000	12.115710000
6	0.638464000	-1.566207000	12.646509000

6	1.716829000	-2.653816000	12.579348000
6	1.233775000	-4.090762000	12.577885000
8	2.464737000	-2.345194000	11.380574000
1	3.148016000	-0.483811000	10.788670000
1	0.800701000	0.468634000	11.764274000
8	2.343888000	0.096246000	13.101683000
1	1.958128000	-0.148788000	13.962418000
1	-0.207290000	-1.812617000	11.997659000
1	2.373710000	-2.532879000	13.451708000
1	0.620372000	-4.234010000	13.476024000
1	2.093978000	-4.762336000	12.648232000
8	0.212846000	-1.376343000	13.986619000
7	0.763487000	1.784854000	6.994628000
6	1.463664000	2.157821000	8.117695000
7	1.816972000	3.456630000	8.203975000
7	1.812542000	1.305186000	9.079259000
6	1.325714000	0.063807000	8.868426000
6	0.551784000	-0.402682000	7.803279000
6	0.260247000	0.499275000	6.736417000
8	-0.353663000	0.263095000	5.683356000
7	0.163321000	-1.717072000	8.014937000
6	0.689766000	-2.037461000	9.173623000
7	1.432427000	-1.003153000	9.732584000
1	0.498743000	2.520026000	6.308834000
1	1.371908000	4.173231000	7.616555000
1	2.247255000	3.749835000	9.068918000
1	0.591966000	-2.984340000	9.678365000
15	-1.364028000	-0.857273000	14.252701000
8	-1.493185000	-0.779025000	15.743054000
8	-2.293104000	-1.616925000	13.354122000
8	3.359842000	9.307629000	3.527938000
6	4.137633000	6.840136000	6.204936000
6	5.640650000	7.195650000	6.117472000
6	5.589901000	8.421560000	5.202614000
6	4.324419000	9.135999000	5.709351000
6	3.619255000	10.046673000	4.724037000
8	3.428034000	8.053320000	6.069987000
1	3.889685000	6.372728000	7.158815000
1	6.224388000	6.369768000	5.694695000
8	6.131439000	7.594744000	7.385565000
1	6.174333000	6.800589000	7.940610000

1	5.412578000	8.074141000	4.176847000
1	4.580406000	9.706298000	6.610997000
1	4.256060000	10.916294000	4.515697000
1	2.676473000	10.392097000	5.160848000
8	6.769206000	9.190425000	5.294129000
7	3.719562000	5.887400000	5.147922000
6	3.879215000	4.535652000	5.453531000
8	4.466342000	4.165910000	6.469167000
7	3.339114000	3.668388000	4.536074000
6	2.712994000	3.997583000	3.336153000
8	2.256067000	3.109192000	2.604173000
6	2.682155000	5.413503000	3.048855000
1	2.252142000	5.757366000	2.118126000
6	3.179938000	6.291800000	3.952504000
1	3.408278000	2.655002000	4.778717000
1	3.185609000	7.360218000	3.775214000
15	2.302213000	9.930790000	2.400694000
8	2.695834000	11.337380000	2.058762000
8	2.140086000	8.830930000	1.389757000
8	1.450660000	-6.271748000	6.841670000
6	4.342935000	-3.649290000	7.379449000
6	3.769000000	-3.493622000	8.796456000
6	2.805900000	-4.682030000	8.834006000
6	3.549683000	-5.753604000	8.038428000
6	2.632397000	-6.806837000	7.418049000
8	4.263403000	-5.015164000	7.022127000
1	5.375996000	-3.292735000	7.329361000
1	3.259164000	-2.533074000	8.893596000
8	4.809249000	-3.616709000	9.749106000
1	4.356732000	-3.565001000	10.610856000
1	1.898400000	-4.399378000	8.297979000
1	4.279212000	-6.248067000	8.693626000
1	2.393118000	-7.539123000	8.203884000
1	3.177126000	-7.333821000	6.627528000
8	2.508922000	-5.136427000	10.139734000
7	3.601761000	0.944740000	5.183959000
6	4.405174000	0.559431000	6.190753000
7	4.536152000	-0.657251000	6.720387000
6	3.707068000	-1.536948000	6.127146000
6	2.791468000	-1.274167000	5.101984000
6	2.772988000	0.046381000	4.599465000

7	2.013749000	0.434290000	3.556662000
7	2.085048000	-2.415128000	4.763521000
6	2.566237000	-3.343437000	5.563171000
7	3.560276000	-2.876978000	6.404444000
1	5.007328000	1.356481000	6.621550000
1	1.215055000	-0.142004000	3.329765000
1	1.952353000	1.430540000	3.330809000
1	2.235306000	-4.372133000	5.619565000
15	0.968639000	-5.662698000	10.489455000
8	1.108327000	-6.896592000	11.328372000
8	0.133325000	-5.621583000	9.229117000
1	-17.723399000	6.623039000	6.859960000
1	-9.450462000	-8.215517000	5.916200000
1	6.777070000	9.810052000	4.547728000
1	0.863849000	-6.028240000	7.596982000

Figure S36. X-Y coordinates for **1:2** at level: B3LYP-GD3/6-31G*. Adjustment of one strand C3'-C2'-O2'-H2' to 180° and another randomized.

8	10.709277000	-2.766336000	16.661583000
6	12.830455000	-2.661939000	13.523356000
6	11.554373000	-2.447237000	12.699856000
6	10.523103000	-2.200909000	13.814443000
6	11.344899000	-1.376042000	14.811857000
6	10.867816000	-1.411486000	16.248815000
8	12.685698000	-1.907421000	14.709026000
1	13.714132000	-2.336269000	12.972045000
1	11.334616000	-3.301609000	12.061171000
8	11.713203000	-1.266955000	11.916980000
1	11.110018000	-0.608840000	12.307248000
1	10.200174000	-3.142722000	14.265098000
1	11.354421000	-0.329049000	14.481114000
1	9.913522000	-0.866293000	16.295455000
1	11.595699000	-0.883123000	16.879928000
8	9.406399000	-1.443918000	13.370445000
7	13.042601000	-4.096812000	13.865187000
6	13.587809000	-4.925981000	12.865314000
8	13.741643000	-4.447202000	11.724179000
7	13.935079000	-6.194623000	13.189233000
6	13.665726000	-6.690578000	14.407506000
7	14.043768000	-7.948544000	14.669478000
6	13.022460000	-5.893127000	15.408493000
6	12.752527000	-4.597304000	15.101285000
1	14.467321000	-8.534573000	13.940243000
1	13.794467000	-8.377171000	15.548653000
1	12.786308000	-6.293906000	16.386322000
1	12.293712000	-3.909838000	15.801694000
8	17.147501000	-13.882884000	6.605871000
6	15.178277000	-10.596689000	6.753988000
6	16.373270000	-9.871392000	6.076209000
6	17.257849000	-11.066251000	5.674637000
6	16.203363000	-12.110418000	5.278451000
6	16.650964000	-13.554254000	5.307405000
8	15.122352000	-11.906852000	6.211280000
1	14.236484000	-10.073552000	6.575261000
1	16.870387000	-9.166117000	6.752480000
8	15.608373000	-8.648078000	5.885016000
1	15.650571000	-8.378513000	4.951208000
1	17.808599000	-11.428575000	6.546669000
1	15.853882000	-11.887005000	4.259787000

1	17.432915000	-13.691285000	4.551312000
1	15.800938000	-14.195812000	5.049012000
8	18.192984000	-10.779492000	4.654689000
7	14.749374000	-8.015698000	11.074854000
6	14.503408000	-7.617580000	9.781134000
7	14.112840000	-6.338597000	9.598397000
7	14.661654000	-8.416293000	8.731204000
6	15.093767000	-9.646600000	9.076681000
6	15.420335000	-10.141015000	10.343795000
6	15.210708000	-9.284484000	11.469213000
8	15.382831000	-9.537139000	12.674950000
7	15.895663000	-11.441511000	10.252957000
6	15.843476000	-11.727990000	8.972216000
7	15.348749000	-10.680838000	8.206828000
1	14.514519000	-7.355619000	11.842173000
1	13.926129000	-5.701635000	10.381118000
1	13.752850000	-6.103535000	8.685381000
1	16.152641000	-12.653359000	8.506706000
8	8.655331000	-2.971464000	11.469364000
6	10.157821000	-5.079609000	8.709419000
6	8.754541000	-5.274108000	8.127034000
6	7.950076000	-4.286148000	8.982838000
6	8.932976000	-3.114000000	9.090425000
6	8.733570000	-2.195742000	10.274977000
8	10.234690000	-3.736997000	9.158146000
1	10.926839000	-5.274340000	7.956256000
1	8.415951000	-6.306755000	8.202416000
8	8.774818000	-4.850159000	6.767743000
1	8.258233000	-4.026088000	6.739025000
1	7.752976000	-4.698937000	9.974665000
1	8.871089000	-2.512370000	8.173574000
1	7.809774000	-1.625360000	10.131411000
1	9.576615000	-1.495678000	10.332236000
8	6.743928000	-3.872988000	8.357209000
7	11.829943000	-9.663269000	10.142371000
6	11.557014000	-9.195540000	8.880575000
7	11.810768000	-10.045689000	7.852409000
7	11.103584000	-7.969921000	8.636582000
6	10.905046000	-7.256750000	9.767156000
6	11.112629000	-7.647811000	11.092381000
6	11.653470000	-8.943348000	11.334752000

8	11.958253000	-9.449077000	12.428496000
7	10.735779000	-6.643996000	11.969954000
6	10.324014000	-5.667391000	11.196290000
7	10.419125000	-5.971971000	9.844211000
1	12.144493000	-10.649634000	10.259745000
1	11.853105000	-11.053811000	8.043800000
1	11.382957000	-9.781331000	6.975279000
1	9.913113000	-4.723332000	11.519426000
15	8.047932000	-2.290551000	12.852685000
8	7.036939000	-1.236454000	12.516089000
8	7.797262000	-3.433480000	13.789828000
8	15.450018000	-17.511495000	10.393963000
6	13.150159000	-15.336321000	8.336817000
6	14.271457000	-15.042633000	7.340390000
6	15.364448000	-16.004937000	7.839325000
6	14.536750000	-17.247969000	8.189679000
6	15.128134000	-18.214243000	9.197148000
8	13.297668000	-16.699669000	8.707951000
1	12.163342000	-15.172556000	7.907405000
1	14.564963000	-13.991700000	7.351448000
8	13.843428000	-15.429583000	6.036400000
1	14.370140000	-16.215130000	5.803331000
1	15.861079000	-15.614837000	8.731165000
1	14.319040000	-17.801455000	7.267344000
1	16.026204000	-18.666707000	8.757802000
1	14.401399000	-19.006489000	9.406955000
8	16.314743000	-16.297845000	6.827011000
7	13.256312000	-14.458059000	9.524311000
6	12.642651000	-13.193646000	9.442524000
8	12.095271000	-12.872388000	8.367055000
7	12.686032000	-12.381698000	10.520913000
6	13.336407000	-12.746821000	11.638165000
7	13.308455000	-11.911069000	12.677997000
6	14.022525000	-14.000963000	11.719627000
6	13.963453000	-14.814578000	10.636945000
1	12.855203000	-10.992246000	12.592053000
1	13.911057000	-12.074248000	13.470456000
1	14.570595000	-14.300035000	12.604289000
1	14.461341000	-15.775202000	10.608994000
15	17.746676000	-15.411934000	6.852029000
8	18.507462000	-15.877044000	5.647095000

8	18.295269000	-15.405060000	8.247678000
8	5.271452000	-5.973928000	8.434261000
6	7.295356000	-8.986668000	7.345785000
6	6.041323000	-9.825308000	7.101240000
6	4.949046000	-8.767983000	7.335304000
6	5.577106000	-7.553815000	6.634799000
6	5.091264000	-6.178284000	7.035073000
8	6.990141000	-7.673975000	6.917667000
1	8.162142000	-9.370678000	6.802435000
1	5.981327000	-10.688727000	7.761173000
8	6.031422000	-10.244640000	5.738672000
1	5.318781000	-9.741390000	5.306809000
1	4.811001000	-8.567852000	8.401388000
1	5.419238000	-7.658656000	5.552656000
1	4.031062000	-6.089235000	6.766770000
1	5.649960000	-5.429227000	6.461066000
8	3.720393000	-9.135619000	6.726696000
7	9.431890000	-11.701849000	11.118111000
6	9.346597000	-11.923192000	9.796716000
7	8.802226000	-11.135530000	8.866680000
6	8.307869000	-10.007897000	9.412633000
6	8.327485000	-9.644827000	10.761960000
6	8.930352000	-10.562638000	11.651163000
7	9.009490000	-10.371818000	12.973769000
7	7.679563000	-8.439259000	10.961068000
6	7.274412000	-8.083310000	9.760063000
7	7.641127000	-8.985042000	8.773915000
1	9.784644000	-12.856796000	9.459847000
1	8.686498000	-9.501064000	13.366858000
1	9.546593000	-11.019415000	13.554923000
1	6.700510000	-7.200582000	9.517472000
15	5.284596000	-4.406636000	8.990900000
8	4.237700000	-3.602172000	8.280817000
8	5.396380000	-4.516926000	10.482930000
8	13.004521000	-18.295862000	15.455341000
6	10.965509000	-17.476203000	12.403966000
6	12.213059000	-17.704576000	11.535637000
6	13.164572000	-18.325360000	12.569335000
6	12.214303000	-19.203936000	13.384245000
6	12.662329000	-19.515155000	14.795326000
8	10.977922000	-18.451124000	13.423893000

1	10.055513000	-17.559540000	11.807514000
1	12.577744000	-16.759920000	11.147744000
8	11.922454000	-18.598281000	10.475167000
1	12.419654000	-19.411417000	10.676819000
1	13.554113000	-17.532195000	13.213684000
1	12.041510000	-20.149074000	12.851649000
1	13.527965000	-20.184900000	14.760539000
1	11.845215000	-20.013803000	15.330123000
8	14.231580000	-19.091630000	12.042337000
7	10.956965000	-16.115309000	13.003874000
6	10.519921000	-15.086986000	12.169605000
8	10.301881000	-15.271008000	10.971920000
7	10.357808000	-13.870573000	12.783238000
6	10.618394000	-13.560159000	14.113085000
8	10.395254000	-12.420464000	14.547466000
6	11.155687000	-14.657465000	14.885173000
1	11.420152000	-14.491250000	15.921123000
6	11.289107000	-15.879785000	14.312486000
1	9.991203000	-13.104382000	12.171275000
1	11.682255000	-16.733788000	14.848393000
15	15.712523000	-18.364748000	11.802943000
8	16.662615000	-19.493668000	11.534541000
8	15.938809000	-17.306180000	12.844597000
8	3.296755000	-11.350081000	7.990841000
6	6.095308000	-13.646305000	8.920019000
6	5.233700000	-14.905262000	8.959061000
6	3.892089000	-14.345185000	8.450526000
6	4.377086000	-13.405616000	7.338525000
6	3.467425000	-12.269753000	6.916099000
8	5.627376000	-12.874617000	7.835455000
1	7.155888000	-13.871123000	8.780231000
1	5.185039000	-15.344760000	9.953906000
8	5.758864000	-15.840891000	8.020466000
1	5.112947000	-15.879191000	7.292197000
1	3.373843000	-13.788912000	9.237232000
1	4.578245000	-14.014042000	6.446183000
1	2.503859000	-12.689267000	6.600460000
1	3.920081000	-11.767402000	6.054255000
8	3.062130000	-15.368470000	7.916411000
7	7.141973000	-13.830911000	13.842879000
6	7.275026000	-14.791560000	12.871533000

7	7.772880000	-15.994598000	13.251856000
7	6.965960000	-14.584878000	11.598882000
6	6.424192000	-13.367987000	11.388976000
6	6.158734000	-12.354150000	12.311594000
6	6.597765000	-12.547365000	13.657463000
8	6.530956000	-11.755358000	14.613911000
7	5.511316000	-11.293327000	11.694658000
6	5.403138000	-11.653190000	10.435001000
7	5.954887000	-12.902959000	10.184169000
1	7.438546000	-14.059925000	14.815509000
1	7.782133000	-16.257961000	14.244518000
1	7.639026000	-16.738394000	12.579824000
1	4.910134000	-11.096983000	9.653307000
15	2.557358000	-9.895365000	7.679503000
8	1.389853000	-10.094528000	6.760708000
8	2.483982000	-9.203326000	9.007940000
8	11.955809000	-16.140526000	20.631353000
6	9.374070000	-17.518698000	18.256437000
6	10.460402000	-18.131535000	17.362708000
6	11.714423000	-17.900750000	18.226560000
6	11.165675000	-18.175437000	19.629632000
6	11.925501000	-17.557816000	20.783980000
8	9.810543000	-17.674933000	19.591517000
1	8.410827000	-18.009430000	18.114333000
1	10.493423000	-17.656794000	16.381367000
8	10.210603000	-19.527790000	17.233367000
1	10.917198000	-19.972386000	17.735700000
1	12.066306000	-16.868772000	18.143357000
1	11.140078000	-19.261853000	19.788261000
1	12.942623000	-17.967604000	20.794165000
1	11.428118000	-17.833097000	21.719630000
8	12.758472000	-18.816974000	17.933516000
7	9.166815000	-16.077555000	17.952205000
6	8.384034000	-15.772764000	16.823654000
8	7.970144000	-16.715083000	16.118735000
7	8.117111000	-14.475182000	16.553138000
6	8.630783000	-13.485780000	17.303863000
7	8.272424000	-12.236332000	17.003756000
6	9.522230000	-13.773070000	18.389464000
6	9.746604000	-15.080252000	18.683841000
1	7.617448000	-12.056636000	16.235614000

1	8.635646000	-11.458096000	17.532877000
1	9.968623000	-12.989022000	18.987501000
1	10.389895000	-15.394051000	19.495449000
15	13.929644000	-18.331764000	16.828784000
8	14.907005000	-19.466128000	16.768129000
8	14.302369000	-16.905653000	17.103516000
8	3.219715000	-16.846891000	10.004771000
6	4.883035000	-18.180577000	13.121729000
6	3.743048000	-19.208515000	13.237474000
6	3.062199000	-19.025395000	11.874050000
6	4.252435000	-18.797667000	10.945032000
6	3.919490000	-18.047363000	9.672357000
8	5.192699000	-18.043461000	11.748887000
1	5.759104000	-18.513406000	13.680238000
1	3.091226000	-18.953891000	14.066843000
8	4.271388000	-20.513874000	13.399162000
1	4.061522000	-20.986435000	12.574067000
1	2.458513000	-18.113893000	11.902266000
1	4.705301000	-19.762373000	10.678658000
1	3.294386000	-18.687958000	9.041789000
1	4.841641000	-17.800189000	9.135140000
8	2.280983000	-20.110697000	11.411916000
7	4.499834000	-16.859082000	13.682307000
6	4.556150000	-16.722933000	15.081501000
8	4.758457000	-17.746048000	15.764968000
7	4.400435000	-15.488248000	15.615858000
6	4.088972000	-14.439513000	14.839357000
7	4.012223000	-13.230167000	15.424028000
6	3.837464000	-14.600285000	13.439962000
6	4.094589000	-15.819777000	12.897324000
1	4.463913000	-13.120620000	16.341247000
1	4.055385000	-12.416463000	14.825035000
1	3.530871000	-13.768742000	12.818852000
1	3.990524000	-16.030038000	11.841528000
15	2.073094000	-16.197045000	9.000555000
8	1.417193000	-17.275051000	8.191163000
8	1.331369000	-15.198939000	9.838582000
8	9.482130000	-12.106523000	23.980454000
6	7.893874000	-15.348389000	22.697107000
6	9.233325000	-15.968850000	22.306074000
6	10.198865000	-14.894875000	22.832945000

6	9.534223000	-14.544326000	24.171160000
6	9.899270000	-13.210117000	24.792381000
8	8.116997000	-14.624470000	23.898227000
1	7.123460000	-16.106944000	22.854323000
1	9.301850000	-16.157669000	21.235210000
8	9.404033000	-17.182036000	23.035351000
1	10.104449000	-17.010038000	23.689448000
1	10.224909000	-14.024899000	22.170400000
1	9.803189000	-15.323769000	24.897568000
1	10.990725000	-13.183115000	24.898329000
1	9.463855000	-13.140733000	25.793166000
8	11.504534000	-15.407700000	23.047498000
7	5.472879000	-15.047723000	18.250406000
6	5.814966000	-16.156325000	18.989765000
7	5.479284000	-17.354033000	18.472540000
7	6.428026000	-16.087876000	20.169625000
6	6.718412000	-14.819319000	20.525695000
6	6.442599000	-13.632163000	19.842896000
6	5.726592000	-13.714584000	18.611368000
8	5.337709000	-12.780276000	17.891422000
7	6.975676000	-12.542360000	20.513880000
6	7.556208000	-13.054617000	21.573332000
7	7.411989000	-14.435908000	21.651351000
1	5.026363000	-15.183445000	17.322128000
1	5.201516000	-17.456648000	17.489434000
1	5.793960000	-18.171208000	18.974070000
1	8.089794000	-12.509210000	22.334476000
15	12.633906000	-15.198637000	21.818883000
8	13.887998000	-15.835599000	22.334115000
8	12.540396000	-13.794676000	21.299915000
8	0.569795000	-20.653290000	13.278549000
6	1.838415000	-20.343427000	16.794635000
6	0.622781000	-21.143619000	17.285105000
6	0.030403000	-21.667594000	15.968960000
6	1.300310000	-21.953668000	15.145968000
6	1.148175000	-21.904991000	13.636990000
8	2.237940000	-20.930767000	15.567523000
1	2.649398000	-20.394150000	17.520257000
1	-0.073879000	-20.516304000	17.853407000
8	1.110739000	-22.221320000	18.071469000
1	0.938446000	-23.033562000	17.563450000

1	-0.568635000	-20.889726000	15.481780000
1	1.693054000	-22.935096000	15.438800000
1	0.505873000	-22.737295000	13.318680000
1	2.128702000	-22.020374000	13.164703000
8	-0.744106000	-22.819836000	16.252416000
7	1.543949000	-18.907173000	16.594266000
6	1.789647000	-18.062443000	17.681663000
8	2.132112000	-18.495434000	18.779067000
7	1.600190000	-16.724525000	17.429980000
6	1.170558000	-16.144535000	16.239065000
8	1.050820000	-14.915611000	16.144814000
6	0.876923000	-17.091453000	15.188014000
1	0.519387000	-16.733675000	14.231849000
6	1.066503000	-18.415489000	15.403238000
1	1.787787000	-16.090151000	18.235733000
1	0.867487000	-19.152633000	14.634653000
15	0.641657000	-20.117506000	11.699186000
8	0.087515000	-21.172964000	10.789477000
8	0.123795000	-18.708285000	11.761575000
8	5.394516000	-9.167253000	23.617886000
6	3.849011000	-12.784524000	23.941734000
6	5.295231000	-13.249257000	24.184264000
6	5.990107000	-11.898295000	24.376576000
6	4.937692000	-11.076689000	25.122009000
6	5.090546000	-9.565800000	24.946065000
8	3.677073000	-11.538809000	24.589996000
1	3.131077000	-13.521104000	24.313767000
1	5.662898000	-13.796270000	23.315405000
8	5.350741000	-14.052954000	25.350845000
1	5.838795000	-13.517198000	26.001370000
1	6.161022000	-11.459105000	23.392493000
1	4.980718000	-11.322972000	26.191725000
1	5.868100000	-9.228241000	25.647654000
1	4.152184000	-9.078747000	25.231581000
8	7.193347000	-11.969466000	25.119430000
7	2.334295000	-14.985236000	19.530382000
6	2.581914000	-15.506333000	20.745003000
7	2.992218000	-14.876025000	21.847081000
6	3.172155000	-13.561169000	21.618251000
6	2.988492000	-12.886785000	20.406133000
6	2.524821000	-13.659948000	19.317963000

7	2.237342000	-13.137059000	18.112179000
7	3.291269000	-11.542715000	20.535149000
6	3.643669000	-11.409488000	21.796003000
7	3.580016000	-12.593476000	22.509224000
1	2.433454000	-16.581509000	20.816640000
1	2.645904000	-12.241516000	17.885683000
1	1.994922000	-13.759314000	17.336236000
1	3.975600000	-10.496540000	22.273159000
15	8.473237000	-10.995640000	24.687621000
8	9.076746000	-10.489459000	25.962444000
8	8.034904000	-10.078373000	23.567701000
1	17.745687000	-10.161054000	4.050396000
1	10.508428000	-2.773119000	17.609987000
1	-1.177621000	-23.118278000	15.437618000
1	6.345498000	-9.393130000	23.476172000

Figure S37. X-Y coordinates for **1:2** at level: B3LYP-GD3/6-31G*. Adjustment of one strand C3'-C2'-O2'-H2' to 360° and another randomized.