Supporting Information

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Synthesis, Characterization and Third-Order Nonlinear Optical Properties of a Dodecaruthenium Organometallic Dendrimer with a Zinc(II) Tetraphenylporphyrin Core

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Including:

1. Synthesis of the Organometallic Dendrons 9 and 10.

Synthesis and characterization of 9. The dendron **8**[1] (75 mgs; 0.35 mmol) was added to a solution of $Me_3SiC{\equiv}C(1,4\text{-}C_6H_4)C{\equiv}C(4\text{-}C_6H_4I)$[2] (0.21 g, 0.52 mmol), CuI (0.01 g, 0.08 mmol), and $Pd(PPh_3)_4$ (0.04 g, 0.03 mmol) in 120 mL of a deoxygenated mixture of CH_2Cl_2/NEt_3 (1:1) under nitrogen. The reaction mixture was stirred at 40 ˚C overnight, concentrated under reduced pressure, and passed through a 10 cm pad of basic alumina, eluting with a CH_2Cl_2/NEt_3 mixture (98:2). The yellow eluate was concentrated and precipitated from hexane, to yield the title compound as a yellow solid (0.69 g, 82%). **^{1}H NMR** (300 MHz, CD_2Cl_2): δ = 7.70–6.50 (m, 101H, CH_{Ar}), 2.77 (s, 16H, C$H_{2/dppe}$), 0.31 (s, 9H, Si(CH_3)$_3$). **^{31}P{^{1}H} NMR** (121 MHz, CD_2Cl_2): δ = 53.3 (s). **^{13}C{^{1}H} NMR** (125 MHz, CD_2Cl_2): δ = 137.7 & 137.3 (m, $C_{ipso/dppe}$), 134.6 & 134.4 (s, CH$_{dppe}$), 132.2 (CH), 132.1 (Ru-C≡C, m), 132.0 (CH), 131.8 (CH), 130.9 (C_q), 130.5 (C_q), 130.2 (CH), 129.8 (CH), 129.1 & 128.9 (s, CH$_{dppe}$), 127.8 (CH), 127.4 & 127.3 (s, CH$_{dppe}$), 124.7 (C_q), 123.5 (C_q), 123.3 (CH), 122.6 (C_q), 121.5 (C_q), 116.9 (C_q), 116.4 (C_q), 104.6 (C_q), 96.8 (C_q), 93.4 (C_q), 91.4 (C_q), 90.9 (C_q), 87.6 (C_q), 31.9 (C_{dppe}), 0.8 (C_{TMS}) [one Ru-C≡C (quintuplet), 1C_q (s) and 2CH (s) not observed]. **FT-IR** (KBr, cm^{-1}): ν = 2202 (vw, C≡C), 2155 (w, C≡C), 2054 (s, RuC≡C). **Raman** (solid, cm^{-1}): ν = 2207 (m, C≡C), 2158 (w, C≡C), 2073 (m, RuC≡C).

Synthesis and characterization of 10. To a solution of **9** (250 mgs, 0.10 mmol) in distilled THF (30 mL), N^{n}Bu$_4$F (1.0 mL of a 1 M solution in THF; 0.10 mmol) was added under nitrogen, and the reaction mixture was stirred at room temperature for 1 h. The reaction mixture was concentrated under reduced pressure, and passed through a 10 cm pad of basic alumina, eluting with a CH_2Cl_2/NEt_3 mixture (98:2). The yellow eluate was concentrated and precipitated from hexane, to yield the title compound as a yellow solid (0.19 g, 81%).[3] **^{1}H NMR** (300 MHz, $CDCl_3$): δ = 7.70–6.50 (m, 101H, CH_{Ar}), 3.19 (s, 1H, -C≡CH), 2.70 (s, 16H, C$H_{2/dppe}$). **^{31}P{^{1}H} NMR** (121 MHz, $CDCl_3$): δ = 53.9 (s). FT-IR (KBr, cm^{-1}): ν = 3282 (m, ≡C-H), 2198 (vw, C≡C), 2049 (vs, C≡CH & RuC≡C). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$): δ = 137.8 & 137.6 (m, C_{dppe}), 135.0 & 134.8 (s, C_{dppe}), 132.8, 132.3, 132.1, 132.0, 131.3, 130.7, 130.3, 129.3 & 129.1 (C_{dppe}), 128.0, 127.2 & 127.1 (s, C_{dppe}), 125.2, 124.3, 123.4, 122.8, 122.7, 121.6, 117.5, 116.8, 94.2, 92.0, 91.1, 87.9, 83.9, 79.7, 32.2 (C_{dppe}) [all Ru-C≡C (quintuplets), 2 C (s) not observed]. **HRMS-ESI** (m/z): calcd for $[C_{148}H_{118}P_8{}^{102}Ru_2]^+$: 2347.5300, Found: 2347.5339 [M + H]$^+$. **Anal.** Calcd. for $C_{148}H_{118}P_8Ru_2$: C 75.76, H 5.07%. Found: C 75.68, H 5.12%.

[1] S. K. Hurst, M. P. Cifuentes, M. G. Humphrey, *Organometallics* 2002, *21*, 2353-2355.
[2] R. P. Hsung, C. E. D. Chidsey and L. R. Sita *Organometallics* 1995, *14*, 4808-4815.
[3] R. L. Roberts, T. Schwich, T. C. Corkery, M. P. Cifuentes, K. A. Green, J. D. Farmer, P. J. Low, T. B. Marder, M. Samoc and M. G. Humphrey, *Adv. Mater.*, 2009, *21*, 2318-2322.

2. ^{1}H, $^{31}P\{^{1}H\}$ and $^{13}C\{^{1}H\}$ NMR spectra of 9

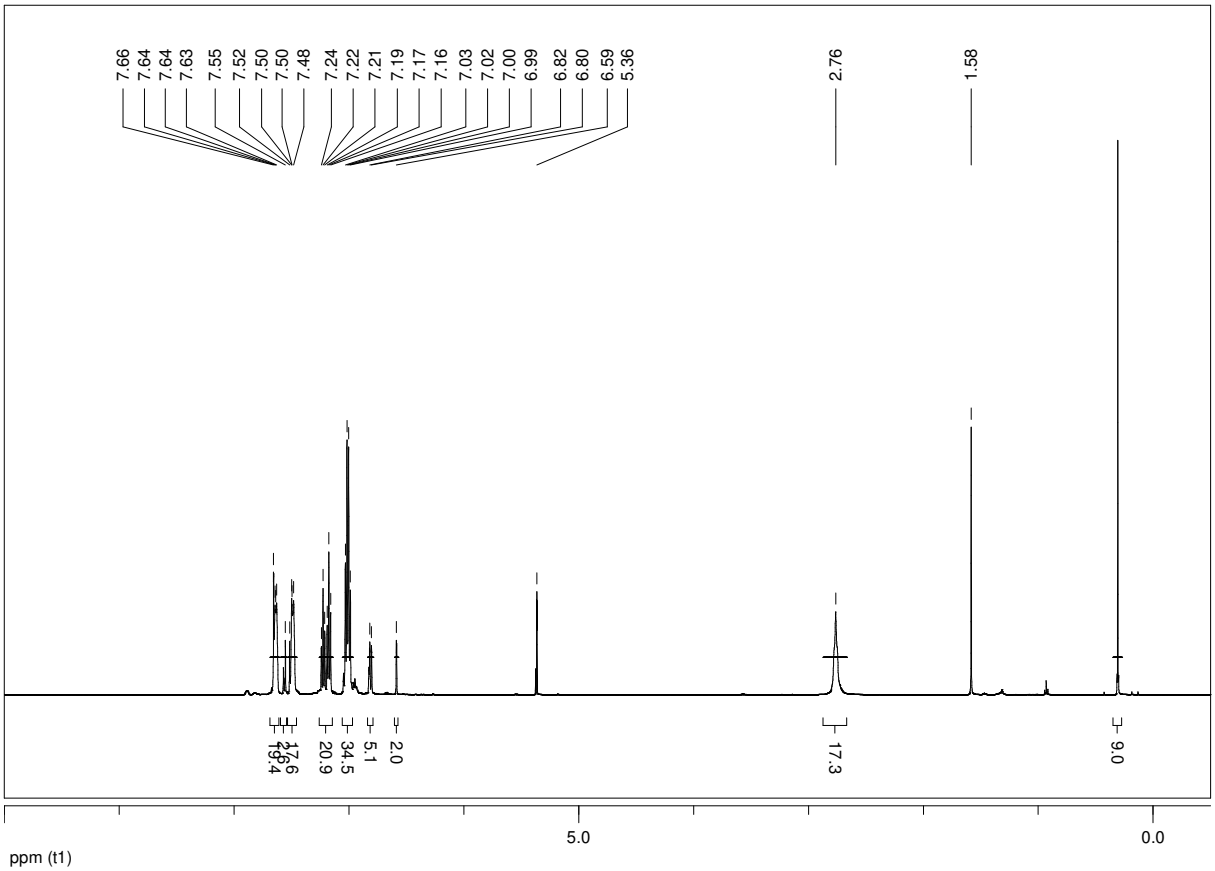


Fig. S1. ^{1}H NMR (300 MHz) spectrum of **9** in CD_2Cl_2.

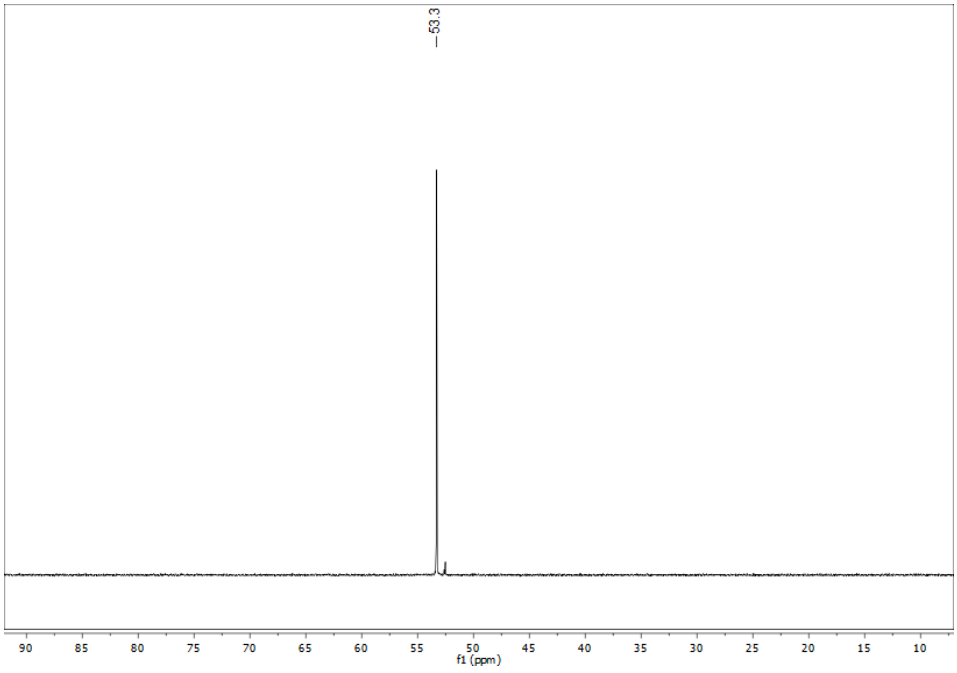


Fig. S2. $^{31}P\{^{1}H\}$ NMR (121 MHz) spectrum of **9** in CD_2Cl_2.

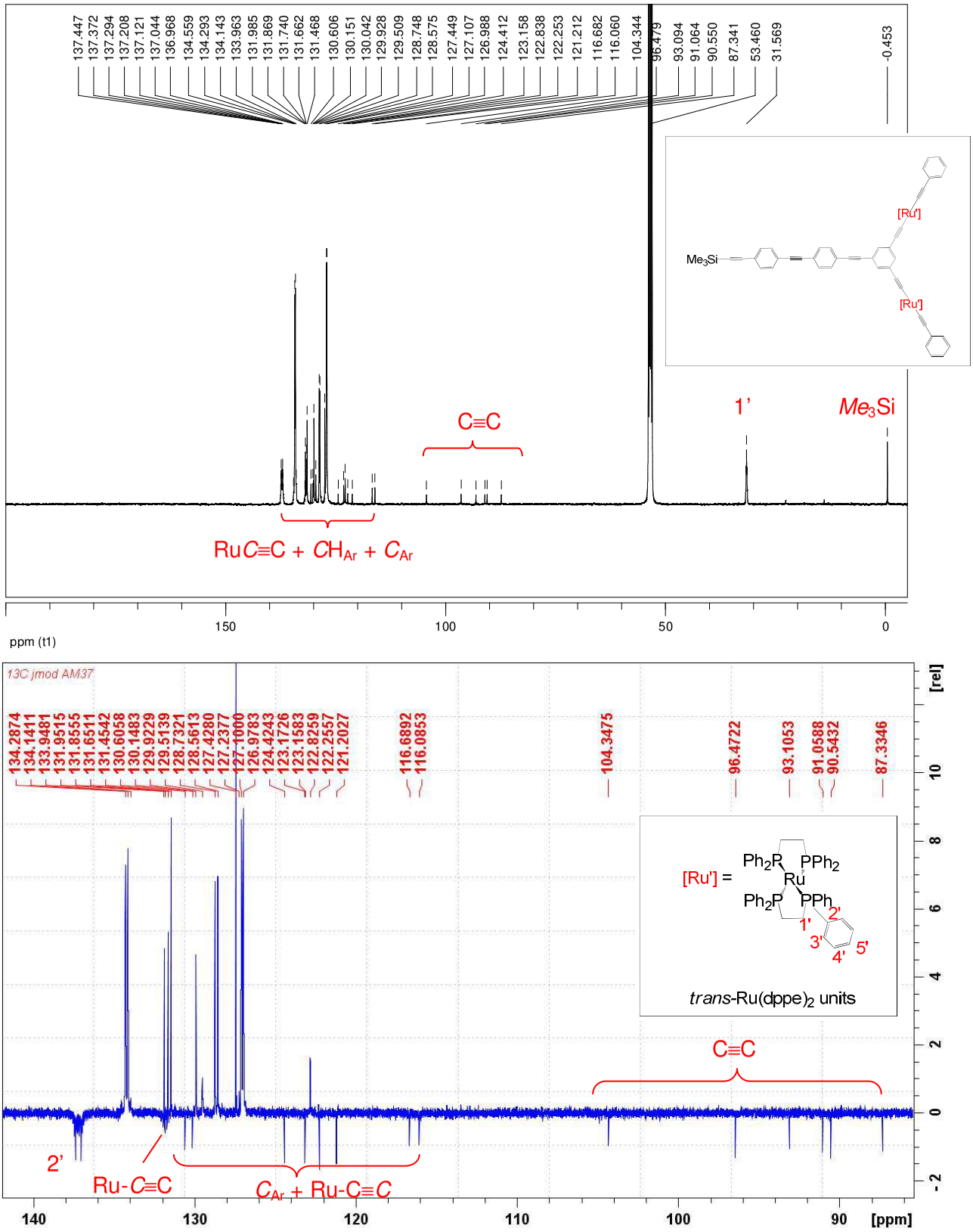


Fig. S3. (a) $^{13}C\{^{1}H\}$ NMR (125 MHz) spectrum of **9** in CD_2Cl_2 and (b) spectral expansion in J-mode (quaternary and secondary carbon atoms shown as negative peaks).

3. ^{1}H, $^{31}P\{^{1}H\}$ and $^{13}C\{^{1}H\}$ NMR spectra of 5_2

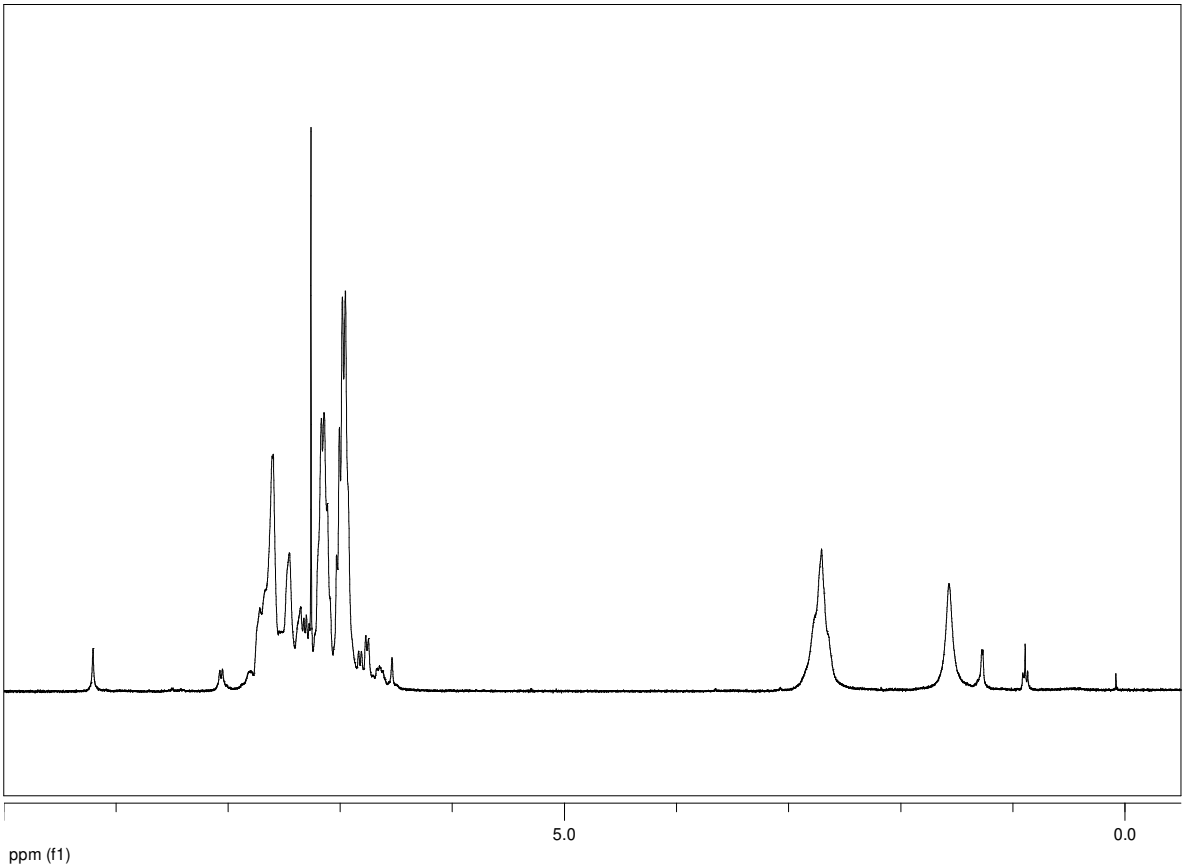


Fig. S4. ^{1}H NMR (300 MHz) spectum of $\mathbf{5_2}$ in $CDCl_3$.

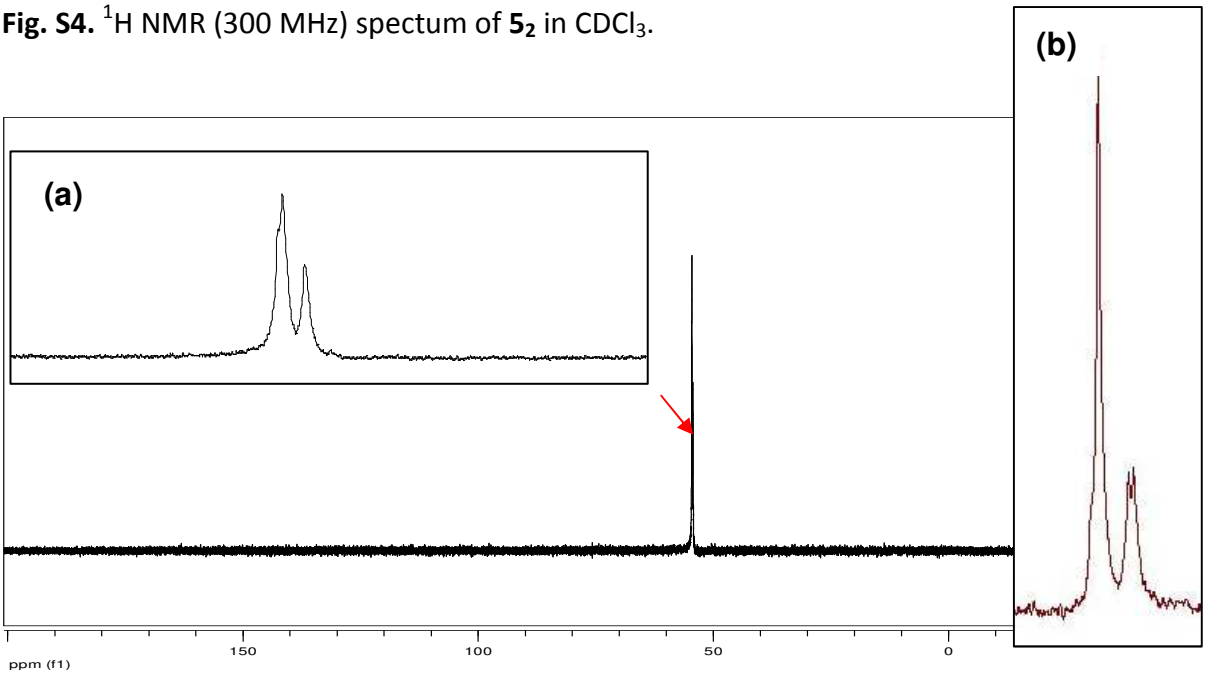


Fig. S5. (a) $^{31}P\{^{1}H\}$ NMR (120 MHz) spectrum of $\mathbf{5_2}$ in $CDCl_3$ showing the expanded ^{31}P signal detected in inset. (b) Expansion of the corresponding $^{31}P\{^{1}H\}$ NMR signal on a 162 MHz spectrometer showing the AB pattern of the inner phosphorus atoms.

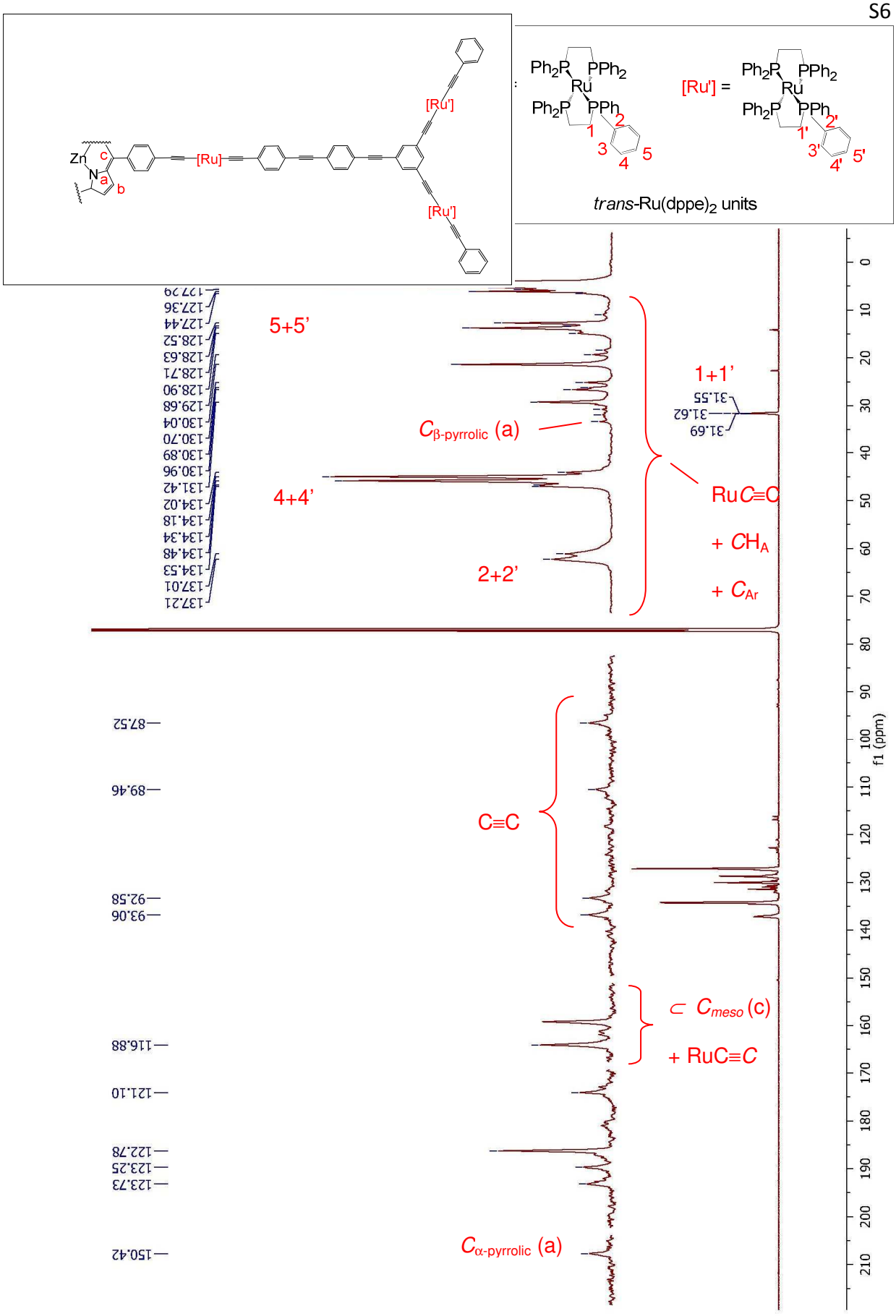


Fig. S6. $^{13}C\{^{1}H\}$ NMR (201 MHz) spectrum of **5_2** in THF, spectral expansions and tentative attributions.

4. Compared $^{13}C\{^{1}H\}$ NMR Spectra of 5_2 and 9

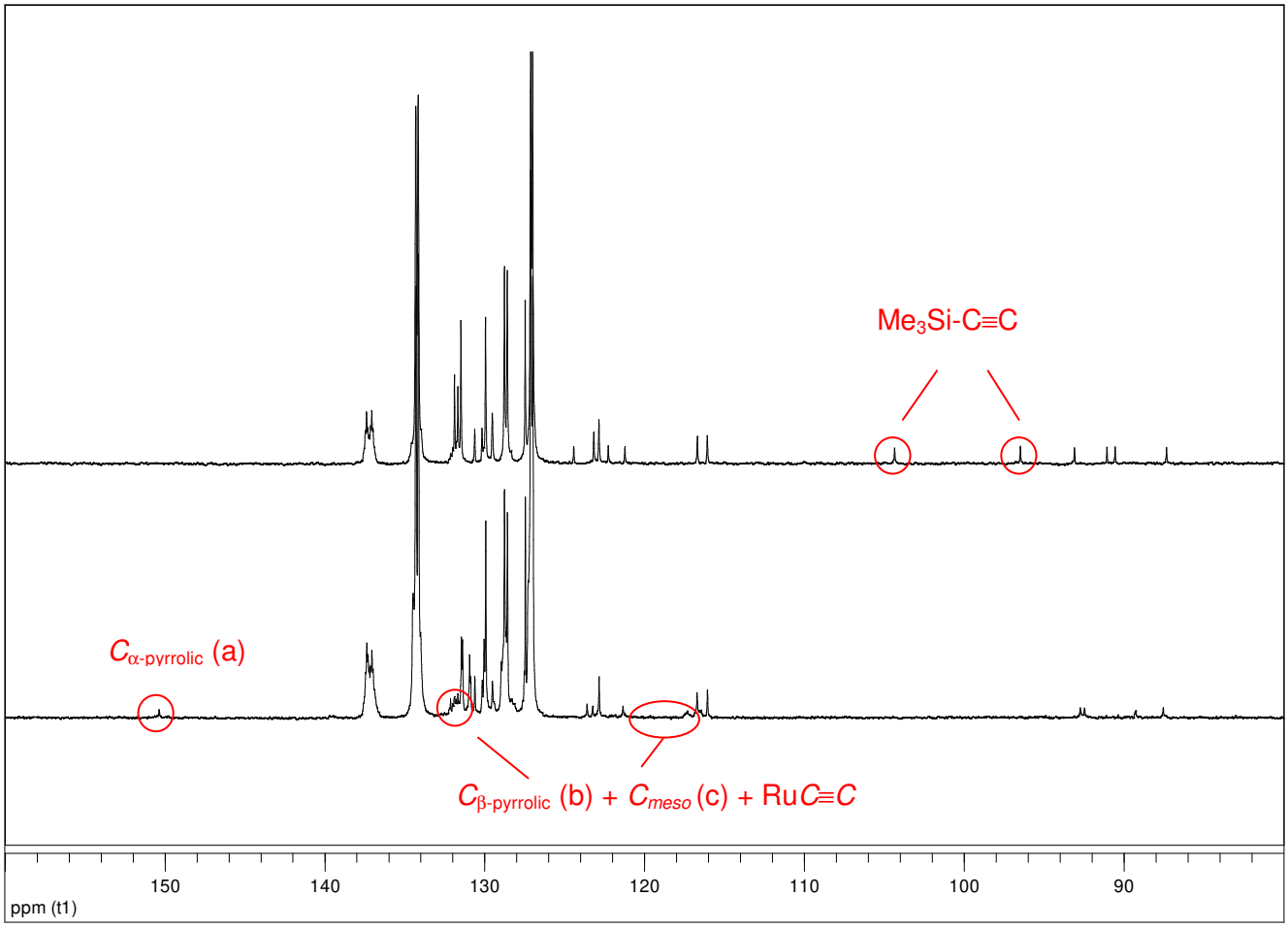


Fig. S7. Overlaid $^{13}C\{^{1}H\}$ NMR (125 MHz) spectra of **5_2** and **9** in CD_2Cl_2 in the 160-80 ppm spectral region with diagnostic signals.

5. Cyclic Voltammetry of 5_2, 9 and 10

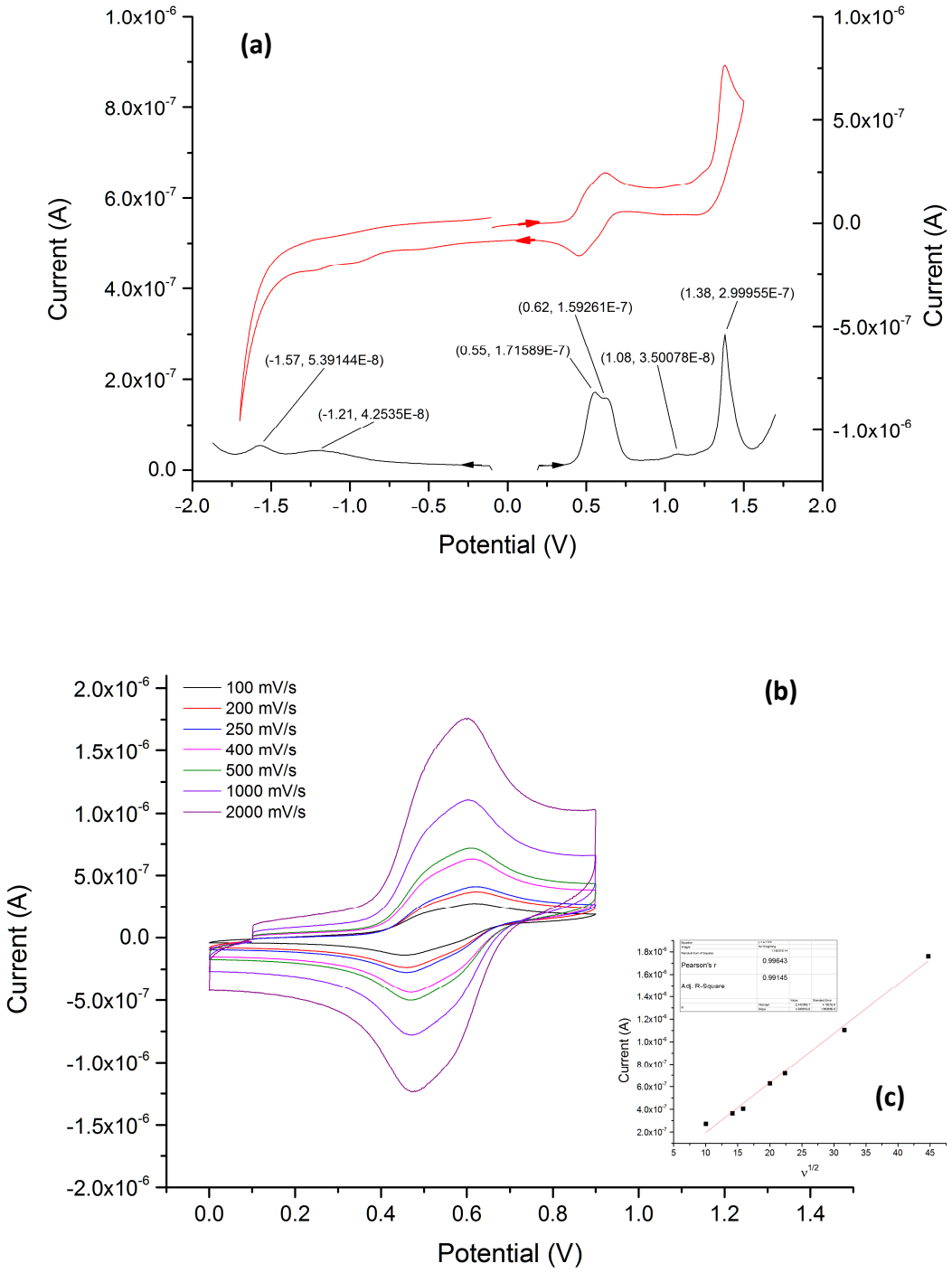


Fig. S8. (a) Cyclic voltammogram of the zinc porphyrin **5_2** in THF/[NBu_4][PF_6] (0.1 M) at 25 °C at 0.1 V/s between -1.5 and 1.6 V *vs.* Ag/AgCl (arrows indicate the porphyrin-based oxidations). (b) Ru(III/II) oxidations/reductions with increasing scanning speeds (v_s). (c) Linear current (I) vs. $(v_s)^{1/2}$ plot.

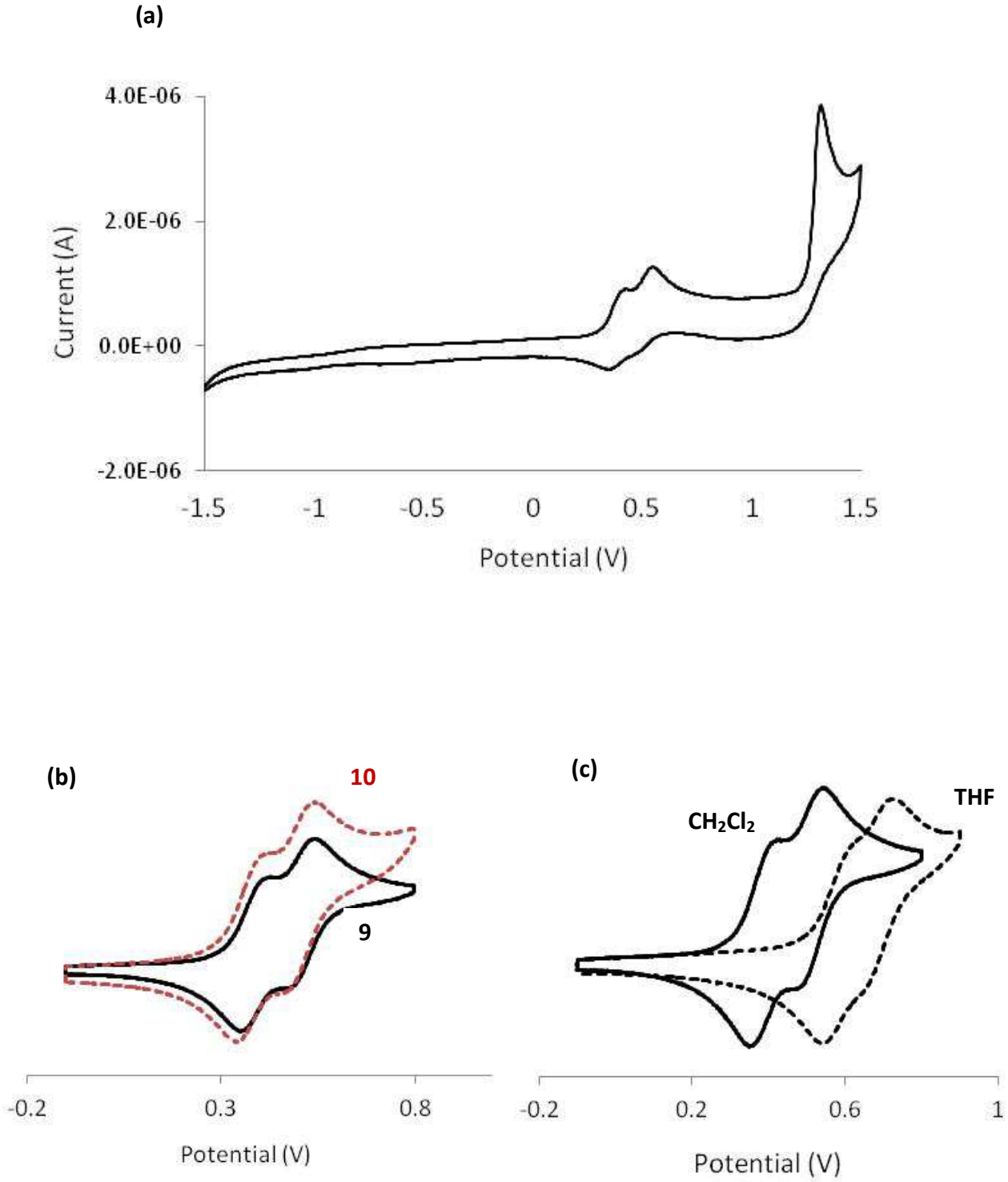


Fig. S9. (a) Cyclic voltammogram of the wedge **9** in CH_2Cl_2/$[NBu_4][PF_6]$ (0.1 M) at 25 °C at 0.1 V/s between -1.0 and 1.5 V *vs.* ECS. (b) Ru(III/II) expansion of the two oxidations of **9** and **10** recorded under previous conditions. (c) Cyclic voltammogram of **9** in CH_2Cl_2 and THF under previous conditions.

6. Cartesian Coordinates of DFT Optimized Geometries for 6, 9, 9', 4-H' and 5_2'

Compound 6:

1	N	-0.0075	-2.0565	-0.0006
2	N	2.0560	-0.0071	-0.0554
3	N	0.0071	2.0566	0.0008
4	N	-2.0564	0.0072	0.0561
5	C	1.0903	-2.8743	0.0004
6	C	2.4342	-2.4516	-0.0046
7	C	2.8653	-1.1104	-0.0155
8	C	4.2472	-0.6967	0.0591
9	H	5.0989	-1.3620	0.1286
10	C	4.2520	0.6668	0.0593
11	H	5.1084	1.3261	0.1289
12	C	2.8732	1.0904	-0.0152
13	C	2.4515	2.4347	-0.0040
14	C	1.1106	2.8668	0.0015
15	C	0.6966	4.2505	-0.0020
16	H	1.3613	5.1053	-0.0156
17	C	-0.6669	4.2552	0.0093
18	H	-1.3256	5.1146	0.0255
19	C	-1.0907	2.8744	0.0021
20	C	-2.4346	2.4517	0.0055
21	C	-2.8657	1.1105	0.0149
22	C	-4.2473	0.6968	-0.0625
23	H	-5.0989	1.3621	-0.1339
24	C	-4.2522	-0.6668	-0.0628
25	H	-5.1084	-1.3259	-0.1343
26	C	-2.8735	-1.0903	0.0145
27	C	-2.4519	-2.4347	0.0047
28	C	-1.1109	-2.8668	0.0009
29	C	-0.6968	-4.2504	0.0083
30	H	-1.3615	-5.1052	0.0246
31	C	0.6667	-4.2551	-0.0029
32	H	1.3254	-5.1146	-0.0164
33	C	3.4861	-3.5068	0.0134
34	C	3.6630	-4.3272	1.1371
35	H	3.0271	-4.1796	2.0081
36	C	4.6477	-5.3106	1.1591
37	H	4.7809	-5.9349	2.0397
38	C	5.4826	-5.5045	0.0455
39	C	5.3079	-4.6869	-1.0840
40	H	5.9469	-4.8339	-1.9518
41	C	-3.4862	3.5071	-0.0126
42	C	-4.3285	3.6990	1.0923
43	H	-4.1993	3.0733	1.9735

44	C	-5.3111	4.6849	1.0823
45	H	-5.9525	4.8300	1.9487
46	C	-5.4823	5.5052	-0.0456
47	C	-4.6442	5.3139	-1.1573
48	H	-4.7747	5.9404	-2.0367
49	C	-3.5109	-3.4825	-0.0133
50	C	-3.6897	-4.3054	-1.1349
51	H	-3.0497	-4.1653	-2.0042
52	C	-4.6815	-5.2817	-1.1572
53	H	-4.8161	-5.9079	-2.0362
54	C	-5.5219	-5.4658	-0.0461
55	C	-5.3451	-4.6459	1.0815
56	H	-5.9882	-4.7855	1.9475
57	C	3.5108	3.4824	0.0135
58	C	4.3512	3.6697	-1.0935
59	H	4.2146	3.0465	-1.9754
60	C	5.3414	4.6479	-1.0847
61	H	5.9815	4.7894	-1.9526
62	C	5.5224	5.4648	0.0442
63	C	4.6859	5.2783	1.1579
64	H	4.8239	5.9022	2.0380
65	Zn	-0.0002	0.0001	0.0001
66	C	6.5411	6.4691	0.0596
67	C	6.4934	-6.5166	0.0615
68	C	-6.5402	-6.4704	-0.0627
69	C	-6.4929	6.5175	-0.0623
70	C	-7.3516	7.3777	-0.0766
71	H	-8.1083	8.1341	-0.0888
72	C	7.4067	7.3223	0.0728
73	H	8.1693	8.0728	0.0844
74	C	7.3522	-7.3766	0.0753
75	H	8.1082	-8.1338	0.0875
76	C	-7.4054	-7.3239	-0.0768
77	H	-8.1674	-8.0750	-0.0893
78	C	-4.3553	-3.6674	1.0913
79	H	-4.2219	-3.0421	1.9721
80	C	4.3251	-3.7012	-1.0936
81	H	4.1933	-3.0776	-1.9758
82	C	3.6937	4.3023	1.1367
83	H	3.0566	4.1603	2.0077
84	C	-3.6597	4.3303	-1.1349
85	H	-3.0213	4.1847	-2.0044

Compound 9:

1	C	17.8735	-0.9849	-0.0924
2	C	16.4477	-0.9180	-0.0936
3	C	15.7888	0.3056	-0.3185
4	C	15.6761	-2.0743	0.1296
5	C	14.4022	0.3711	-0.3205
6	H	16.3805	1.2017	-0.4913
7	C	14.2895	-2.0093	0.1277
8	H	16.1807	-3.0219	0.3039
9	C	13.6294	-0.7854	-0.0976
10	H	13.8981	1.3188	-0.4949
11	H	13.6981	-2.9055	0.3005
12	C	12.2070	-0.7176	-0.1005
13	C	10.9873	-0.6572	-0.1041
14	C	9.5657	-0.5834	-0.1102
15	C	8.9120	0.6446	-0.3330
16	C	8.7843	-1.7357	0.1056
17	C	7.5264	0.7169	-0.3401
18	H	9.5082	1.5387	-0.5010
19	C	7.3986	-1.6621	0.0979
20	H	9.2815	-2.6873	0.2796
21	C	6.7427	-0.4348	-0.1254
22	H	7.0283	1.6677	-0.5169
23	H	6.8019	-2.5553	0.2691
24	C	5.3211	-0.3572	-0.1349
25	C	4.1024	-0.2820	-0.1455
26	C	2.6780	-0.1849	-0.1592
27	C	1.8962	-1.3508	-0.1367
28	C	2.0679	1.0793	-0.1882
29	C	0.4926	-1.2638	-0.1463
30	H	2.3733	-2.3268	-0.1130
31	C	0.6662	1.1882	-0.2136
32	H	2.6761	1.9796	-0.1824
33	C	-0.1032	0.0101	-0.1982
34	H	-1.1879	0.0917	-0.2297
35	C	-0.3133	-2.4412	-0.0744
36	C	-1.0045	-3.4594	0.0559
37	C	0.0301	2.4676	-0.2354
38	C	-0.5357	3.5676	-0.2475
39	Ru	-2.2094	-5.1131	0.1819
40	P	-1.5430	-5.8341	2.3578
41	P	-0.4931	-6.5973	-0.5377
42	C	-3.3588	-6.8083	0.1526
43	P	-3.8600	-3.6007	1.0002
44	P	-3.0946	-4.4012	-1.9440
45	C	-0.4041	-7.3258	2.2122
46	C	-0.3343	-7.8886	0.8042

47	C	-3.9735	-7.8794	0.0734
48	C	-3.9761	-2.2939	-0.3081
49	C	-4.2702	-2.9669	-1.6367
50	H	0.5811	-6.9880	2.5466
51	H	-0.7317	-8.0874	2.9284
52	H	-1.1913	-8.5431	0.6097
53	H	0.5839	-8.4665	0.6473
54	C	-4.6930	-9.1092	-0.0226
55	H	-4.7179	-1.5271	-0.0600
56	H	-2.9901	-1.8179	-0.3274
57	H	-4.1818	-2.2554	-2.4635
58	H	-5.2879	-3.3727	-1.6488
59	C	-6.0799	-9.1666	0.2309
60	C	-4.0359	-10.3082	-0.3724
61	C	-6.7749	-10.3713	0.1457
62	H	-6.6015	-8.2479	0.4906
63	C	-4.7351	-11.5107	-0.4551
64	H	-2.9699	-10.2793	-0.5914
65	C	-6.1083	-11.5527	-0.1946
66	H	-7.8456	-10.3908	0.3452
67	H	-4.2056	-12.4225	-0.7280
68	H	-6.6527	-12.4931	-0.2599
69	Ru	-1.5411	5.3528	-0.1695
70	P	-1.8063	4.6684	2.1021
71	P	-3.5826	4.1590	-0.4373
72	C	-2.5463	7.1389	-0.0883
73	P	0.4974	6.5549	0.0845
74	P	-1.2861	6.0329	-2.4392
75	C	-2.6948	3.0393	1.9870
76	C	-3.9591	3.2523	1.1656
77	C	-3.1162	8.2371	-0.1001
78	C	0.8473	7.4861	-1.5108
79	C	-0.4215	7.6754	-2.3312
80	H	-2.0203	2.3422	1.4810
81	H	-2.9311	2.6529	2.9848
82	H	-4.6818	3.8491	1.7322
83	H	-4.4384	2.2977	0.9253
84	C	-3.7692	9.5084	-0.1142
85	H	1.3019	8.4498	-1.2594
86	H	1.5850	6.9150	-2.0838
87	H	-0.1939	8.0576	-3.3326
88	H	-1.1057	8.3637	-1.8262
89	C	-3.1211	10.6615	0.3775
90	C	-5.0758	9.6470	-0.6294
91	C	-3.7562	11.9016	0.3541
92	H	-2.1127	10.5664	0.7766
93	C	-5.7046	10.8907	-0.6498

94	H	-5.5861	8.7627	-1.0062
95	C	-5.0513	12.0258	-0.1593
96	H	-3.2374	12.7792	0.7376
97	H	-6.7137	10.9763	-1.0512
98	H	-5.5448	12.9959	-0.1775
99	C	19.0976	-1.0421	-0.0917
100	Si	20.9382	-1.1265	-0.0924
101	C	21.4467	-2.8797	0.3345
102	H	21.0725	-3.1689	1.3232
103	H	21.0515	-3.5937	-0.3971
104	H	22.5396	-2.9751	0.3446
105	C	21.5504	-0.6596	-1.8020
106	H	21.1582	-1.3450	-2.5619
107	H	21.2346	0.3551	-2.0701
108	H	22.6461	-0.6961	-1.8450
109	C	21.5854	0.0793	1.1893
110	H	21.2715	1.1040	0.9601
111	H	21.2126	-0.1704	2.1892
112	H	22.6819	0.0599	1.2211
113	C	-4.2263	-5.5033	-2.9138
114	C	-5.3963	-5.9565	-2.2851
115	C	-3.9600	-5.9263	-4.2225
116	C	-6.2907	-6.7864	-2.9592
117	H	-5.6024	-5.6832	-1.2521
118	C	-4.8564	-6.7577	-4.8983
119	H	-3.0450	-5.6165	-4.7216
120	C	-6.0277	-7.1862	-4.2716
121	H	-7.1872	-7.1338	-2.4491
122	H	-4.6334	-7.0698	-5.9173
123	H	-6.7255	-7.8363	-4.7967
124	C	-2.0080	-3.6942	-3.2620
125	C	-2.5699	-3.0962	-4.4031
126	C	-0.6188	-3.7139	-3.1296
127	C	-1.7572	-2.5412	-5.3898
128	H	-3.6512	-3.0786	-4.5362
129	C	0.1988	-3.1579	-4.1171
130	H	-0.1744	-4.1210	-2.2269
131	C	-0.3655	-2.5716	-5.2490
132	H	-2.2089	-2.0889	-6.2713
133	H	1.2792	-3.1712	-3.9837
135	C	-5.6140	-4.1516	1.1995
136	C	-6.6957	-3.3070	0.9010
137	C	-5.8796	-5.4219	1.7267
138	C	-8.0093	-3.7223	1.1184
139	H	-6.5230	-2.3088	0.5044
140	C	-7.1947	-5.8299	1.9652
141	H	-5.0583	-6.1013	1.9361

142	C	-8.2628	-4.9859	1.6598
143	H	-8.8340	-3.0544	0.8754
144	H	-7.3766	-6.8135	2.3956
145	H	-9.2871	-5.3077	1.8413
146	C	-3.6452	-2.5511	2.5107
147	C	-2.5197	-1.7183	2.6038
148	C	-4.5978	-2.5185	3.5395
149	C	-2.3552	-0.8689	3.6980
150	H	-1.7641	-1.7470	1.8207
151	C	-4.4274	-1.6718	4.6369
152	H	-5.4782	-3.1550	3.4901
153	C	-3.3070	-0.8423	4.7197
154	H	-1.4728	-0.2330	3.7536
155	H	-5.1771	-1.6598	5.4265
156	H	-3.1747	-0.1828	5.5758
157	C	-2.8770	-6.4564	3.4734
158	C	-3.3850	-7.7550	3.3256
159	C	-3.4408	-5.6183	4.4456
160	C	-4.4265	-8.2075	4.1371
161	H	-2.9882	-8.4156	2.5591
162	C	-4.4835	-6.0698	5.2554
163	H	-0.8498	-6.1815	5.2228
164	C	-4.9803	-7.3663	5.1051
165	H	-4.8077	-9.2181	4.0018
166	H	-4.9051	-5.4039	6.0065
167	H	-5.7920	-7.7196	5.7389
168	C	-0.5144	-4.8493	3.5457
169	C	-0.3127	-5.3069	4.8597
170	C	0.1953	-3.7281	3.1039
171	C	0.5699	-4.6469	5.7128
172	H	-3.0604	-4.6088	4.5831
173	C	1.0829	-3.0690	3.9599
174	H	0.0551	-3.3760	2.0829
175	C	1.2716	-3.5225	5.2650
176	H	0.7117	-5.0121	6.7286
177	H	1.6252	-2.1977	3.5957
178	H	1.9612	-3.0074	5.9320
179	C	-0.6080	-7.7815	-1.9546
180	C	0.4839	-8.6024	-2.2875
181	C	-1.8233	-7.9793	-2.6137
182	C	0.3656	-9.5750	-3.2786
183	H	1.4377	-8.4799	-1.7772
184	C	-1.9426	-8.9534	-3.6086
185	H	-2.6922	-7.3993	-2.3214
186	C	-0.8501	-9.7505	-3.9476
187	H	1.2232	-10.1982	-3.5269
188	H	-2.9016	-9.0886	-4.1052

189	H	-0.9437	-10.5106	-4.7216
190	C	1.2272	-5.9349	-0.7322
191	C	1.9283	-5.4743	0.3912
192	C	1.8389	-5.8143	-1.9887
193	C	3.2175	-4.9552	0.2715
194	H	1.4701	-5.4944	1.3759
195	C	3.1222	-5.2791	-2.1140
196	H	1.3157	-6.1452	-2.8833
197	C	3.8225	-4.8558	-0.9832
198	H	3.7403	-4.6118	1.1627
199	H	3.5754	-5.1981	-3.1007
200	H	4.8239	-4.4398	-1.0813
201	C	-2.7338	6.3813	-3.5309
202	C	-3.4377	7.5899	-3.4412
203	C	-3.1446	5.4291	-4.4765
204	C	-4.5102	7.8498	-4.2959
205	H	-3.1621	8.3305	-2.6957
206	C	-4.2193	5.6883	-5.3274
207	H	-2.6149	4.4828	-4.5650
208	C	-4.9029	6.9042	-5.2445
209	H	-5.0385	8.7980	-4.2127
210	H	-4.5160	4.9396	-6.0601
211	H	-5.7346	7.1125	-5.9157
212	C	-0.1662	5.1821	-3.6542
213	C	0.0256	5.7371	-4.9321
214	C	0.5408	4.0258	-3.3101
215	C	0.9027	5.1475	-5.8398
216	H	-0.5255	6.6285	-5.2287
217	C	1.4163	3.4289	-4.2243
218	H	0.4120	3.5934	-2.3176
219	C	1.6012	3.9865	-5.4886
220	H	1.0387	5.5912	-6.8247
221	H	1.9514	2.5251	-3.9367
222	H	2.2831	3.5229	-6.1998
223	C	-3.7301	2.7793	-1.6633
224	C	-2.6493	2.4135	-2.4683
225	C	-4.9284	2.0527	-1.7666
226	C	-2.7570	1.3470	-3.3652
227	H	-1.7086	2.9452	-2.3643
228	C	-5.0414	0.9933	-2.6653
229	H	-5.7877	2.3276	-1.1560
230	C	-3.9529	0.6376	-3.4694
231	H	-1.8982	1.0651	-3.9718
232	H	-5.9807	0.4475	-2.7418
233	H	-4.0354	-0.1908	-4.1714
234	C	-5.1713	5.0654	-0.7259
235	C	-5.7994	5.7496	0.3246

236	C	-5.7495	5.1272	-2.0000
237	C	-6.9956	6.4358	0.1181
238	H	-5.3603	5.7623	1.3189
239	C	-6.9410	5.8226	-2.2113
240	H	-5.2759	4.6263	-2.8404
241	C	-7.5768	6.4709	-1.1515
242	H	-7.4675	6.9519	0.9524
243	H	-7.3690	5.8536	-3.2117
244	H	-8.5122	7.0041	-1.3133
245	C	0.6520	7.9164	1.3297
246	C	1.8374	8.6655	1.4136
247	C	-0.4099	8.2397	2.1759
248	C	1.9544	9.7102	2.3288
249	H	2.6840	8.4219	0.7726
250	C	-0.2952	9.2847	3.0970
251	H	-1.3407	7.6885	2.0891
252	C	0.8860	10.0224	3.1766
253	H	2.8811	10.2788	2.3839
254	H	-1.1374	9.5218	3.7454
255	H	0.9769	10.8380	3.8923
256	C	2.0976	5.6612	0.3494
257	C	2.6469	5.5471	1.6330
258	C	2.7636	5.0410	-0.7171
259	C	3.8420	4.8579	1.8409
260	H	2.1459	6.0011	2.4844
261	C	3.9658	4.3633	-0.5134
262	H	2.3513	5.0693	-1.7227
263	C	4.5131	4.2699	0.7681
264	H	4.2445	4.7817	2.8493
265	H	4.4685	3.8995	-1.3608
266	H	5.4476	3.7352	0.9310
267	C	-2.9172	5.5281	3.3205
268	C	-3.6019	6.7007	2.9857
269	C	-3.1243	4.9646	4.5921
270	C	-4.4692	7.3046	3.9030
271	H	-3.4622	7.1405	1.9978
272	C	-3.9929	5.5615	5.5031
273	H	-2.5909	4.0600	4.8814
274	C	-4.6685	6.7386	5.1614
275	H	-4.9872	8.2204	3.6222
276	H	-4.1402	5.1111	6.4833
277	H	-5.3437	7.2081	5.8751
278	C	-0.3630	4.2972	3.1932
279	C	0.0481	5.2296	4.1582
280	C	0.3458	3.0935	3.0748
281	C	1.1274	4.9565	4.9989
282	H	-0.4835	6.1723	4.2688

283	C	1.4235	2.8198	3.9185
284	H	0.0744	2.3726	2.3089
285	C	1.8164	3.7461	4.8862
286	H	1.4249	5.6909	5.7456
287	H	1.9619	1.8803	3.8069
288	H	2.6540	3.5280	5.5470

Compound 9':

1	C	15.7948	-0.0012	-0.0305
2	C	14.3675	-0.0012	-0.0214
3	C	13.6513	-1.2133	-0.0168
4	C	13.6515	1.2110	-0.0172
5	C	12.2631	-1.2133	-0.0083
6	H	14.1999	-2.1524	-0.0200
7	C	12.2633	1.2113	-0.0088
8	H	14.2003	2.1500	-0.0208
9	C	11.5458	-0.0010	-0.0042
10	H	11.7147	-2.1525	-0.0048
11	H	11.7150	2.1505	-0.0056
12	C	10.1219	-0.0008	0.0039
13	C	8.9007	-0.0007	0.0103
14	C	7.4770	-0.0006	0.0170
15	C	6.7587	-1.2126	0.0204
16	C	6.7589	1.2115	0.0198
17	C	5.3710	-1.2121	0.0259
18	H	7.3062	-2.1524	0.0183
19	C	5.3712	1.2112	0.0254
20	H	7.3065	2.1512	0.0173
21	C	4.6514	-0.0004	0.0283
22	H	4.8226	-2.1512	0.0282
23	H	4.8229	2.1504	0.0272
24	C	3.2277	-0.0003	0.0327
25	C	2.0067	-0.0002	0.0353
26	C	0.5795	-0.0001	0.0367
27	C	-0.1207	1.2166	0.0366
28	C	-0.1208	-1.2167	0.0366
29	C	-1.5262	1.2290	0.0364
30	H	0.4255	2.1561	0.0357
31	C	-1.5263	-1.2289	0.0364
32	H	0.4253	-2.1563	0.0357
33	C	-2.2104	0.0000	0.0370
34	H	-3.2977	0.0001	0.0374
35	C	-2.2429	2.4674	0.0338
36	C	-2.8458	3.5464	0.0279
37	C	-2.2432	-2.4673	0.0338

38	C	-2.8462	-3.5462	0.0279
39	Ru	-3.8569	5.3338	0.0125
40	P	-5.2737	4.4434	-1.5800
41	P	-2.6481	6.0683	-1.8148
42	C	-4.8677	7.1203	-0.0061
43	P	-5.0601	4.5971	1.8420
44	P	-2.4345	6.2210	1.6027
45	C	-4.4489	4.5256	-3.2507
46	H	-5.7011	3.0877	-1.5399
47	H	-6.5305	5.0598	-1.8386
48	C	-3.6670	5.8355	-3.3593
49	H	-2.2281	7.4198	-1.9512
50	H	-1.4279	5.4239	-2.1630
51	C	-5.4703	8.1998	-0.0186
52	C	-4.0331	4.8202	3.3825
53	H	-5.4842	3.2465	1.9755
54	H	-6.2769	5.2434	2.1998
55	C	-3.2504	6.1299	3.2773
56	H	-1.1760	5.6044	1.8509
57	H	-2.0094	7.5773	1.5660
58	H	-3.7685	3.6662	-3.2966
59	H	-5.1817	4.4263	-4.0587
60	H	-4.3525	6.6910	-3.4036
61	H	-3.0367	5.8549	-4.2548
62	C	-6.1768	9.4437	-0.0319
63	H	-4.6585	4.7964	4.2815
64	H	-3.3482	3.9639	3.4179
65	H	-2.5127	6.2236	4.0815
66	H	-3.9291	6.9901	3.3326
67	C	-7.5826	9.4816	0.0741
68	C	-5.4896	10.6694	-0.1513
69	C	-8.2694	10.6941	0.0611
70	H	-8.1253	8.5430	0.1668
71	C	-6.1802	11.8797	-0.1639
72	H	-4.4045	10.6549	-0.2338
73	C	-7.5742	11.9015	-0.0579
74	H	-9.3554	10.6990	0.1444
75	H	-5.6282	12.8140	-0.2571
76	H	-8.1122	12.8477	-0.0679
77	Ru	-3.8574	-5.3335	0.0124
78	P	-5.0612	-4.5972	1.8416
79	P	-2.4357	-6.2213	1.6028
80	C	-4.8685	-7.1199	-0.0064
81	P	-5.2737	-4.4426	-1.5804
82	P	-2.6482	-6.0678	-1.8148
83	C	-4.0349	-4.8212	3.3826
84	H	-5.4850	-3.2465	1.9755

85	H	-6.2783	-5.2432	2.1986
86	C	-3.2523	-6.1310	3.2770
87	H	-2.0105	-7.5776	1.5656
88	H	-1.1773	-5.6048	1.8518
89	C	-5.4712	-8.1994	-0.0189
90	C	-4.4481	-4.5241	-3.2507
91	H	-5.7012	-3.0869	-1.5399
92	H	-6.5303	-5.0589	-1.8398
93	C	-3.6664	-5.8341	-3.3596
94	H	-1.4277	-5.4235	-2.1622
95	H	-2.2285	-7.4193	-1.9516
96	H	-3.3499	-3.9650	3.4187
97	H	-4.6607	-4.7977	4.2812
98	H	-3.9312	-6.9911	3.3316
99	H	-2.5150	-6.2251	4.0815
100	C	-6.1779	-9.4431	-0.0320
101	H	-5.1805	-4.4242	-4.0590
102	H	-3.7676	-3.6647	-3.2958
103	H	-3.0357	-5.8531	-4.2549
104	H	-4.3520	-6.6894	-3.4046
105	C	-7.5835	-9.4810	0.0771
106	C	-5.4911	-10.6687	-0.1544
107	C	-8.2705	-10.6933	0.0642
108	H	-8.1258	-8.5423	0.1721
109	C	-6.1820	-11.8790	-0.1670
110	H	-4.4063	-10.6544	-0.2394
111	C	-7.5758	-11.9007	-0.0578
112	H	-9.3563	-10.6982	0.1499
113	H	-5.6304	-12.8133	-0.2624
114	H	-8.1139	-12.8468	-0.0677
115	C	17.0203	-0.0006	-0.0384
116	Si	18.8625	0.0002	-0.0506
117	C	19.4499	1.7806	-0.0549
118	H	19.0823	2.3145	-0.9386
119	H	19.0940	2.3149	0.8334
120	H	20.5460	1.8277	-0.0622
121	C	19.4647	-0.8893	1.4862
122	H	19.1092	-0.3906	2.3950
123	H	19.1049	-1.9244	1.5087
124	H	20.5612	-0.9109	1.5174
125	C	19.4442	-0.8900	-1.5950
126	H	19.0841	-1.9250	-1.6123
127	H	19.0768	-0.3916	-2.4992
128	H	20.5402	-0.9116	-1.6406

Compound 4-H':

1	N	0.1171	-2.0487	0.0342
2	N	2.0578	0.1161	-0.0591
3	N	-0.1060	2.0584	0.0308
4	N	-2.0469	-0.1062	0.1242
5	C	1.2609	-2.8019	0.0155
6	C	2.5800	-2.3051	-0.0085
7	C	2.9298	-0.9395	-0.0246
8	C	4.2851	-0.4460	0.0413
9	H	5.1719	-1.0644	0.1060
10	C	4.2111	0.9162	0.0427
11	H	5.0256	1.6269	0.1086
12	C	2.8104	1.2599	-0.0228
13	C	2.3148	2.5795	-0.0058
14	C	0.9498	2.9307	0.0146
15	C	0.4563	4.2875	0.0138
16	H	1.0737	5.1768	-0.0110
17	C	-0.9056	4.2138	0.0449
18	H	-1.6154	5.0313	0.0689
19	C	-1.2498	2.8116	0.0454
20	C	-2.5689	2.3149	0.0653
21	C	-2.9187	0.9494	0.0845
22	C	-4.2739	0.4559	0.0166
23	H	-5.1604	1.0742	-0.0528
24	C	-4.2001	-0.9063	0.0200
25	H	-5.0146	-1.6169	-0.0461
26	C	-2.7994	-1.2500	0.0895
27	C	-2.3038	-2.5697	0.0752
28	C	-0.9387	-2.9209	0.0531
29	C	-0.4452	-4.2777	0.0529
30	H	-1.0624	-5.1671	0.0801
31	C	0.9166	-4.2040	0.0169
32	H	1.6261	-5.0217	-0.0096
33	C	3.6909	-3.2969	-0.0049
34	C	3.9187	-4.1277	1.1025
35	H	3.2751	-4.0332	1.9760
36	C	4.9603	-5.0511	1.1088
37	H	5.1265	-5.6785	1.9823
38	C	5.8178	-5.1903	-0.0016
39	C	5.5834	-4.3553	-1.1131
40	H	6.2285	-4.4487	-1.9844
41	C	-3.6795	3.3068	0.0495
42	C	-4.5391	3.4493	1.1490
43	H	-4.3769	2.8303	2.0303
44	C	-5.5775	4.3763	1.1375
45	H	-6.2249	4.4791	2.0060
46	C	-5.8092	5.1977	0.0153

47	C	-4.9460	5.0468	-1.0892
48	H	-5.1090	5.6632	-1.9711
49	C	-3.3008	-3.6759	0.0684
50	C	-3.4343	-4.5248	-1.0408
51	H	-2.8019	-4.3601	-1.9120
52	C	-4.3707	-5.5546	-1.0521
53	H	-4.4666	-6.1944	-1.9270
54	C	-5.2120	-5.7868	0.0552
55	C	-5.0717	-4.9338	1.1688
56	H	-5.7050	-5.0973	2.0385
57	C	3.3112	3.6862	0.0042
58	C	4.1458	3.9184	-1.0993
59	H	4.0491	3.2824	-1.9781
60	C	5.0755	4.9544	-1.0951
61	H	5.7041	5.1256	-1.9666
62	C	5.2192	5.8003	0.0237
63	C	4.3828	5.5589	1.1326
64	H	4.4805	6.1926	2.0118
65	Zn	0.0054	0.0049	0.0327
66	C	6.1765	6.8613	0.0336
67	C	6.8836	-6.1426	-0.0012
68	C	-6.1711	-6.8465	0.0476
69	C	-6.8781	6.1459	-0.0038
70	C	-7.8013	6.9686	-0.0197
71	C	7.0032	7.7811	0.0371
72	C	7.8054	-6.9670	-0.0101
73	C	-7.0006	-7.7636	0.0312
74	C	-4.1399	-3.8996	1.1702
75	H	-4.0458	-3.2579	2.0451
76	C	4.5458	-3.4275	-1.1097
77	H	4.3804	-2.7983	-1.9831
78	C	3.4477	4.5280	1.1182
79	H	2.8183	4.3571	1.9904
80	C	-3.9031	4.1255	-1.0677
81	H	-3.2553	4.0222	-1.9371
82	Ru	8.3841	9.2995	0.0510
83	P	7.7325	9.8025	2.2097
84	P	6.7866	10.8608	-0.5423
85	C	9.7669	10.8172	0.0629
86	P	9.9888	7.7461	0.6460
87	P	9.0397	8.7995	-2.1070
88	C	6.1790	10.8341	2.1613
89	H	7.3766	8.7949	3.1479
90	H	8.5815	10.5848	3.0421
91	C	6.2554	11.8000	0.9782
92	H	7.0656	11.9196	-1.4492
93	H	5.5398	10.4347	-1.0806

94	C	10.5950	11.7354	0.0627
95	C	10.5436	6.8226	-0.8762
96	H	9.7132	6.6785	1.5434
97	H	11.2268	8.1817	1.1968
98	C	10.6095	7.7939	-2.0557
99	H	8.2020	8.0008	-2.9356
100	H	9.3785	9.8087	-3.0495
101	H	5.3482	10.1297	2.0297
102	H	6.0291	11.3664	3.1068
103	H	7.0276	12.5601	1.1505
104	H	5.3010	12.3116	0.8138
105	C	11.5556	12.7954	0.0705
106	H	11.5058	6.3269	-0.7085
107	H	9.7862	6.0493	-1.0552
108	H	10.7728	7.2675	-3.0022
109	H	11.4269	8.5126	-1.9177
110	C	11.6976	13.6561	-1.0376
111	C	12.3895	13.0119	1.1870
112	C	12.6336	14.6884	-1.0277
113	H	11.0603	13.5005	-1.9060
114	C	13.3244	14.0454	1.1929
115	H	12.2906	12.3548	2.0487
116	C	13.4535	14.8909	0.0867
117	H	12.7255	15.3409	-1.8949
118	H	13.9579	14.1937	2.0664
119	Ru	9.3288	-8.3429	-0.0149
120	P	10.2667	-7.2296	1.7799
121	P	10.6689	-6.9477	-1.2775
122	C	10.8484	-9.7232	-0.0227
123	P	7.9885	-9.7380	1.2481
124	P	8.3923	-9.4578	-1.8096
125	C	11.1924	-5.7341	1.1599
126	H	9.4769	-6.6656	2.8189
127	H	11.2496	-7.8773	2.5800
128	C	11.8850	-6.0838	-0.1580
129	H	11.5244	-7.4403	-2.3008
130	H	10.0893	-5.8571	-1.9852
131	C	11.7635	-10.5546	-0.0356
132	C	6.7736	-10.6030	0.1281
133	H	7.1321	-9.2448	2.2705
134	H	8.5680	-10.8280	1.9566
135	C	7.4679	-10.9537	-1.1886
136	H	7.4096	-8.8116	-2.6110
137	H	9.1838	-10.0223	-2.8472
138	H	10.4383	-4.9527	1.0038
139	H	11.9078	-5.3747	1.9075
140	H	12.7008	-6.7972	0.0128

141	H	12.3036	-5.1944	-0.6411
142	C	12.8215	-11.5173	-0.0401
143	H	6.3547	-11.4921	0.6115
144	H	5.9579	-9.8899	-0.0445
145	H	6.7536	-11.3148	-1.9364
146	H	8.2228	-11.7339	-1.0305
147	C	13.2275	-12.1565	1.1496
148	C	13.4906	-11.8565	-1.2344
149	C	14.2585	-13.0941	1.1430
150	H	12.7196	-11.9040	2.0783
151	C	14.5211	-12.7947	-1.2367
152	H	13.1876	-11.3708	-2.1599
153	C	14.9126	-13.4202	-0.0490
154	H	14.5552	-13.5751	2.0741
155	H	15.0235	-13.0409	-2.1711
156	Ru	-8.3762	-9.2871	0.0180
157	P	-7.0490	-10.4121	1.5393
158	P	-7.1535	-10.4557	-1.5556
159	C	-9.7506	-10.8121	0.0041
160	P	-9.6004	-8.1196	1.5911
161	P	-9.7054	-8.1648	-1.5034
162	C	-5.6432	-11.2375	0.6338
163	H	-6.3595	-9.7403	2.5855
164	H	-7.5921	-11.4909	2.2924
165	C	-6.1564	-11.7800	-0.7009
166	H	-7.7732	-11.1948	-2.6003
167	H	-6.1600	-9.7851	-2.3234
168	C	-10.5783	-11.7304	-0.0139
169	C	-10.6046	-6.8008	0.7359
170	H	-8.9816	-7.3756	2.6331
171	H	-10.5897	-8.7921	2.3625
172	C	-11.1154	-7.3464	-0.5983
173	H	-9.1662	-7.0837	-2.2558
174	H	-10.3914	-8.8390	-2.5505
175	H	-4.8893	-10.4578	0.4688
176	H	-5.1910	-12.0279	1.2424
177	H	-6.8425	-12.6203	-0.5372
178	H	-5.3350	-12.1279	-1.3364
179	C	-11.5353	-12.7937	-0.0266
180	H	-11.4277	-6.4569	1.3716
181	H	-9.9232	-5.9568	0.5713
182	H	-11.5716	-6.5585	-1.2072
183	H	-11.8653	-8.1299	-0.4326
184	C	-12.0532	-13.3190	1.1754
185	C	-11.9895	-13.3489	-1.2408
186	C	-12.9852	-14.3550	1.1613
187	H	-11.7109	-12.8998	2.1195

188	C	-12.9216	-14.3848	-1.2505
189	H	-11.5982	-12.9530	-2.1759
190	C	-13.4262	-14.8954	-0.0506
191	H	-13.3713	-14.7450	2.1020
192	H	-13.2581	-14.7980	-2.2004
193	Ru	-9.3369	8.3296	-0.0623
194	P	-9.0567	8.4806	-2.3510
195	P	-7.8544	10.1016	-0.0024
196	C	-10.8710	9.6936	-0.1080
197	P	-10.8319	6.5683	-0.1245
198	P	-9.6239	8.1826	2.2250
199	C	-7.6283	9.6210	-2.7226
200	H	-8.7346	7.3500	-3.1508
201	H	-10.0925	9.0305	-3.1573
202	C	-7.6397	10.7807	-1.7258
203	H	-8.1214	11.2847	0.7395
204	H	-6.5073	9.8878	0.4041
205	C	-11.7917	10.5186	-0.1303
206	C	-11.0857	5.9113	1.6029
207	H	-10.5668	5.3734	-0.8480
208	H	-12.1696	6.7929	-0.5555
209	C	-11.0822	7.0794	2.5899
210	H	-8.6042	7.6060	3.0338
211	H	-9.9194	9.3194	3.0262
212	H	-6.7187	9.0197	-2.6022
213	H	-7.6674	9.9788	-3.7571
214	H	-8.5021	11.4347	-1.9051
215	H	-6.7296	11.3854	-1.8015
216	C	-12.8619	11.4674	-0.1653
217	H	-12.0111	5.3294	1.6712
218	H	-10.2429	5.2373	1.8000
219	H	-11.0641	6.7298	3.6278
220	H	-11.9751	7.7021	2.4530
221	C	-12.8723	12.5841	0.6958
222	C	-13.9390	11.3141	-1.0626
223	C	-13.9159	13.5070	0.6595
224	H	-12.0474	12.7146	1.3936
225	C	-14.9807	12.2392	-1.0957
226	H	-13.9431	10.4569	-1.7330
227	C	-14.9772	13.3418	-0.2357
228	H	-13.9028	14.3620	1.3340
229	H	-15.8022	12.1005	-1.7972
230	H	14.1842	15.6977	0.0930
231	H	-15.7916	14.0634	-0.2629
232	H	-14.1542	-15.7045	-0.0598
233	H	15.7177	-14.1528	-0.0524

Compound 5_2':

1	N	-1.9903	-0.0552	-0.1732
2	N	0.0680	1.9983	-0.0819
3	N	2.1230	-0.0571	-0.2077
4	N	0.0641	-2.1108	-0.2988
5	C	-2.8035	1.0464	-0.1426
6	C	-2.3779	2.3901	-0.1153
7	C	-1.0330	2.8126	-0.1047
8	C	-0.6133	4.1929	-0.1622
9	H	-1.2784	5.0458	-0.2175
10	C	0.7508	4.1921	-0.1685
11	H	1.4163	5.0443	-0.2301
12	C	1.1695	2.8113	-0.1159
13	C	2.5139	2.3876	-0.1427
14	C	2.9377	1.0436	-0.1830
15	C	4.3189	0.6234	-0.1990
16	H	5.1744	1.2866	-0.1712
17	C	4.3178	-0.7398	-0.2510
18	H	5.1720	-1.4040	-0.2926
19	C	2.9361	-1.1586	-0.2450
20	C	2.5104	-2.5022	-0.2774
21	C	1.1654	-2.9248	-0.2824
22	C	0.7464	-4.3052	-0.2216
23	H	1.4120	-5.1579	-0.1706
24	C	-0.6177	-4.3047	-0.2049
25	H	-1.2825	-5.1569	-0.1375
26	C	-1.0371	-2.9241	-0.2565
27	C	-2.3812	-2.5003	-0.2228
28	C	-2.8049	-1.1561	-0.1896
29	C	-4.1861	-0.7360	-0.1750
30	H	-5.0414	-1.3998	-0.1972
31	C	-4.1851	0.6276	-0.1338
32	H	-5.0393	1.2922	-0.0972
33	Zn	0.0663	-0.0562	-0.1908
34	C	3.5600	-3.5583	-0.2952
35	C	4.4159	-3.7498	0.8000
36	C	3.7212	-4.3970	-1.4084
37	H	4.2989	-3.1183	1.6795
38	C	5.3932	-4.7408	0.7863
39	C	4.7019	-5.3846	-1.4314
40	H	3.0729	-4.2589	-2.2725
41	H	6.0409	-4.8788	1.6498
42	C	5.5622	-5.5821	-0.3322
43	H	4.8167	-6.0187	-2.3081
44	C	6.5676	-6.5981	-0.3508

45	C	7.4344	-7.4797	-0.3735
46	Ru	8.8794	-8.9382	-0.3956
47	P	10.4172	-7.3127	0.1865
48	P	9.4718	-8.3886	-2.5607
49	C	10.3230	-10.3926	-0.4109
50	P	8.2690	-9.4729	1.7683
51	P	7.3203	-10.5435	-0.9788
52	C	10.8791	-6.3375	-1.3339
53	H	10.1053	-6.2767	1.1086
54	H	11.6906	-7.6875	0.6999
55	C	10.9775	-7.2881	-2.5280
56	H	9.8570	-9.3704	-3.5146
57	H	8.5726	-7.6396	-3.3703
58	C	11.1926	-11.2729	-0.4228
60	H	7.9191	-8.4784	2.7219
61	H	9.1374	-10.2566	2.5794
62	C	6.8028	-11.4829	0.5468
63	H	6.0675	-10.1432	-1.5222
64	H	7.6209	-11.6027	-1.8783
65	H	10.0716	-5.6104	-1.4853
66	H	11.8130	-5.7861	-1.1810
67	H	11.8414	-7.9553	-2.4184
68	H	11.0864	-6.7405	-3.4702
69	C	12.1976	-12.2849	-0.4239
70	H	6.5828	-11.0488	2.6758
71	H	5.8887	-9.8170	1.6007
72	H	5.8513	-12.0012	0.3867
73	H	7.5793	-12.2389	0.7176
74	C	12.6921	-12.8237	0.7841
75	C	12.7336	-12.7833	-1.6313
76	C	13.6701	-13.8084	0.7863
77	H	12.2920	-12.4503	1.7243
78	C	13.7130	-13.7668	-1.6331
79	H	12.3633	-12.3815	-2.5722
80	C	14.2009	-14.2995	-0.4232
81	H	14.0396	-14.2115	1.7271
82	H	14.1144	-14.1385	-2.5736
83	C	15.2055	-15.3079	-0.4217
84	C	16.0685	-16.1730	-0.4179
85	C	17.0745	-17.1800	-0.4100
86	C	17.5073	-17.7551	0.8017
87	C	17.6606	-17.6237	-1.6124
88	C	18.4886	-18.7363	0.8104
89	H	17.0606	-17.4190	1.7348
90	C	18.6427	-18.6043	-1.6030
91	H	17.3330	-17.1857	-2.5526
92	C	19.0755	-19.1793	-0.3916

93	H	18.8168	-19.1745	1.7502
94	H	19.0899	-18.9405	-2.5358
95	C	20.0839	-20.1852	-0.3810
96	C	20.9490	-21.0467	-0.3688
97	C	21.9611	-22.0533	-0.3509
98	C	22.6095	-22.4185	-1.5411
99	C	22.3077	-22.6759	0.8586
100	C	23.6092	-23.4065	-1.5336
101	H	22.3394	-21.9338	-2.4756
102	C	23.3027	-23.6682	0.8899
103	H	21.8042	-22.3901	1.7783
104	C	23.9415	-24.0202	-0.3125
105	C	24.2754	-23.7761	-2.7452
106	C	23.6555	-24.3043	2.1224
107	H	24.7127	-24.7867	-0.2978
108	C	24.8436	-24.0788	-3.8002
109	C	23.9450	-24.8404	3.1978
110	Ru	25.8020	-24.5793	-5.5467
111	Ru	24.4269	-25.7342	4.9833
112	P	27.8049	-24.3924	-4.4111
113	P	26.1509	-22.3511	-6.0499
114	C	26.7638	-25.0759	-7.2907
115	P	25.4413	-26.8022	-5.0325
116	P	23.7907	-24.7576	-6.6698
117	P	23.9727	-27.7777	4.0062
118	P	22.2031	-25.8047	5.6067
119	C	24.9069	-26.6260	6.7687
120	P	26.6460	-25.6522	4.3478
121	P	24.8727	-23.6825	5.9486
122	C	28.2618	-22.5901	-4.2684
123	H	27.9556	-24.8319	-3.0672
124	H	28.9913	-24.9573	-4.9587
125	C	27.8886	-21.8749	-5.5676
126	H	26.0780	-21.8534	-7.3798
127	H	25.3766	-21.3502	-5.3989
128	C	27.3391	-25.3697	-8.3449
129	C	23.6892	-27.2591	-5.4788
130	H	25.5342	-27.2958	-3.7021
131	H	26.1900	-27.8169	-5.6931
132	C	23.3045	-26.5548	-6.7806
133	H	22.6186	-24.1655	-6.1211
134	H	23.6361	-24.3372	-8.0193
135	C	22.1278	-28.0478	3.9793
136	H	24.3226	-28.0666	2.6586
137	H	24.4399	-28.9773	4.6139
138	C	21.5243	-27.5104	5.2777
139	H	21.7840	-25.5853	6.9476

140	H	21.2564	-24.9746	4.9433
141	C	25.1916	-27.1579	7.8480
142	C	27.3046	-23.9323	4.6408
143	H	27.0584	-25.8904	3.0079
144	H	27.6101	-26.4573	5.0176
145	C	26.7140	-23.3854	5.9411
146	H	24.3768	-22.4939	5.3432
147	H	24.5433	-23.3928	7.3011
148	H	27.6764	-22.1945	-3.4291
149	H	29.3246	-22.4687	-4.0332
150	H	28.5352	-22.2063	-6.3896
151	H	27.9873	-20.7883	-5.4714
152	C	28.0107	-25.7163	-9.5594
153	H	23.5721	-28.3452	-5.5592
154	H	23.0625	-26.9066	-4.6502
155	H	22.2359	-26.6620	-6.9957
156	H	23.8678	-26.9711	-7.6250
157	H	21.7512	-27.4838	3.1170
158	H	21.8850	-29.1054	3.8302
159	H	21.8298	-28.1297	6.1302
160	H	20.4298	-27.4985	5.2379
161	C	25.5266	-27.7793	9.0920
162	H	28.3997	-23.9264	4.6625
163	H	26.9745	-23.3308	3.7848
164	H	26.9426	-22.3221	6.0712
165	H	27.1141	-23.9303	6.8052
166	C	29.0002	-26.7211	-9.5813
167	C	27.7044	-25.0641	-10.7717
168	C	26.4033	-28.8831	9.1402
169	C	24.9907	-27.3076	10.3083
170	C	29.6536	-27.0576	-10.7653
171	H	29.2464	-27.2322	-8.6527
172	C	28.3602	-25.4036	-11.9536
173	H	26.9429	-24.2867	-10.7696
174	C	26.7286	-29.4872	10.3531
175	H	26.8240	-29.2573	8.2089
176	C	25.3186	-27.9146	11.5191
177	H	24.3129	-26.4565	10.2860
178	C	29.3390	-26.4021	-11.9596
179	H	30.4144	-27.8370	-10.7580
180	H	28.1069	-24.8862	-12.8780
181	C	26.1893	-29.0082	11.5510
182	H	27.4079	-30.3385	10.3658
183	H	24.8924	-27.5328	12.4459
184	H	29.8503	-26.6661	-12.8836
185	H	26.4444	-29.4812	12.4975
186	C	3.5647	3.4427	-0.1380

187	C	3.7419	4.2784	0.9749
188	C	4.4062	3.6356	-1.2440
189	H	3.1048	4.1394	1.8472
190	C	4.7247	5.2640	0.9873
191	C	5.3856	4.6247	-1.2409
192	H	4.2765	3.0065	-2.1235
193	H	4.8519	5.8954	1.8644
194	C	5.5712	5.4624	-0.1224
195	H	6.0224	4.7639	-2.1122
196	C	6.5801	6.4751	-0.1132
197	C	7.4565	7.3475	-0.1100
198	Ru	8.9072	8.8003	-0.0871
199	P	7.2631	10.3223	0.4844
200	P	8.3940	9.4177	-2.2542
201	C	10.3539	10.2514	-0.0564
202	P	9.4053	8.1651	2.0783
203	P	10.5311	7.2567	-0.6603
204	C	6.3136	10.7991	-1.0476
205	H	6.2121	9.9934	1.3832
206	H	7.6219	11.5908	1.0209
207	C	7.2854	10.9174	-2.2226
208	H	9.3908	9.8196	-3.1853
209	H	7.6643	8.5252	-3.0885
210	C	11.2294	11.1257	-0.0392
211	C	10.4569	6.6261	2.0391
212	H	8.3952	7.7985	3.0092
213	H	10.1696	9.0272	2.9144
214	C	11.4448	6.7243	0.8758
215	H	10.1471	6.0091	-1.2269
216	H	11.6051	7.5741	-1.5361
217	H	5.5935	9.9902	-1.2227
218	H	5.7548	11.7283	-0.8928
219	H	7.9461	11.7831	-2.0897
220	H	6.7546	11.0357	-3.1734
221	C	12.2352	12.1363	-0.0061
222	H	10.9727	6.4752	2.9935
223	H	9.7644	5.7889	1.8872
224	H	11.9707	5.7774	0.7133
225	H	12.1936	7.5022	1.0704
226	C	12.7719	12.5919	1.2180
227	C	12.7292	12.7172	-1.1944
228	C	13.7504	13.5754	1.2537
229	H	12.4018	12.1570	2.1440
230	C	13.7065	13.7023	-1.1626
231	H	12.3292	12.3772	-2.1474
232	C	14.2370	14.1512	0.0632
233	H	14.1518	13.9145	2.2066

234	H	14.0749	14.1387	-2.0888
235	C	15.2390	15.1617	0.0990
236	C	16.0985	16.0296	0.1322
237	C	17.0991	17.0412	0.1736
238	C	17.6763	17.4326	1.3983
239	C	17.5342	17.6740	-1.0080
240	C	18.6516	18.4190	1.4394
241	H	17.3469	16.9497	2.3155
242	C	18.5089	18.6611	-0.9662
243	H	17.0943	17.3787	-1.9579
244	C	19.0864	19.0524	0.2581
245	H	19.0919	18.7148	2.3890
246	H	18.8384	19.1446	-1.8831
247	C	20.0866	20.0655	0.3015
248	C	20.9438	20.9341	0.3406
249	C	21.9461	21.9495	0.3883
250	C	22.3100	22.6318	-0.7832
251	C	22.5664	22.2649	1.6074
252	C	23.2950	23.6338	-0.7475
253	H	21.8268	22.3862	-1.7251
254	C	23.5549	23.2623	1.6671
255	H	22.2822	21.7346	2.5125
256	C	23.9060	23.9350	0.4830
257	C	23.6651	24.3323	-1.9406
258	C	24.1891	23.5831	2.9093
259	H	24.6700	24.7079	0.5197
260	C	23.9683	24.9266	-2.9810
261	C	24.7252	23.8437	3.9920
262	Ru	24.4727	25.9227	-4.7050
263	Ru	25.6204	24.2787	5.7889
264	P	24.6462	27.8536	-3.4497
265	P	22.2842	26.5992	-5.0099
266	C	24.9745	26.9204	-6.4272
267	P	26.6555	25.2350	-4.3901
268	P	24.2907	23.9835	-5.9477
269	P	27.6627	24.1880	4.7135
270	P	26.0032	22.0369	6.1985
271	C	26.5147	24.7117	7.5850
272	P	25.2266	26.5153	5.3676
273	P	23.5702	24.3610	6.8513
274	C	22.9392	28.5364	-3.1376
275	H	25.1978	27.8563	-2.1390
276	H	25.3283	28.9876	-3.9743
277	C	22.0879	28.3488	-4.3941
278	H	21.6883	26.6825	-6.2982
279	H	21.2347	25.9236	-4.3264
280	C	25.2715	27.5186	-7.4678

281	C	26.8339	23.4716	-4.9701
282	H	27.2504	25.1721	-3.1002
283	H	27.7136	25.8850	-5.0860
284	C	25.9911	23.2714	-6.2304
285	H	23.5848	22.8670	-5.4180
286	H	23.7558	23.9743	-7.2651
287	C	28.1656	22.4047	4.5028
288	H	27.8477	24.6934	3.3973
289	H	28.8171	24.7518	5.3268
290	C	27.7661	21.6209	5.7537
291	H	25.8979	21.4754	7.5005
292	H	25.2734	21.0518	5.4758
293	C	27.0492	24.9674	8.6702
294	C	23.4505	26.9130	5.7743
295	H	25.3523	27.0733	4.0657
296	H	25.9294	27.5133	6.1002
297	C	23.0391	26.1402	7.0282
298	H	22.4309	23.7700	6.2363
299	H	23.3811	23.8749	8.1740
300	H	22.5278	27.9546	-2.3034
301	H	22.9829	29.5880	-2.8344
302	H	22.4453	28.9988	-5.2025
303	H	21.0351	28.5847	-4.2057
304	C	25.6228	28.2161	-8.6662
305	H	27.8850	23.2174	-5.1445
306	H	26.4599	22.8432	-4.1524
307	H	25.9345	22.2147	-6.5130
308	H	26.4186	23.8294	-7.0727
309	H	27.6180	22.0366	3.6263
310	H	29.2383	22.3176	4.2988
311	H	28.3775	21.9264	6.6119
312	H	27.8925	20.5424	5.6102
313	C	27.6730	25.2699	9.9214
314	H	23.3057	27.9913	5.9007
315	H	22.8601	26.5862	4.9092
316	H	21.9618	26.2141	7.2111
317	H	23.5641	26.5286	7.9097
318	C	26.7255	29.0949	-8.6984
319	C	24.8778	28.0470	-9.8516
320	C	28.6582	26.2745	10.0181
321	C	27.3224	24.5730	11.0963
322	C	27.0664	29.7740	-9.8665
323	H	27.3091	29.2345	-7.7906
324	C	25.2221	28.7281	-11.0177
325	H	24.0244	27.3720	-9.8411
326	C	29.2651	26.5677	11.2378
327	H	28.9382	26.8200	9.1191

328	C	27.9318	24.8693	12.3141
329	H	26.5637	23.7951	11.0364
330	C	26.3181	29.5962	-11.0343
331	H	27.9222	30.4477	-9.8677
332	H	24.6320	28.5817	-11.9213
333	C	28.9070	25.8681	12.3943
334	H	30.0236	27.3478	11.2884
335	H	27.6448	24.3178	13.2084
336	H	26.5857	30.1274	-11.9458
337	H	29.3820	26.0984	13.3462
338	C	-3.4281	3.4459	-0.1094
339	C	-4.2749	3.6316	-1.2126
340	C	-3.5990	4.2897	0.9984
341	H	-4.1505	2.9957	-2.0879
342	C	-5.2523	4.6226	-1.2121
343	C	-4.5801	5.2771	1.0083
344	H	-2.9582	4.1558	1.8687
345	H	-5.8922	4.7567	-2.0820
346	C	-5.4307	5.4695	-0.0993
347	H	-4.7030	5.9149	1.8813
348	C	-6.4363	6.4855	-0.0952
349	C	-7.3048	7.3657	-0.0871
350	Ru	-8.7526	8.8216	-0.0944
351	P	-7.8879	9.5608	-2.1078
352	P	-7.2900	10.3564	0.8256
353	C	-10.2000	10.2723	-0.1117
354	P	-10.1995	7.2712	-1.0122
355	P	-9.5958	8.0631	1.9209
356	C	-6.3676	10.5887	-1.7793
357	H	-7.4165	8.6597	-3.1012
358	H	-8.6571	10.4222	-2.9395
359	C	-6.5978	11.4371	-0.5279
360	H	-7.7072	11.3255	1.7789
361	H	-6.1093	9.9036	1.4783
362	C	-11.0732	11.1490	-0.1222
363	C	-10.8368	6.1542	0.3379
364	H	-9.7764	6.3283	-1.9884
365	H	-11.4044	7.7036	-1.6348
366	C	-11.0817	6.9828	1.5997
367	H	-8.7942	7.2295	2.7501
368	H	-10.0950	8.9472	2.9160
369	H	-5.5486	9.8768	-1.6176
370	H	-6.1161	11.2097	-2.6457
371	H	-7.3539	12.2085	-0.7200
372	H	-5.6773	11.9343	-0.2038
373	C	-12.0832	12.1555	-0.1501
374	H	-11.7430	5.6273	0.0203

375	H	-10.0501	5.4097	0.5125
376	H	-11.2997	6.3458	2.4635
377	H	-11.9290	7.6646	1.4552
378	C	-13.1964	12.0482	-1.0122
379	C	-12.0054	13.2947	0.6805
380	C	-14.1797	13.0271	-1.0440
381	H	-13.2722	11.1778	-1.6604
382	C	-12.9860	14.2766	0.6504
383	H	-11.1560	13.3935	1.3532
384	C	-14.0934	14.1622	-0.2134
385	H	-15.0300	12.9279	-1.7156
386	H	-12.9088	15.1480	1.2974
387	C	-15.0998	15.1683	-0.2481
388	C	-15.9641	16.0315	-0.2815
389	C	-16.9718	17.0359	-0.3245
390	C	-18.1045	16.8835	-1.1490
391	C	-16.8592	18.2047	0.4548
392	C	-19.0869	17.8628	-1.1926
393	H	-18.2001	15.9846	-1.7539
394	C	-17.8416	19.1841	0.4102
395	H	-15.9885	18.3312	1.0943
396	C	-18.9741	19.0320	-0.4143
397	H	-19.9577	17.7370	-1.8320
398	H	-17.7463	20.0833	1.0146
399	C	-19.9822	20.0371	-0.4609
400	C	-20.8472	20.8978	-0.5026
401	C	-21.8596	21.9029	-0.5528
402	C	-21.7012	23.0953	0.1709
403	C	-23.0129	21.6975	-1.3262
404	C	-22.6917	24.0917	0.1282
405	H	-20.8070	23.2512	0.7684
406	C	-24.0172	22.6791	-1.3828
407	H	-23.1323	20.7731	-1.8851
408	C	-23.8404	23.8674	-0.6516
409	C	-22.5312	25.3081	0.8650
410	C	-25.1950	22.4695	-2.1685
411	H	-24.6121	24.6325	-0.6898
412	C	-22.3741	26.3517	1.5083
413	C	-26.2056	22.2691	-2.8512
414	Ru	-22.1195	28.0870	2.5774
415	Ru	-27.8907	21.9406	-3.9788
416	P	-22.7101	29.2646	0.6800
417	P	-19.9673	28.3315	1.7728
418	C	-21.8638	29.8214	3.6448
419	P	-24.2709	27.8267	3.3769
420	P	-21.5263	26.8953	4.4662
421	P	-29.1502	22.5292	-2.1341

422	P	-28.0945	19.7974	-3.1393
423	C	-29.5745	21.6099	-5.1051
424	P	-27.6712	24.0837	-4.8121
425	P	-26.6180	21.3500	-5.8147
426	C	-21.2404	29.3625	-0.4638
427	H	-23.7291	28.8142	-0.2035
428	H	-23.0987	30.6302	0.7815
429	C	-19.9716	29.5574	0.3673
430	H	-18.9077	28.8282	2.5805
431	H	-19.2972	27.2173	1.1942
432	C	-21.7022	30.8653	4.2875
433	C	-24.2646	26.5699	4.7544
434	H	-25.3291	27.3461	2.5577
435	H	-24.9455	28.9255	3.9803
436	C	-23.0027	26.7579	5.5977
437	H	-21.1169	25.5377	4.3452
438	H	-20.5208	27.3474	5.3641
439	C	-29.2311	21.0821	-0.9608
440	H	-28.7650	23.5831	-1.2607
441	H	-30.5252	22.8651	-2.2864
442	C	-29.3596	19.7899	-1.7686
443	H	-28.5354	18.7080	-3.9397
444	H	-26.9774	19.1732	-2.5165
445	C	-30.5847	21.4022	-5.7872
446	C	-26.3764	24.0907	-6.1545
447	H	-27.2458	25.1709	-4.0004
448	H	-28.7721	24.7134	-5.4586
449	C	-26.4988	22.8056	-6.9745
450	H	-25.2509	20.9933	-5.6435
451	H	-27.0056	20.3093	-6.7026
452	H	-21.2073	28.4054	-0.9990
453	H	-21.3656	30.1633	-1.2006
454	H	-19.9635	30.5518	0.8308
455	H	-19.0696	29.4580	-0.2459
456	C	-21.5241	32.0769	5.0268
457	H	-25.1712	26.6466	5.3643
458	H	-24.2597	25.5866	4.2678
459	H	-22.8739	25.9417	6.3166
460	H	-23.0487	27.7016	6.1553
461	H	-28.2886	21.0936	-0.3994
462	H	-30.0560	21.1954	-0.2492
463	H	-30.3398	19.7376	-2.2587
464	H	-29.2472	18.9051	-1.1329
465	C	-31.7562	21.1681	-6.5739
466	H	-26.4663	24.9811	-6.7860
467	H	-25.4073	24.1295	-5.6418
468	H	-25.6595	22.6897	-7.6686

469	H	-27.4283	22.8075	-7.5574
470	C	-22.5211	33.0743	5.0379
471	C	-20.3464	32.3115	5.7664
472	C	-32.8091	22.1059	-6.6072
473	C	-31.8942	19.9921	-7.3402
474	C	-22.3459	34.2544	5.7580
475	H	-23.4348	32.9061	4.4713
476	C	-20.1751	33.4931	6.4851
477	H	-19.5687	31.5503	5.7669
478	C	-33.9495	21.8755	-7.3743
479	H	-32.7157	23.0176	-6.0205
480	C	-33.0362	19.7656	-8.1060
481	H	-31.0894	19.2597	-7.3238
482	C	-21.1726	34.4729	6.4865
483	H	-23.1297	35.0107	5.7519
484	H	-19.2569	33.6523	7.0490
485	C	-34.0719	20.7047	-8.1290
486	H	-34.7500	22.6140	-7.3846
487	H	-33.1206	18.8500	-8.6898
488	H	-21.0372	35.3953	7.0484
489	H	-34.9634	20.5264	-8.7276
490	C	-3.4326	-3.5547	-0.2072
491	C	-4.2598	-3.7353	0.9116
492	C	-3.6251	-4.4017	-1.3091
493	H	-4.1183	-3.0970	1.7825
494	C	-5.2394	-4.7238	0.9317
495	C	-4.6086	-5.3868	-1.2983
496	H	-2.9997	-4.2719	-2.1912
497	H	-5.8640	-4.8537	1.8132
498	C	-5.4399	-5.5734	-0.1753
499	H	-4.7485	-6.0269	-2.1670
500	C	-6.4487	-6.5862	-0.1579
501	C	-7.3214	-7.4621	-0.1456
502	Ru	-8.7744	-8.9122	-0.1012
503	P	-7.8835	-9.6253	1.9100
504	P	-7.3264	-10.4611	-1.0202
505	C	-10.2288	-10.3549	-0.0462
506	P	-10.2064	-7.3470	0.8152
507	P	-9.6443	-8.1797	-2.1147
508	C	-6.3659	-10.6547	1.5743
509	H	-7.4007	-8.7111	2.8856
510	H	-8.6403	-10.4772	2.7628
511	C	-6.6120	-11.5210	0.3383
512	H	-7.7576	-11.4448	-1.9522
513	H	-6.1566	-10.0174	-1.6982
514	C	-11.1100	-11.2230	-0.0134
515	C	-10.8657	-6.2507	-0.5414

516	H	-9.7685	-6.3892	1.7701
517	H	-11.4011	-7.7703	1.4630
518	C	-11.1276	-7.0980	-1.7873
519	H	-8.8554	-7.3553	-2.9650
520	H	-10.1551	-9.0771	-3.0919
521	H	-5.5511	-9.9434	1.3910
522	H	-6.1007	-11.2631	2.4456
523	H	-7.3633	-12.2915	0.5520
524	H	-5.6951	-12.0206	0.0080
525	C	-12.1327	-12.2156	0.0406
526	H	-11.7681	-5.7209	-0.2180
527	H	-10.0833	-5.5073	-0.7385
528	H	-11.3600	-6.4739	-2.6569
529	H	-11.9710	-7.7795	-1.6203
530	C	-13.2225	-12.0913	0.9301
531	C	-12.0927	-13.3561	-0.7909
532	C	-14.2200	-13.0544	0.9861
533	H	-13.2686	-11.2198	1.5797
534	C	-13.0878	-14.3223	-0.7367
535	H	-11.2616	-13.4681	-1.4840
536	C	-14.1722	-14.1904	0.1534
537	H	-15.0520	-12.9419	1.6782
538	H	-13.0402	-15.1947	-1.3852
539	C	-15.1945	-15.1791	0.2116
540	C	-16.0738	-16.0260	0.2647
541	C	-17.1002	-17.0100	0.3301
542	C	-18.2132	-16.8328	1.1763
543	C	-17.0270	-18.1824	-0.4485
544	C	-19.2149	-17.7911	1.2407
545	H	-18.2784	-15.9310	1.7810
546	C	-18.0286	-19.1409	-0.3830
547	H	-16.1716	-18.3281	-1.1044
548	C	-19.1418	-18.9636	0.4625
549	H	-20.0705	-17.6460	1.8964
550	H	-17.9638	-20.0430	-0.9873
551	C	-20.1705	-19.9463	0.5296
552	C	-21.0539	-20.7871	0.5885
553	C	-22.0888	-21.7678	0.6586
554	C	-21.9695	-22.9669	-0.0616
555	C	-23.2253	-21.5313	1.4478
556	C	-22.9829	-23.9389	0.0002
557	H	-21.0878	-23.1471	-0.6709
558	C	-24.2521	-22.4881	1.5236
559	H	-23.3143	-20.6018	2.0039
560	C	-24.1145	-23.6834	0.7954
561	C	-22.8633	-25.1630	-0.7316
562	C	-25.4135	-22.2471	2.3244

563	H	-24.9040	-24.4292	0.8479
564	C	-22.7444	-26.2160	-1.3677
565	C	-26.4113	-22.0212	3.0180
566	Ru	-22.5575	-27.9721	-2.4168
567	Ru	-28.0774	-21.6528	4.1614
568	P	-23.4531	-29.0673	-0.5911
569	P	-20.5336	-28.4231	-1.3964
570	C	-22.3719	-29.7286	-3.4622
571	P	-24.5793	-27.5038	-3.4319
572	P	-21.6583	-26.8618	-4.2324
573	P	-29.3661	-22.2821	2.3505
574	P	-28.2813	-19.5310	3.2690
575	C	-29.7437	-21.2839	5.3017
576	P	-27.8579	-23.7746	5.0476
577	P	-26.7755	-21.0218	5.9629
578	C	-22.1274	-29.2868	0.7016
579	H	-24.5123	-28.5125	0.1785
580	H	-23.9559	-30.3921	-0.7287
581	C	-20.8044	-29.6182	0.0098
582	H	-19.4552	-29.0384	-2.0893
583	H	-19.8142	-27.3730	-0.7601
584	C	-22.2534	-30.7850	-4.0937
585	C	-24.3058	-26.2723	-4.8053
586	H	-25.6600	-26.9078	-2.7257
587	H	-25.2980	-28.5365	-4.0978
588	C	-22.9886	-26.5953	-5.5121
589	H	-21.1341	-25.5486	-4.0706
590	H	-20.6132	-27.4180	-5.0199
591	C	-29.4541	-20.8660	1.1406
592	H	-28.9994	-23.3612	1.5003
593	H	-30.7408	-22.6049	2.5307
594	C	-29.5645	-19.5521	1.9155
595	H	-28.7057	-18.4187	4.0465
596	H	-27.1694	-18.9295	2.6154
597	C	-30.7440	-21.0545	5.9914
598	C	-26.5455	-23.7539	6.3725
599	H	-27.4492	-24.8851	4.2591
600	H	-28.9535	-24.3809	5.7249
601	C	-26.6495	-22.4468	7.1594
602	H	-25.4087	-20.6787	5.7636
603	H	-27.1442	-19.9553	6.8281
604	H	-22.0564	-28.3274	1.2291
605	H	-22.4062	-30.0582	1.4276
606	H	-20.8453	-30.6171	-0.4421
607	H	-19.9655	-29.5954	0.7136
608	C	-22.1261	-32.0103	-4.8208
609	H	-25.1478	-26.2678	-5.5058

610	H	-24.2538	-25.2876	-4.3245
611	H	-22.7059	-25.8059	-6.2168
612	H	-23.0704	-27.5378	-6.0676
613	H	-28.5190	-20.8981	0.5678
614	H	-30.2888	-20.9929	0.4428
615	H	-30.5378	-19.4807	2.4166
616	H	-29.4554	-18.6851	1.2551
617	C	-31.9045	-20.7968	6.7869
618	H	-26.6323	-24.6266	7.0287
619	H	-25.5833	-23.8126	5.8485
620	H	-25.8005	-22.3176	7.8393
621	H	-27.5713	-22.4273	7.7540
622	C	-23.1893	-32.9352	-4.8775
623	C	-20.9340	-32.3311	-5.5028
624	C	-32.9694	-21.7200	6.8394
625	C	-32.0194	-19.6118	7.5431
626	C	-23.0637	-34.1286	-5.5861
627	H	-24.1149	-32.7000	-4.3558
628	C	-20.8125	-33.5257	-6.2103
629	H	-20.1053	-31.6267	-5.4674
630	C	-34.0991	-21.4672	7.6153
631	H	-32.8938	-22.6385	6.2607
632	C	-33.1508	-19.3629	8.3178
633	H	-31.2052	-18.8904	7.5118
634	C	-21.8754	-34.4329	-6.2574
635	H	-23.8983	-34.8278	-5.6159
636	H	-19.8821	-33.7521	-6.7293
637	C	-34.1985	-20.2879	8.3599
638	H	-34.9091	-22.1949	7.6404
639	H	-33.2173	-18.4408	8.8935
640	H	-21.7790	-35.3655	-6.8104
641	H	-35.0816	-20.0920	8.9654

7. Selected Frontier MO Diagrams for 6, 9, 9', 4-H' and 5_2'

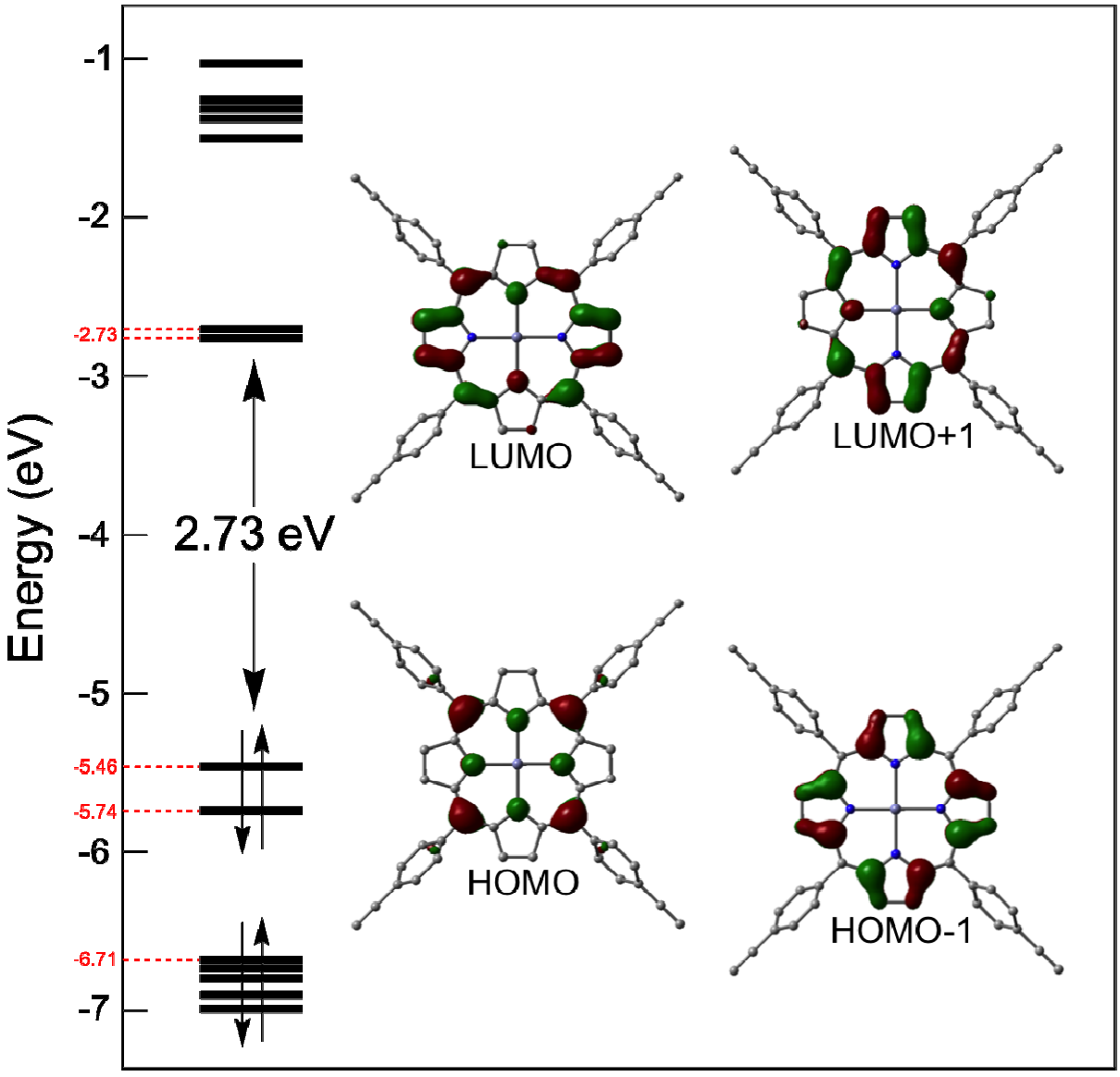


Fig. S10. B3PW91 DFT molecular orbital diagram of PBE0 optimized compound **6** (isocontour value: 0.04 $(e.bohr^{-3})^{1/2}$).

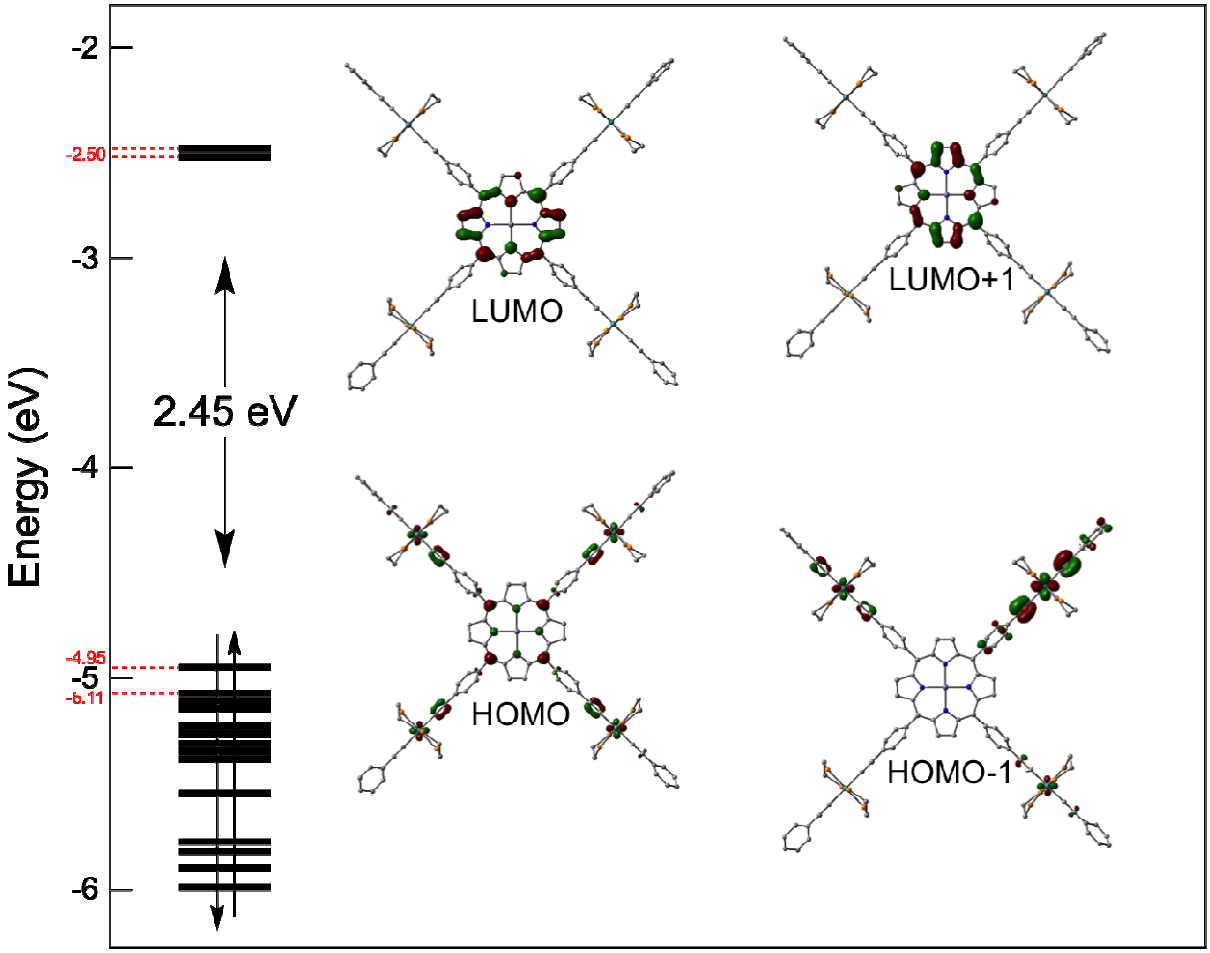


Fig. S11. B3PW91 DFT molecular orbital diagram of PBE0 optimized compound **4-H'** (isocontour value: 0.04 (e.bohr^{-3})$^{1/2}$).

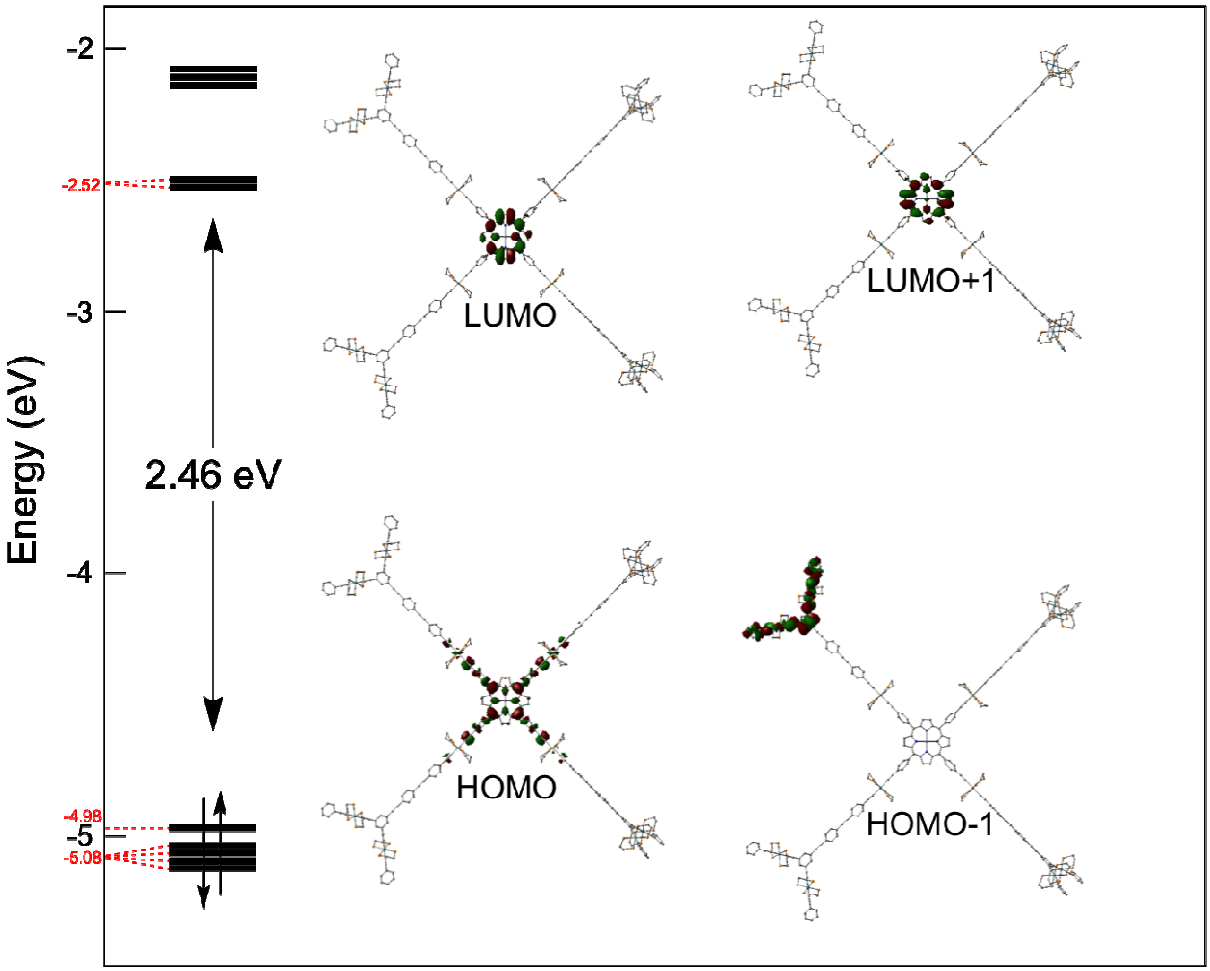


Fig. S12. B3PW91 DFT molecular orbital diagram of PBE0 optimized compound **5_2'** (isocontour value: 0.04 (e.bohr^{-3})$^{1/2}$).

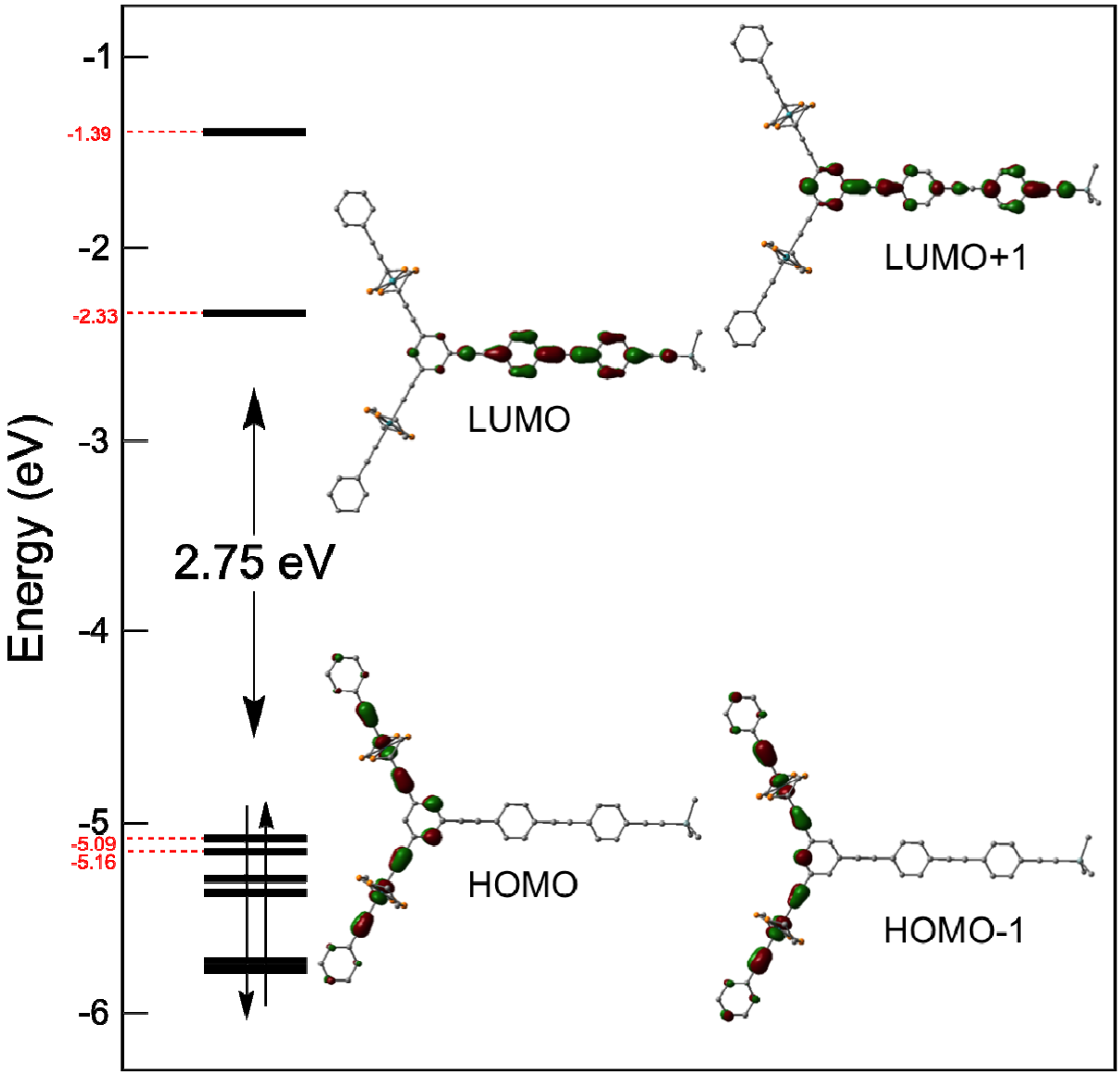


Fig. S13. B3PW91 DFT molecular orbital diagram of PBE0 optimized compound **9'** (isocontour value: 0.04 $(e.bohr^{-3})^{1/2}$).

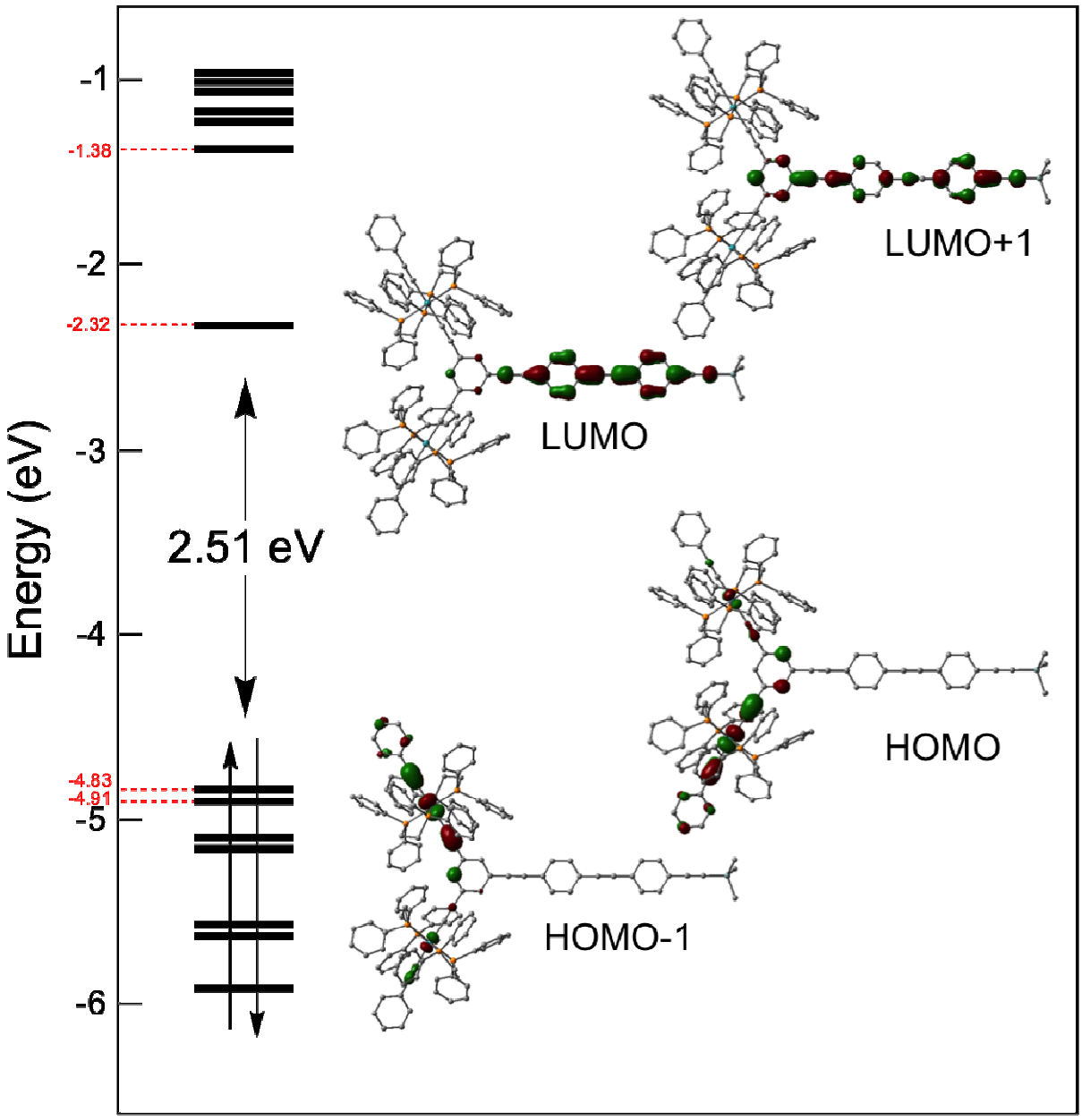


Fig. S14. B3PW91 DFT molecular orbital diagram of PBE0 optimized compound **9** (isocontour value: 0.04 (e.bohr^{-3})$^{1/2}$).

8. Selected TD-DFT Data and Ionization Potentials (in eV)

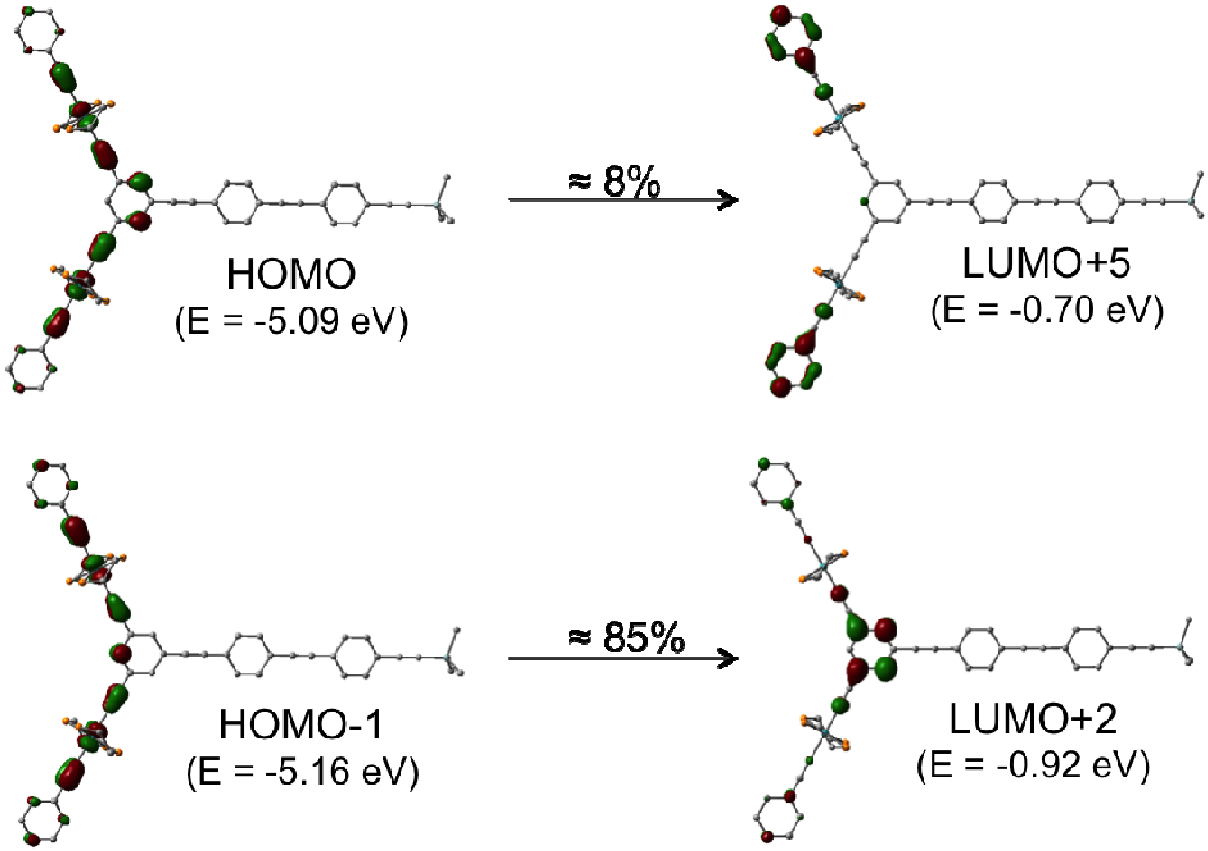


Fig. S15. Main electronic transitions involved in the λ = 336 nm electronic excitation of 9' (isocontour value: 0.04 **(**e.bohr^{-3})$^{1/2}$).

Table S1. Calculated vertical ionisation potentials (VIP) for **6**, **4-H'**, **5_2'**, and **9'**.

Compound	VIP (eV)
6	6.37
4-H'	5.24
5_2'	5.05
9'	5.65

9. THG Measurements in $CHCl_3$

The measurements were carried out using a wedge-shaped cell, consisting of two fused silica windows assembled on a stainless steel support, their inner interfaces with the liquid forming a small angle α. This cell follows the classic design implemented by Levine and Bethea for electric-field induced second-harmonic generation.[4] The wedge shapes are to measure the intensity of the harmonic radiation 3ω as a function of the cell displacement, i.e. without changing the incidence angle, resulting in fringes with constant amplitudes, and thereby making data processing much easier than is the case for a rotating cell with parallel windows. The whole cell was translated horizontally relative to the incident beam, producing a periodic third-harmonic generation signal (Maker fringes). The schematic diagram of the THG experimental set-up is shown in Fig. S16 together with a sketch of the cell used for the measurements.

After passing through the cell, the fundamental radiation was removed by filters, and only the third-harmonic radiation was detected by a photomultiplier and processed by a home-made computer program to calculate the inter-fringe distance and the fringe amplitude. These data were then used to calculate the γvalue of the sample.

In our THG experiments, the fundamental field E^{ω} was polarized along the vertical direction. The generated third-harmonic was therefore also polarized along this direction, because of the symmetry properties of an isotropic medium.

The resulting cubic susceptibility $\Gamma(x)$ of a solution was deduced from the fringe amplitude $I^{3\omega}$ and period δ. From δ, the value of the coherence length $l_c = \pi/\Delta k$, Δk being the wavevector mismatch between the fundamental and third-harmonic waves in the nonlinear medium, can be inferred using the relation $l_c = 2\delta \mathrm{tg}(\alpha/2)$. If x is the concentration of the molecule of interest in a solvent taken as reference material:

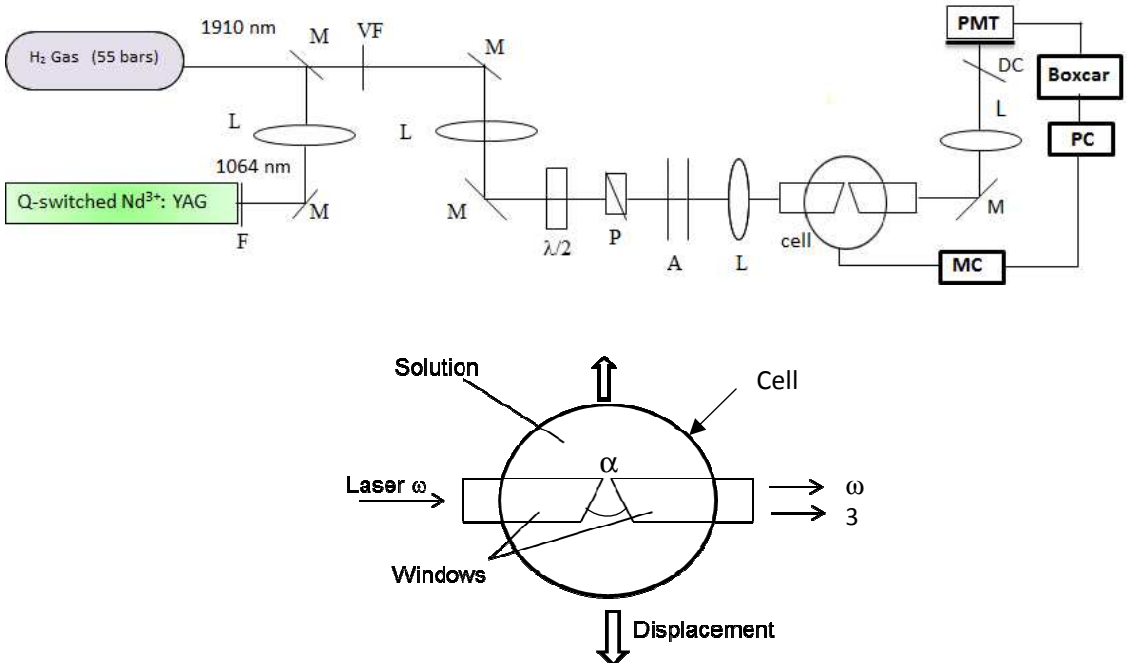
$$\Gamma(x) = \frac{1}{l_c(x)}\left[A\frac{\sqrt{I^{3\omega}(x)}}{\sqrt{I^{3\omega}(0)}} + B \right] \qquad \text{(in } 10^{-12} \text{ esu)}$$

Then, the cubic hyperpolarizability $\gamma$of the molecule can be inferred using:

[4] B. F. Levine, C. G. Bethea, *J. Chem. Phys.* **1975**, *63*, 2666-2682.

$$\gamma = \frac{M}{\rho N_A f^{3\omega} (f^{\omega})^3 x} [(1+x)\Gamma(x) - \Gamma(0))]$$

where N_A is Avogadro's number (6.02×10^{23}), M the molecular weight of the compound, ρ the density of the solvent, x the molar fraction of the compound, $\Gamma(0)$ the susceptibility of the pure solvent and $f^{\omega,3\omega}$ are local field corrections factors for the E^{ω} and $E^{3\omega}$ electric fields, respectively.



THG Cell (top view)

Fig. S16. (a) THG experimental set-up at 1907 nm. [F: Filter; M: Mirrors; L: Lens; $\lambda/2$: Half wave plate; P: Polarizer; A: Attenuator; PMT: Photomultiplier tube: DC: dichroic mirror; MC: Micro controller; PC: personal computer]. (b) THG measurement cell.

10. Z-scan Data for 7 in CH_2Cl_2

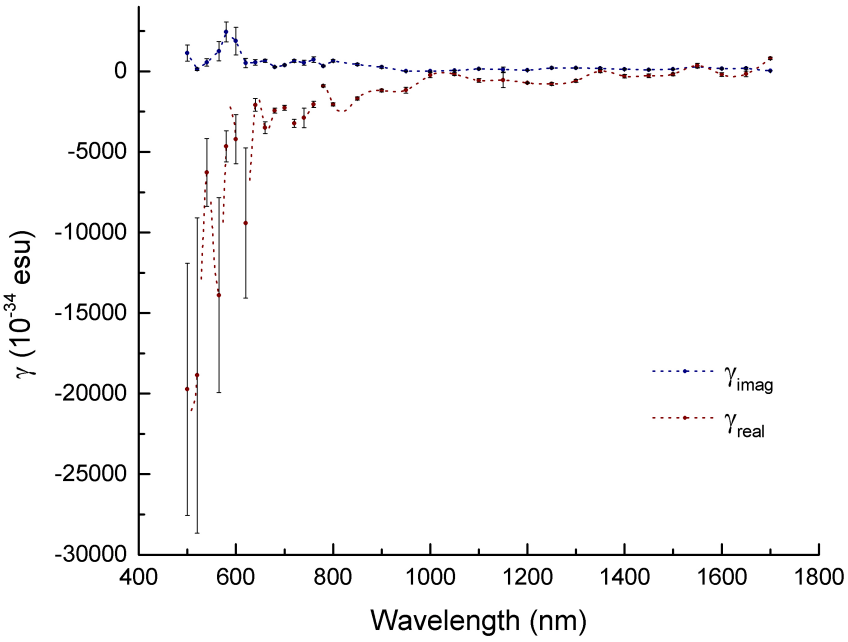


Fig. S17. Plots of the real (red) and imaginary (blue) components of the second hyper-polarizability over the range 500-1700 nm for **7.**

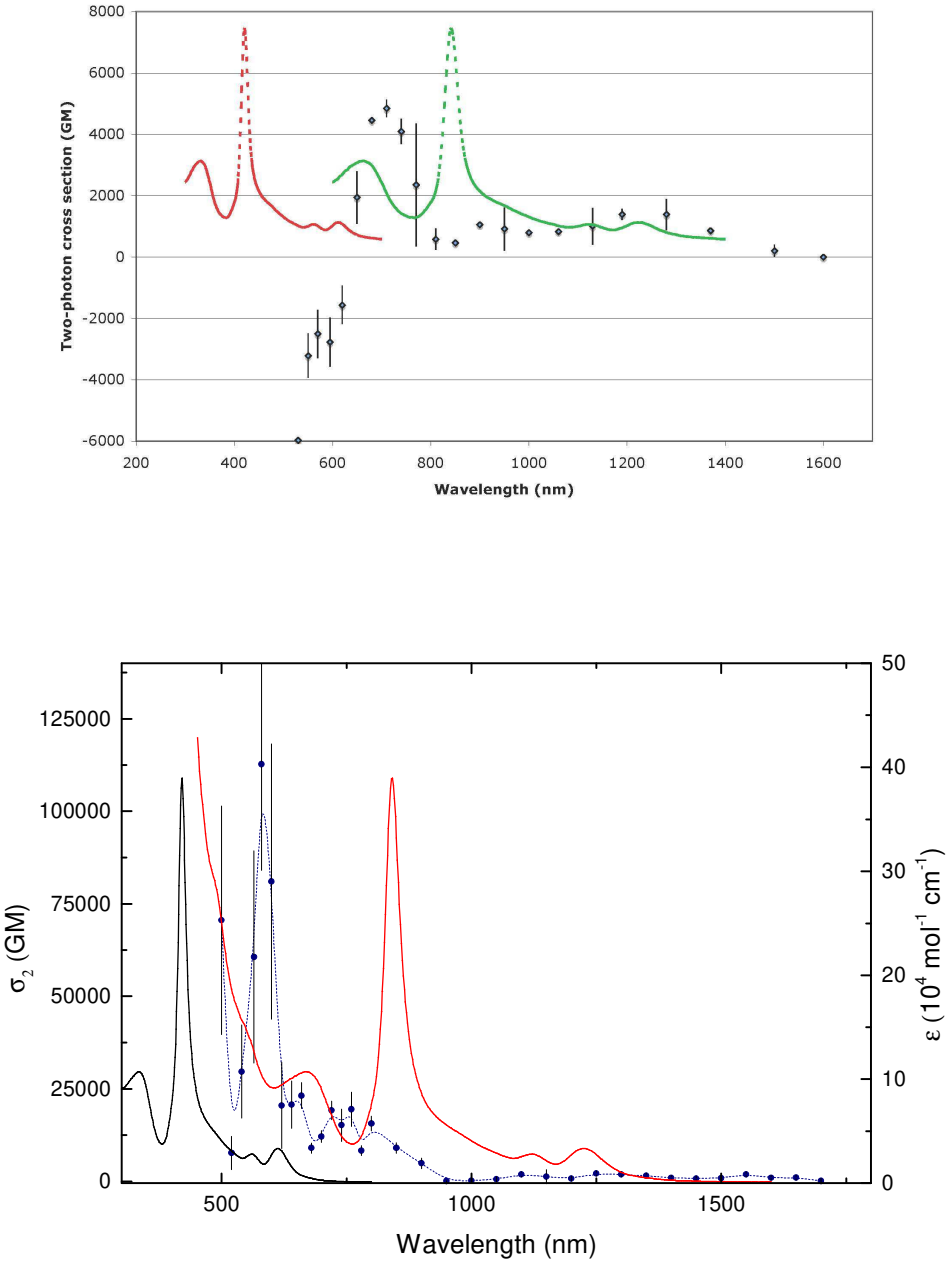


Fig. S18. Compared apparent TPA cross-section plots (blue) overlaid on one-photon absorption (OPA) spectra (red/black) and the same OPA plotted at twice the wavelength (green/red) for **4-H**[5] (a) and **7** (b).

[5] S. Drouet, A. Merhi, D. Yao, M. P. Cifuentes, M. G. Humphrey, M. Wielgus, J. Olesiak-Banska, K. Matczyszyn, M. Samoc, F. Paul and C. O. Paul-Roth, *Tetrahedron*, 2012, **68**, 10351-10359.

11. *SPARTAN* Modelling of 5_1, 5_2 and of their tetra-Vinylidene Complexes

The supplementary file *SPARTAN_Structures_52_52vin_51_51vin.pdb* contains the computed Cartesian coordinates of all the molecules reported in this study in ".pdb" format for convenient visualization via *Mercury*.

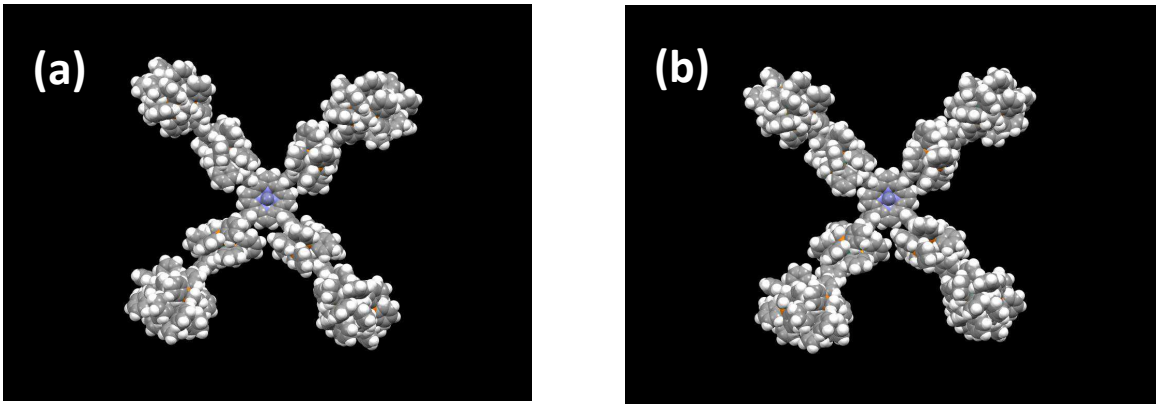


Fig. S19. *SPARTAN* modelization of $\mathbf{5_1}$ (a) and its tetra-vinylidene derivative (b) with couter-anions omitted.

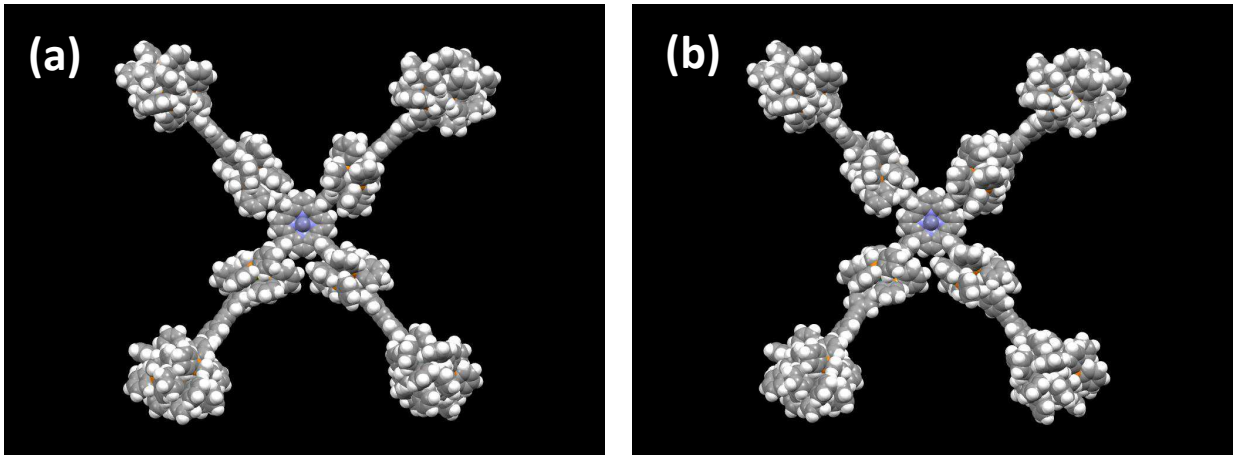


Fig. S20. *SPARTAN* modelization of $\mathbf{5_2}$ (a) and its tetra-vinylidene derivative (b) with couter-anions omitted.