Electronic Supplementary Material (ESI) for ChemComm.

- Electronic Supplementary Information -

Absorption of Chemicals in Amorphous Trisresorcinarene

Daisuke Shimoyama, Ryo Sekiya, and Takeharu Haino*

Department of Chemistry, Graduate School of Advanced Science and Engineering, Hiroshima University,

1-3-1 Kagamiyama, Higashi-Hiroshima, Hiroshima 739-8526, Japan

To whom correspondence should be addressed

haino@hiroshima-u.ac.jp

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General

All chemicals and solvents were purchased from Kanto Chemical Co., Ltd., Wako Pure Chemical Co., Ltd., Tokyo Kasei Kogyo Co., Ltd., and Sigma-Aldrich Co., Ltd., and were used as received without further purification. ^{1}H NMR spectra were recorded on VARIAN 300 MHz spectrometers. Chemical shifts are quoted as parts per million (ppm) relative to DMSO (δ = 2.48 ppm), D_2O (δ = 4.79 ppm), and chloroform (δ = 7.26 ppm). Thermogravimetric analysis was carried out on a SEIKO Instrument EXSTAR6200 TG/DTA system. Scanning electron microscope image of the apohost and (pyrene)⊂**1** were obtained on JEOL-S5200.

Trisresorcinarenes **1** and **2** were synthesized by the procedures reported previously.[1] ^{1}H and ^{13}C-NMR spectra can be found in the previous paper.

Computational methods

The energy minimizations of the host-guest complexes were carried out by the *MacroMode*l Ver. 9.0 program using MMFFs force field.[2] The cartesian coordinates of the host-guest complexes were listed in Tables S2–S10.

Experimental Procedure of the Absorption

Typical procedure of the absorption experiment: 0.1 mol L^{-1} of the chemical was dissolved in 2 mL of acetone. 10 mg of the apohost was added to it. The solution was standing for 24 h at room temperature. The filtration of the mixture offered the solid host-guest complex. The solid was dissolved in DMSO-d_6 and subjected to be NMR analysis. The integration of the signals of **1** and the chemical provided the host-to-guest ratio.

X-ray Crystallography

Powder X-ray diffraction was collected on a Rigaku ULTIMA III diffractometer using Cu Kα radiation (λ = 1.5418 Å) at 298 K.

X-ray crystallographic data of (hexane)⊂**2**· were collected on a Bruker SMART AEPX II ULTRA CCD diffractometer using graphite-monochromatized Mo Kα radiation (λ = 0.71073 Å) at 93 K. The crystal structure was solved by the direct method using the *SHELXS-2014* program and refined by successive differential Fourier syntheses and full-matrix least-squares procedures using the *SHELXL-2018* program.[3] Anisotropic thermal factors were applied to all non-hydrogen atoms except for some carbon atoms (C57, C230-C233, and C601-C606). The hydrogen atoms were generated geometrically. Electron densities arising from the disordered solvents and protecting groups were treated by the *SQUEEZE* routine on the *PLATON* program.[4] Crystallographic parameters are listed in Table S1.

Table S1. Crystallographic parameters of (hexane)⊂**2**. [a]

Parameters	(hexane)⊂**2**
Formula	$C_{279}H_{381}O_{48}$
Formula weight	4502.82
Crystal system	Monoclinic
Space group	$P2_1/c$ (#14)
a / Å	21.609(5)
b / Å	49.509(12)
c / Å	28.125(7)
α / °	90
β / °	111.398(3)
γ / °	90
V/ Å^3	28015(12)
$d_{calc.}$ /g cm^{-3}	1.068
Z	4
$2\theta_{max}$/°	50.314
ρ (MoKα) /mm^{-1}	0.071
Temperature /K	–170
Crystal form	Block
Crystal size /mm^3	0.15 × 0.10 × 0.04
Crystal color	Colorless
# of total reflections	268149
# of unique reflections	49871
# of observed reflections	19026
R_{int}	0.150
Criterion for observed reflections	2σ
$R1(F_o)$	0.1611
$wR2(F_o^2)$	0.3963
G. O. F.	1.185
# of parameters used	2760
$\Delta\rho_{max}$ (eÅ^{-3})	+1.246
$\Delta\rho_{min}$ (eÅ^{-3})	–0.437
CCDC number	2014628

[a] Formula, formula weight, and density are known contents only.

Supporting Figures and Tables

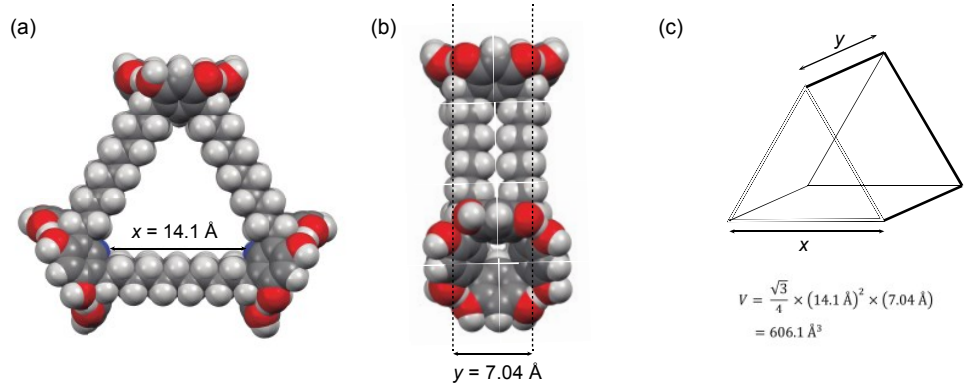

Figure S1. Calculation of the cavity volume of **1**.

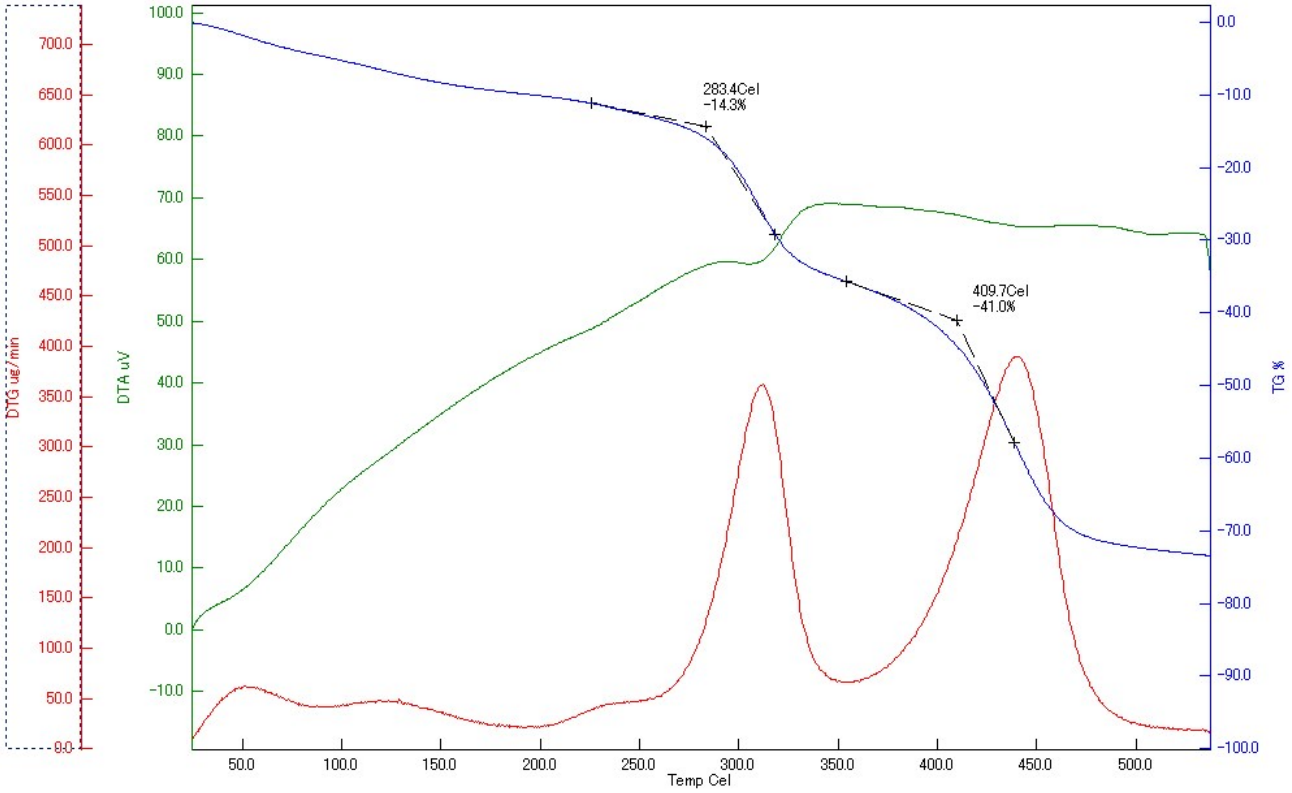

Figure S2. TG analysis of as produced **1**. 12.88 mg of **1** was used for the analysis. Conditions: N_2 atmosphere, 5 °C min^{-1}.

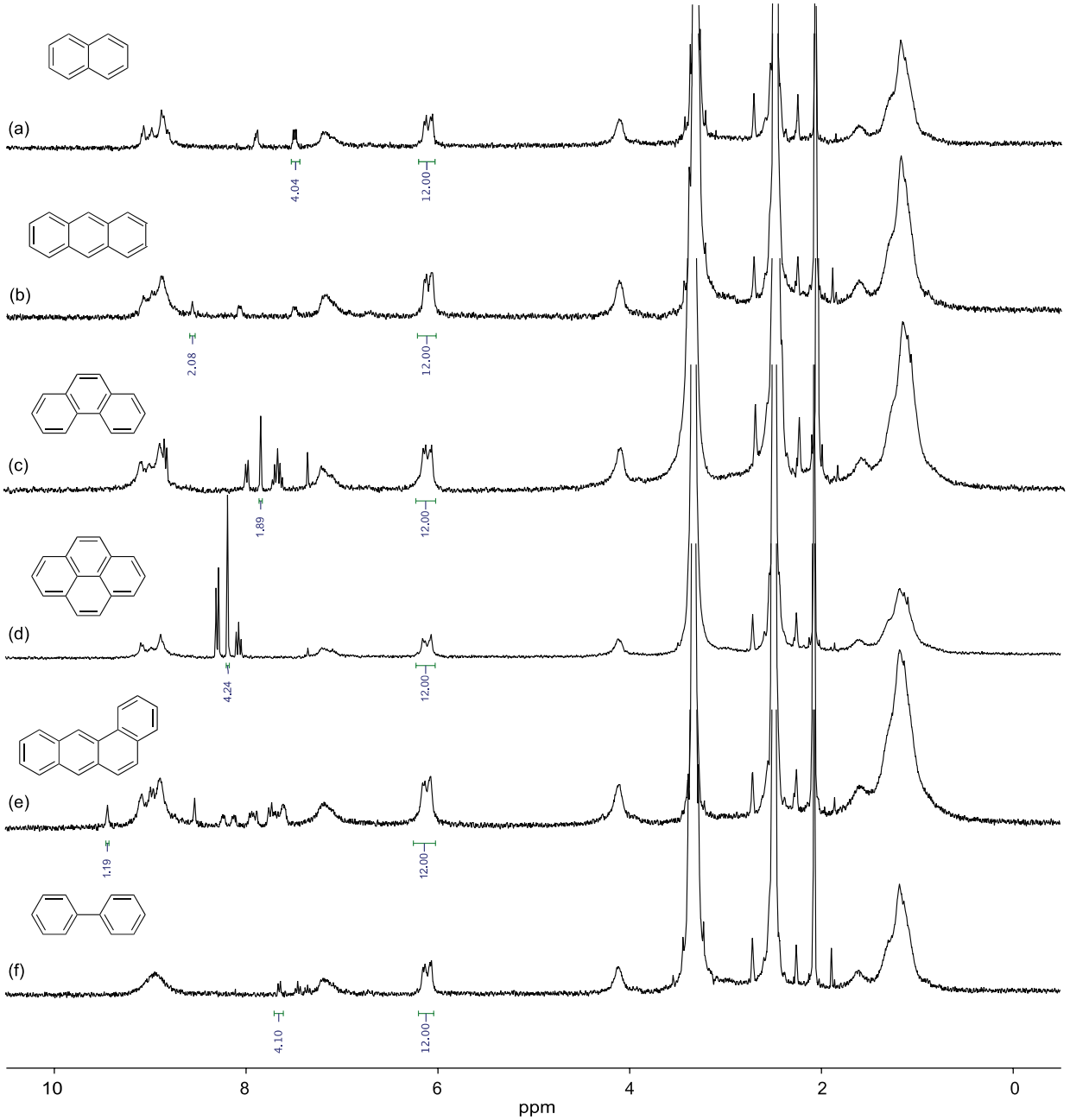

Figure S3. ^{1}H NMR spectra (300 MHz, DMSO-d_6, 298 K) of (a) (naphthalene)⊂**1**, (b) (anthracene)⊂**1**, (c) (phenanthrene)⊂**1**, (d) (pyrene)⊂**1**, (e) (benz[*a*]anthracene)⊂**1**, and (f) (biphenyl)⊂**1**.

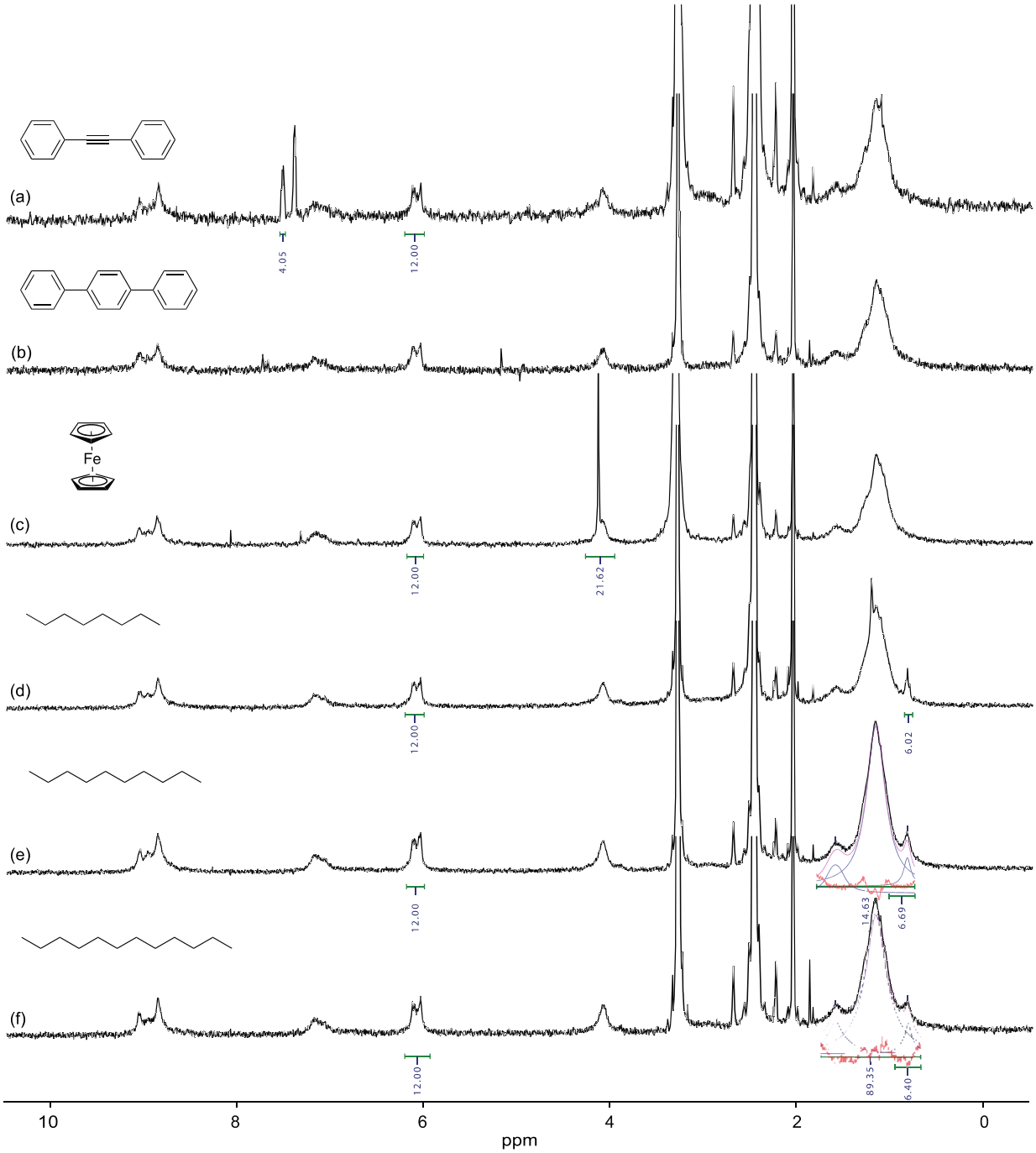

Figure S4. ^{1}H NMR spectra (300 MHz, DMSO-d_6, 298 K) of (a) (diphenylacetylene)⊂**1**, (b) (*p*-terphenyl)⊂**1**, (c) (ferrocene)⊂**1**, (d) (octane)⊂**1**, (e) (decane)⊂**1**, and (f) (dodecane)⊂**1**.

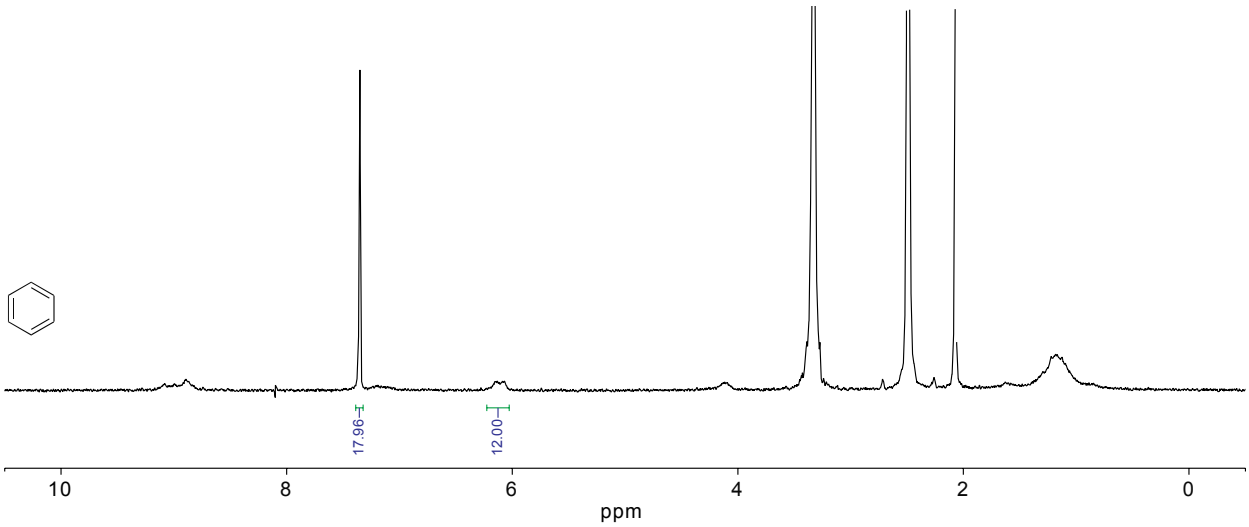

Figure S5. ^{1}H NMR spectrum (300 MHz, DMSO-d_6, 298 K) of (benzene)$_x$⊂**1**.

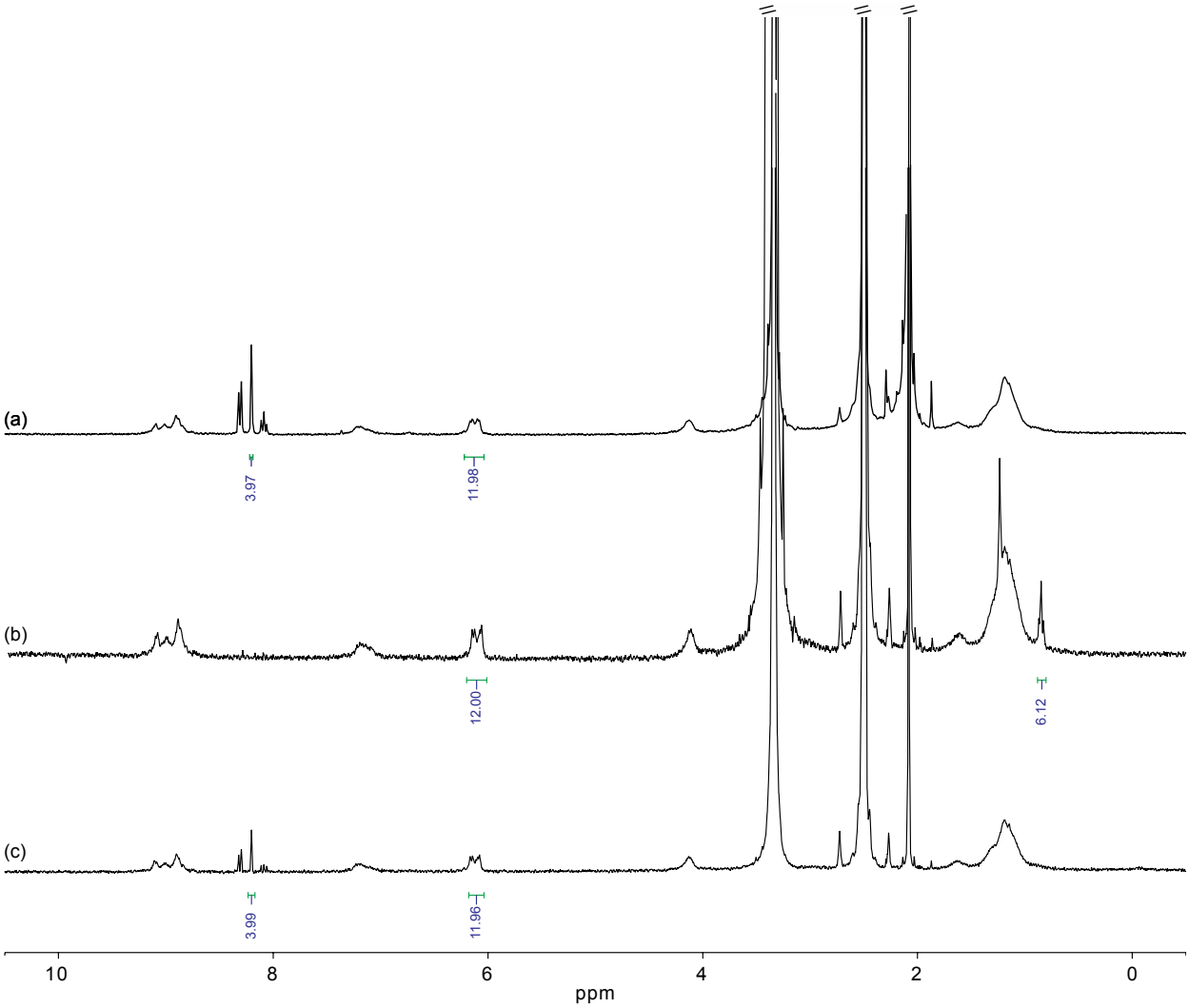

Figure S6. (a)–(c) ^{1}H NMR spectra (300 MHz, DMSO-d_6, 298 K). (a) (pyrene)⊂**1**, (b) (pyrene)⊂**1** after contacting with octane for 5 min, and (c) the solid of (b) after contacting with pyrene for 5 min.

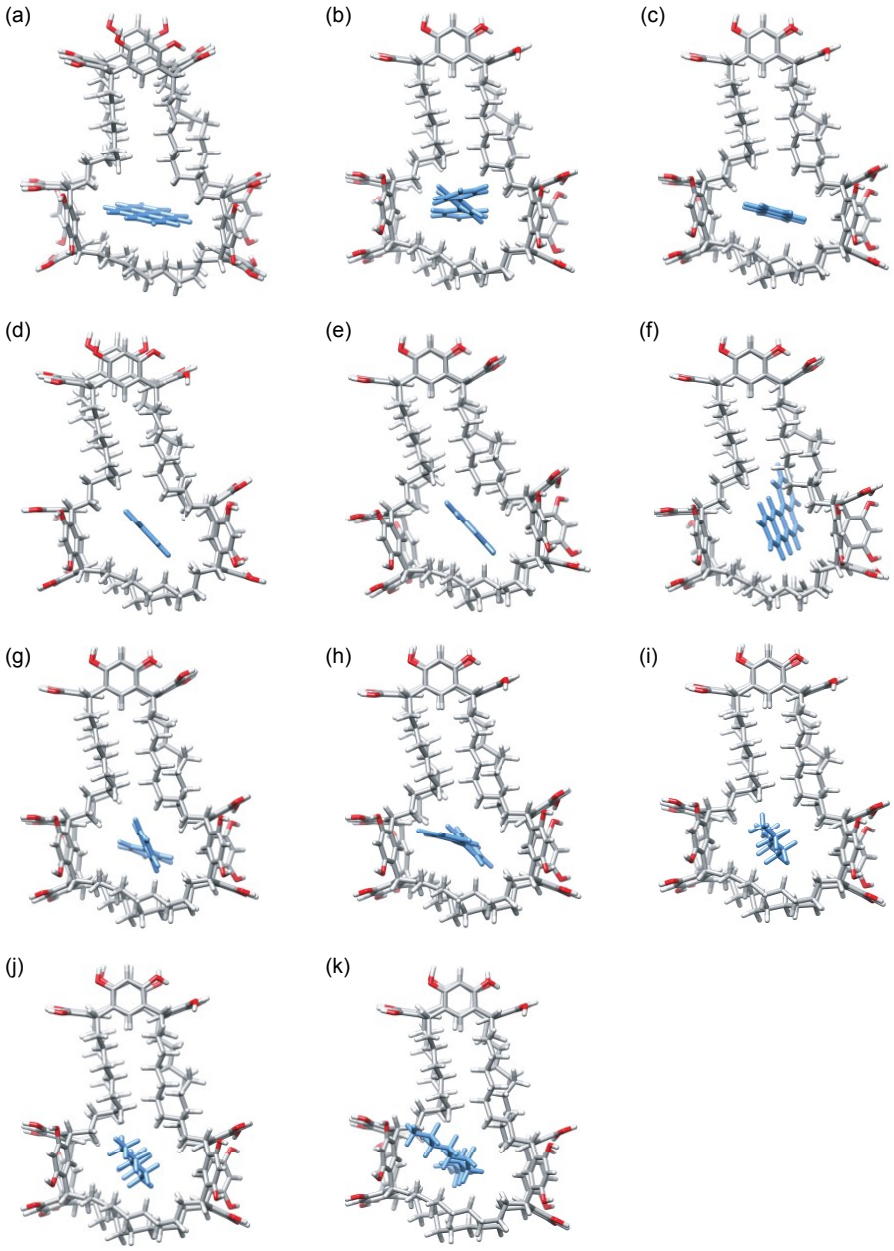

Figure S7. Energy minimized structures of (a) (pyrene)⊂**1**, (b) (*p*-terphenyl)⊂**1**, (c) (naphthalene)⊂**1**, (d) (anthracene)⊂**1**, (e) (phenanthrene)⊂**1**, (f) (benz[*a*]anthracene)⊂**1**, (g) (biphenyl)⊂**1**, (h) (diphenylacetylene)⊂**1**, (i) (octane)⊂**1**, (j) (decane)⊂**1**, and (k) (dodecane)⊂**1** by MacroModel Ver. 9.0 using the MMFFs force field. MMFFs force field cannot be applied to (ferrocene)⊂**1**. Color scheme: gray (carbon), white (hydrogen), red (oxygen). The guests are drawn with blue for clarity.

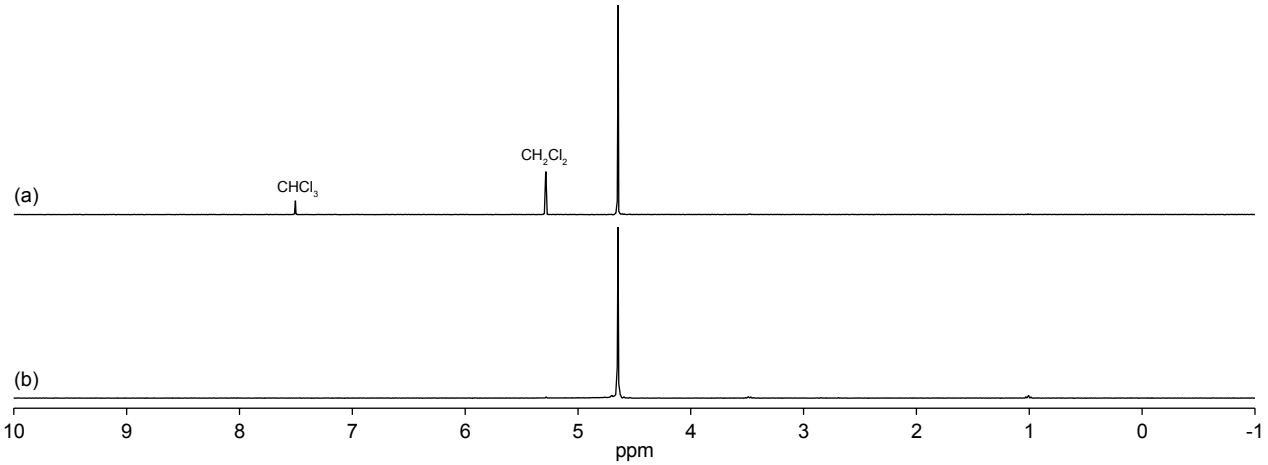

Figure S8. Decontamination of dichloromethane and chloroform saturated D_2O with the apohost. ^1H NMR spectra (300 MHz, D_2O, 298 K) of (a) The polluted D_2O solution and (b) the D_2O solution after addition of the apohost followed by stirring for 1 h at room temperature.

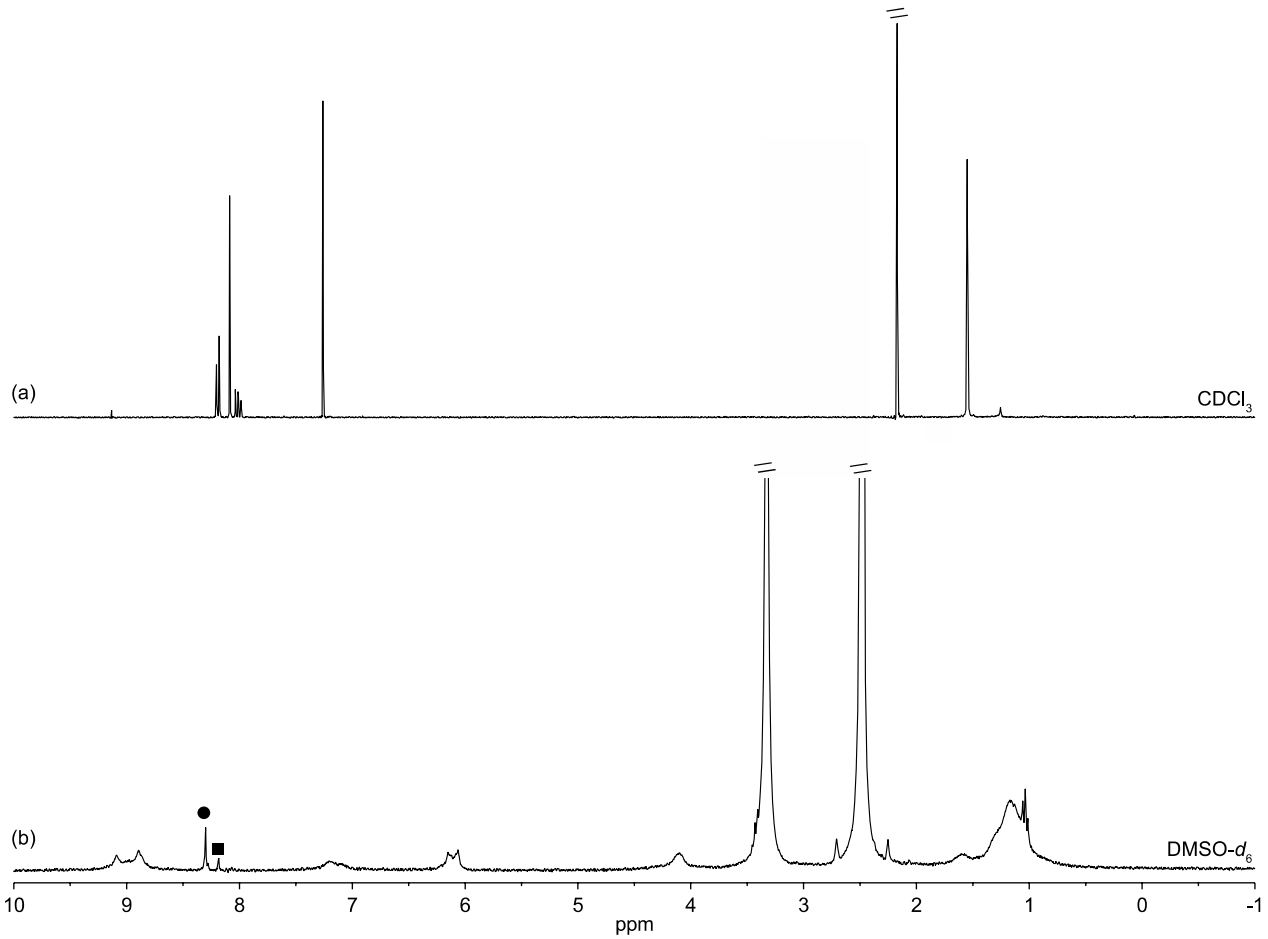

Figure S9. Extraction of pyrene from (pyrene)⊂**1**. ^1H NMR spectrum (300 MHz, 298 K) of (a) a filtrate (chloroform-d_1) and (b) the residual solid dissolved in DMSO-d_6. A filled circle and a filled square denote chloroform and pyrene, respectively.

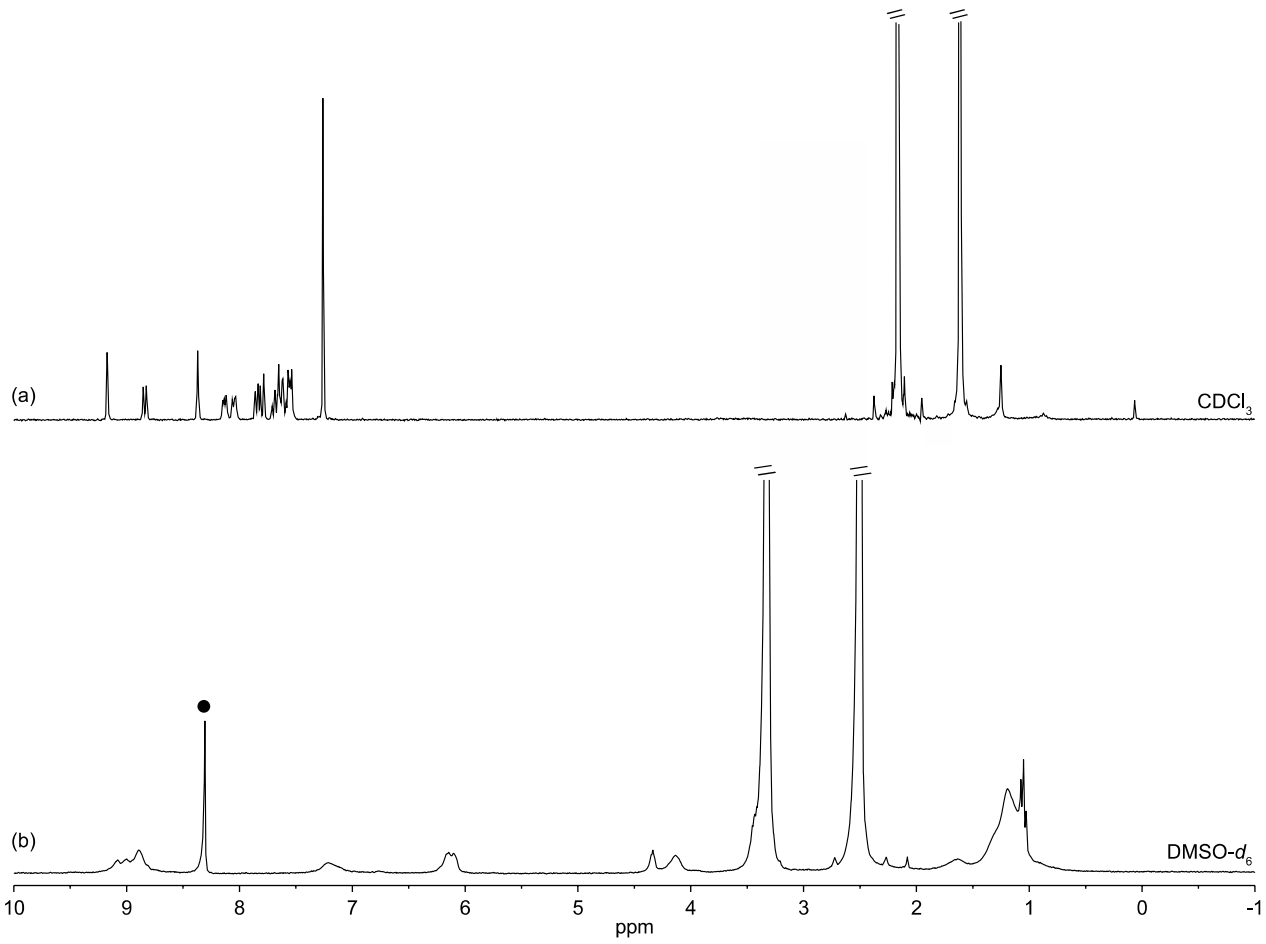

Figure S10. Extraction of pyrene from (benz[*a*]anthracene)⊂**1**. ^{1}H NMR spectrum (300 MHz, 298 K) of (a) a filtrate (chloroform-d_1) and (b) the residual solid dissolved in DMSO-d_6. A filled circle denotes chloroform.

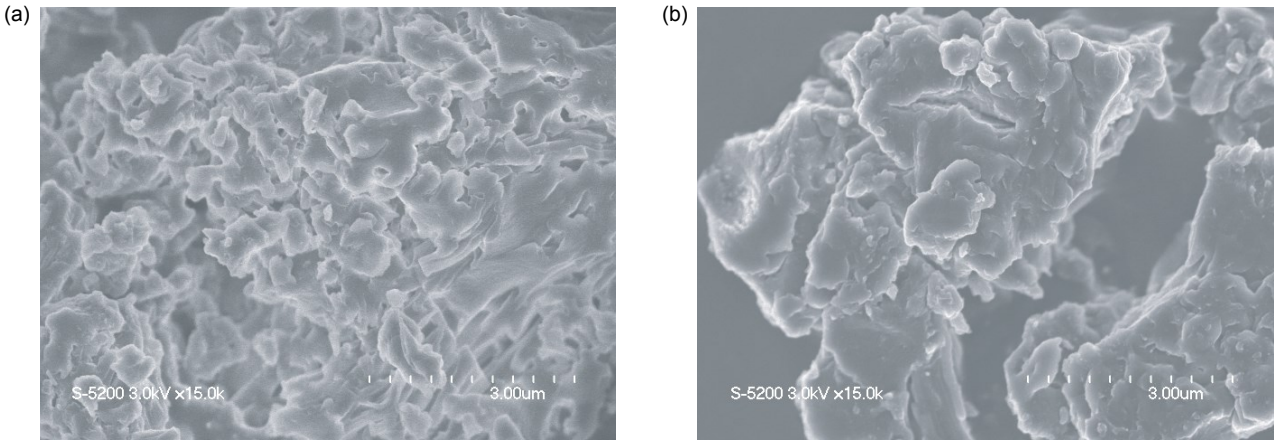

Figure S11. SEM images of (a) the apohost and (b) (pyrene)⊂**1**.

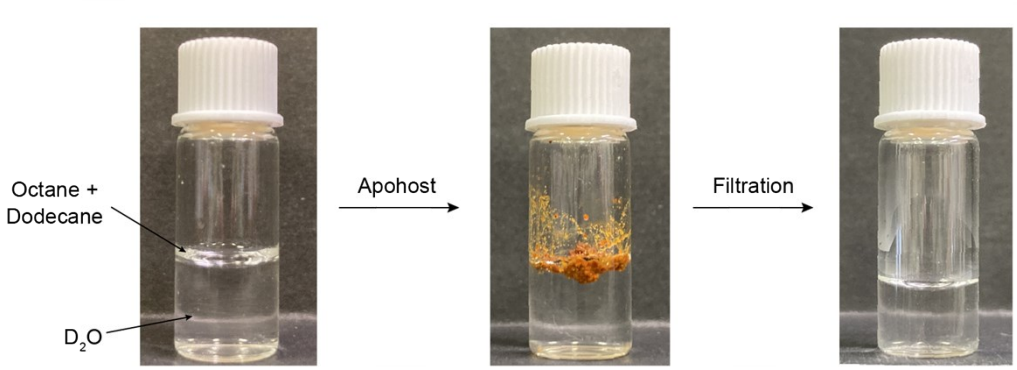

Figure S12. Digital images of the removal of a mixture of octane and dodecane on the surface of D_2O with the apohost.

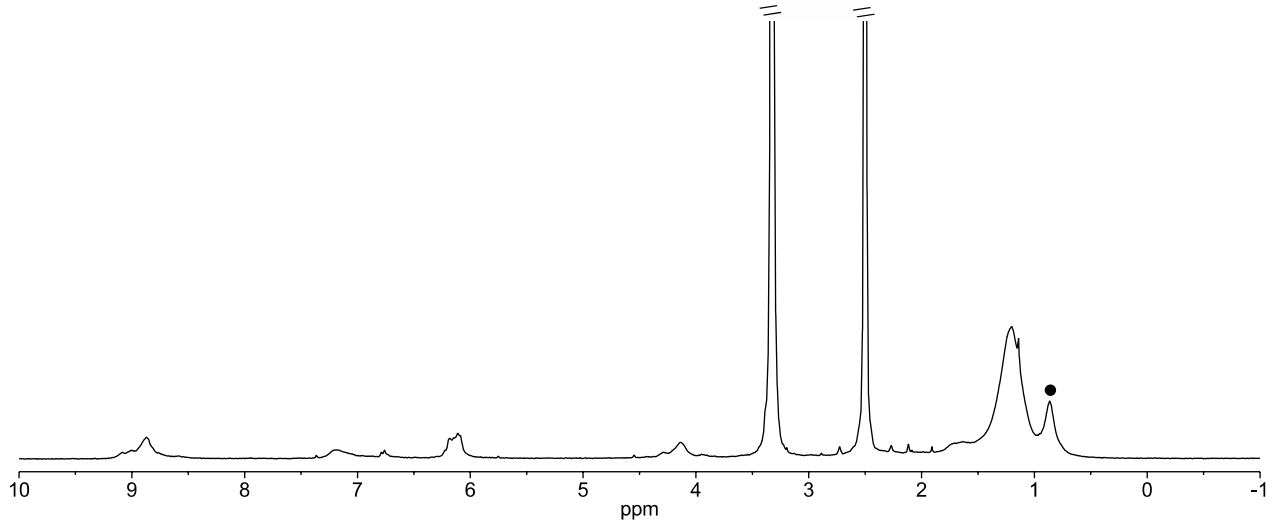

Figure S13. ^{1}H NMR spectrum (300 MHz, DMSO-d_6, 298 K) of the solid that absorbed the mixture of octane and dodecane dissolved in DMSO-d_6. A filled circle denotes the signals of octane and dodecane.

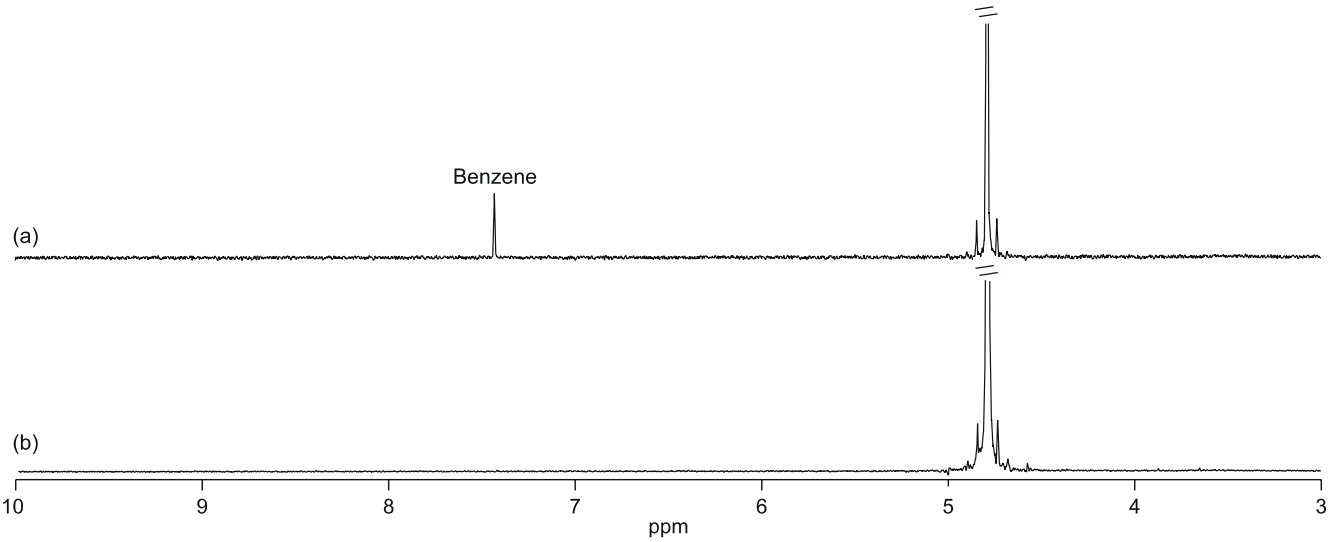

Figure S14. Decontamination of benzene saturated D_2O with the apohost. ^{1}H NMR spectra (300 MHz, D_2O, 298 K) of (a) The polluted D_2O solution and (b) the D_2O solution after addition of the apohost followed by stirring for 1 h at room temperature.

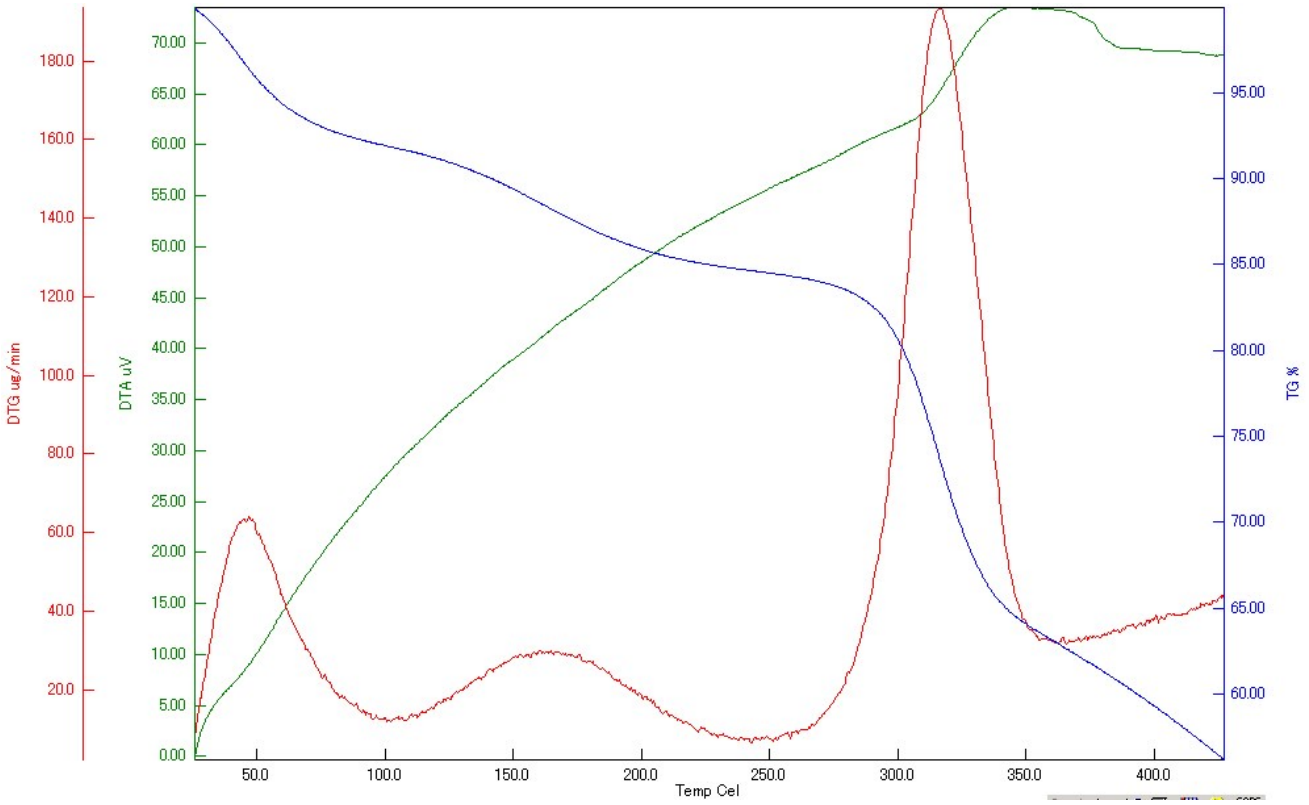

Figure S15. TG analysis of (naphthalene)⊂**1**. 3.308 mg of (naphthalene)⊂**1** was used for the analysis. Conditions: N_2 atmosphere, 10 °C min^{-1}. The weight loss at low temperature (<60 °C) is caused by evaporation of acetone.

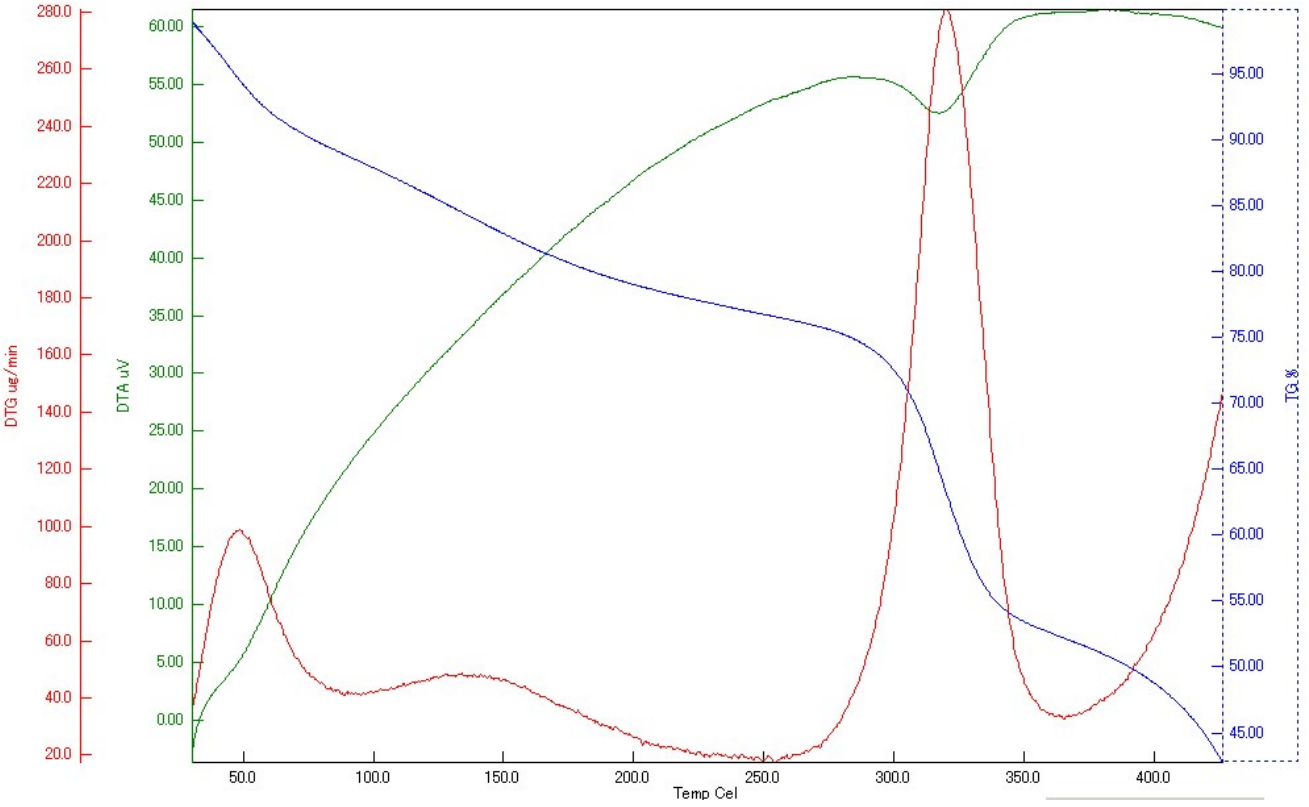

Figure S16. TG analysis of (octane)⊂**1**. 4.095 mg of (octane)⊂**1** was used for the analysis. Conditions: N_2 atmosphere, 10 °C min^{-1}. The weight loss at low temperature (<60 °C) is caused by evaporation of acetone.

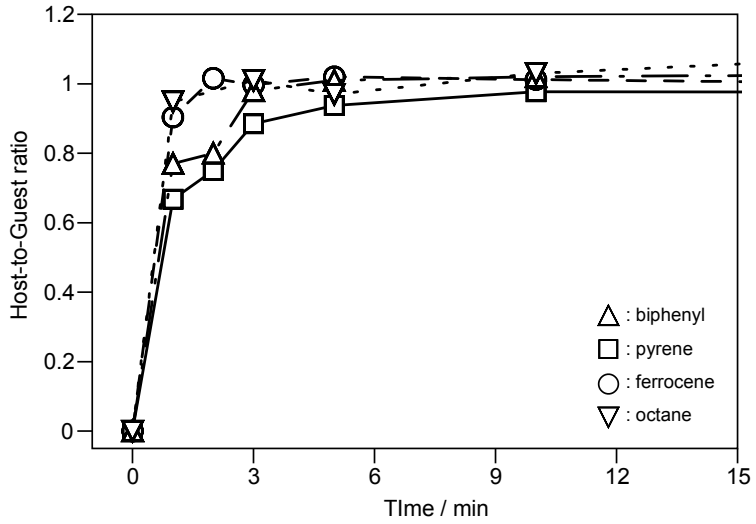

Figure S17. Change of the relative ratio of **1** and the guest (biphenyl = triangle, pyrene = square, ferrocene = circle, octane = inverted triangle).

The absorption processes of four structurally distinct chemicals, namely, biphenyl, pyrene, ferrocene, and octane, were investigated by ^{1}H NMR spectroscopy. The apohost (10 mg) immersed in the acetone solution containing the chemical (0.1 mol L^{-1}) was collected and dissolved in DMSO-d_6. The amount of the absorbed chemical relative to that of **1** was plotted as a function of time (Figure S17). The guests were found to be quickly absorbed in the apohost under the given conditions irrespective of their structures to form the host-guest complexes with the 1:1 host-to-guest ratio. For example, the apohost was saturated with octane within a minute. The other chemicals were absorbed at similar rates. However, pyrene was absorbed slowly compared to the other compounds. The apohost was saturated by pyrene within 5 min.

Table S2. Cartesian coordinates of the structure of (naphthalene)⊂**1** optimized by MacroModel Ver 9.1 using the MMFFs force field.

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	C1	10.525	4.346	9.678
2	C2	9.5	4.451	10.631
3	C02B	0.405	19.479	13.167
4	C3	9.084	5.738	11.019
5	C4	9.668	6.894	10.47
6	C5	10.685	6.73	9.515
7	C6	11.108	5.47	9.102
8	C18	6.815	18.907	10.447
9	C19	8.154	19.311	10.352
10	C20	8.906	19.583	11.492
11	C21	8.329	19.427	12.748
12	C22	6.998	19.02	12.898
13	C23	6.257	18.755	11.73
14	C35	9.69	7.339	16.811
15	C36	9.27	6.105	16.277
16	C37	9.448	4.894	16.978
17	C38	10.08	4.944	18.229
18	C39	10.527	6.148	18.769
19	C40	10.321	7.333	18.064
20	C41	10.096	8.77	14.725
21	C42	11.398	9.283	14.637
22	C43	12.026	9.462	13.407
23	C44	11.355	9.132	12.233
24	C45	10.049	8.619	12.258
25	C46	9.455	8.41	13.522
26	C48	9.61	3.159	15.116
27	C49	10.828	2.462	15.148
28	C50	11.454	2.039	13.978
29	C51	10.863	2.297	12.744
30	C52	9.639	2.976	12.654
31	C53	9.055	3.438	13.855
32	C64	-1.559	4.136	8.141
33	C65	-1.922	5.301	7.226
34	C66	-1.597	6.623	7.573
35	C67	-1.961	7.708	6.754
36	C68	-2.606	7.435	5.538
37	C69	-2.96	6.135	5.183
38	C70	-2.643	5.088	6.044
39	C82	2.309	19.928	9.201
40	C83	3.437	19.093	9.325
41	C84	4.749	19.563	9.123
42	C85	4.908	20.928	8.838
43	C86	3.816	21.793	8.762
44	C87	2.529	21.288	8.941
45	C88	0.256	19.569	10.711
46	C89	-1.109	19.872	10.836
47	C91	-0.964	19.776	13.236
48	C93	0.996	19.371	11.892
49	C95	2.607	19.874	14.444
50	C96	2.733	21.268	14.56
51	C97	3.981	21.884	14.586
52	C98	5.136	21.112	14.491
53	C99	5.073	19.712	14.383
54	C100	3.793	19.121	14.352
55	C111	-2.548	9.798	10.949
56	C112	-1.856	9.442	9.773

57	C113	-2.472	9.468	8.505
58	C114	-3.837	9.792	8.451
59	C115	-4.561	10.101	9.6
60	C116	-3.912	10.11	10.833
61	C117	-2.201	8.691	13.229
62	C118	-1.988	7.362	12.81
63	C119	-2.29	6.266	13.643
64	C120	-2.804	6.535	14.922
65	C121	-3.007	7.84	15.367
66	C122	-2.696	8.905	14.524
67	C124	-2.659	4.488	11.836
68	C125	-3.997	4.086	11.739
69	C126	-4.552	3.71	10.516
70	C127	-3.771	3.726	9.361
71	C128	-2.43	4.137	9.399
72	C129	-1.909	4.542	10.647
73	C1	6.262	17.356	14.6
74	C2	5.884	17.05	16.056
75	C3	6.296	15.64	16.494
76	C4	5.688	14.517	15.649
77	C5	6.167	13.147	16.137
78	C6	5.633	12.019	15.251
79	C7	6.025	10.62	15.735
80	C8	7.534	10.372	15.705
81	C9	7.872	8.923	16.08
82	C10	5.972	18.634	9.201
83	C11	0.689	17.909	8.876
84	C12	0.881	19.385	9.325
85	C13	1.033	17.679	7.396
86	C14	0.692	16.267	6.909
87	C15	1.545	15.175	7.559
88	C16	1.179	13.795	7.005
89	C17	1.592	11.27	7.252
90	C18	1.944	12.684	7.729
91	C19	0.101	10.949	7.383
92	C20	-0.187	9.452	7.209
93	C21	-1.708	9.145	7.212
94	C22	-1.866	9.877	12.32
95	C23	-0.332	10.099	12.326
96	C24	0.086	11.452	11.737
97	C25	1.604	11.648	11.713
98	C26	2.281	11.728	13.084
99	C27	1.739	12.811	14.023
100	C28	1.802	14.218	13.425
101	C29	1.43	15.279	14.461
102	C30	1.375	16.673	13.83
103	C31	1.129	17.748	14.9
104	C32	1.213	19.231	14.441
105	C33	-0.526	4.444	13.303
106	C34	-0.024	4.063	8.37
107	C35	0.393	2.725	8.999
108	C36	1.668	2.846	9.834
109	C37	1.335	3.725	14.901
110	C38	2.91	2.784	16.699
111	C39	1.943	1.529	10.561
112	C40	4.28	3.09	16.084
113	C41	5.309	2.069	16.584
114	C42	3.018	1.642	11.637
115	C43	5.443	1.736	12.218
116	C44	6.897	1.751	11.757
117	C45	4.429	1.848	11.081
118	C46	1.815	3.793	16.355
119	C47	-0.006	4.454	14.748

120	C48	6.729	2.253	16.041
121	C49	7.361	3.605	16.402
122	C50	9.402	8.654	16.085
123	C51	8.918	3.573	16.416
124	C52	8.949	3.199	11.307
125	C53	9.296	8.293	10.968
126	C54	7.762	8.546	10.986
127	C55	7.33	9.98	11.346
128	C56	7.934	11.065	10.45
129	C57	7.539	12.471	10.915
130	C58	6.343	18.871	14.272
131	C59	7.396	3.146	11.344
132	C60	-1.721	19.982	12.084
133	O1	12.057	9.355	11.079
134	O2	12.061	9.63	15.783
135	O3	11.407	2.181	16.355
136	O4	10.709	8.519	18.626
137	O5	10.231	3.791	18.951
138	O6	11.551	1.833	11.655
139	O7	11.012	3.098	9.373
140	O8	11.328	7.847	9.039
141	O9	-4.469	9.816	7.237
142	O10	-4.615	10.447	11.958
143	O11	-4.766	4.046	12.869
144	O12	-4.404	3.304	8.221
145	O13	-3.089	5.492	15.761
146	O14	-2.856	10.187	14.976
147	O15	-1.568	19.844	14.463
148	O16	-1.859	20.036	9.702
149	O17	1.604	22.035	14.661
150	O18	1.453	22.128	8.846
151	O19	6.167	21.419	8.619
152	O20	8.736	19.42	9.119
153	O21	9.121	19.71	13.824
154	O22	6.309	21.817	14.516
155	O23	-2.904	8.468	4.693
156	O24	-3.098	3.821	5.78
157	C61	-2.034	4.826	13.196
158	C62	8.283	13.564	10.136
159	C63	5.636	17.12	9.077
160	C64	6.491	14.758	8.742
161	C65	6.877	16.228	8.949
162	C66	7.713	13.832	8.738
163	H1	5.57	16.845	13.92
164	H2	7.251	16.915	14.408
165	H3	4.805	17.171	16.201
166	H4	6.376	17.767	16.724
167	H5	6.003	15.503	17.542
168	H6	7.391	15.566	16.464
169	H7	5.973	14.638	14.598
170	H8	4.594	14.569	15.698
171	H9	5.841	12.99	17.172
172	H10	7.262	13.135	16.134
173	H11	5.98	12.16	14.22
174	H12	4.539	12.075	15.228
175	H13	5.526	9.884	15.091
176	H14	5.643	10.462	16.751
177	H15	8.034	11.043	16.412
178	H16	7.919	10.61	14.708
179	H17	7.343	8.23	15.416
180	H18	7.473	8.734	17.086
181	H19	6.56	18.866	8.302
182	H20	-0.362	17.624	9.024

183	H21	1.267	17.236	9.519
184	H22	0.29	19.977	8.612
185	H23	2.093	17.873	7.207
186	H24	0.468	18.394	6.786
187	H25	0.838	16.234	5.822
188	H26	-0.371	16.066	7.09
189	H27	1.391	15.175	8.643
190	H28	2.608	15.376	7.38
191	H29	1.396	13.753	5.931
192	H30	0.101	13.648	7.126
193	H31	2.175	10.556	7.846
194	H32	1.903	11.145	6.208
195	H33	3.022	12.84	7.6
196	H34	1.744	12.753	8.804
197	H35	-0.457	11.508	6.623
198	H36	-0.256	11.289	8.359
199	H37	0.341	8.877	7.978
200	H38	0.237	9.13	6.248
201	H39	-2.117	9.827	6.455
202	H40	-2.273	10.789	12.777
203	H41	0.183	9.29	11.799
204	H42	0.021	10.053	13.365
205	H43	-0.396	12.264	12.293
206	H44	-0.274	11.539	10.708
207	H45	1.827	12.564	11.155
208	H46	2.063	10.83	11.142
209	H47	3.352	11.905	12.923
210	H48	2.211	10.757	13.588
211	H49	2.324	12.785	14.95
212	H50	0.707	12.576	14.309
213	H51	1.117	14.292	12.573
214	H52	2.813	14.416	13.049
215	H53	2.169	15.266	15.271
216	H54	0.456	15.042	14.906
217	H55	0.562	16.69	13.094
218	H56	2.301	16.861	13.281
219	H57	1.809	17.594	15.748
220	H58	0.119	17.574	15.298
221	H59	0.707	19.768	15.258
222	H60	-0.389	3.435	12.891
223	H61	0.095	5.119	12.703
224	H62	0.323	4.905	8.976
225	H63	0.498	4.161	7.408
226	H64	0.536	1.982	8.205
227	H65	-0.406	2.336	9.64
228	H66	1.547	3.648	10.571
229	H67	2.514	3.113	9.191
230	H68	1.208	2.678	14.6
231	H69	2.086	4.165	14.236
232	H70	3.015	2.768	17.792
233	H71	2.587	1.778	16.404
234	H72	2.212	0.751	9.837
235	H73	1.021	1.193	11.054
236	H74	4.586	4.103	16.368
237	H75	4.218	3.056	14.992
238	H76	4.97	1.061	16.312
239	H77	5.346	2.098	17.68
240	H78	2.997	0.715	12.225
241	H79	2.771	2.456	12.329
242	H80	5.274	0.791	12.75
243	H81	5.274	2.538	12.945
244	H82	7.041	1.047	10.929
245	H83	7.497	1.368	12.589

246	H84	4.64	1.087	10.321
247	H85	4.509	2.828	10.599
248	H86	2.152	4.81	16.587
249	H87	0.964	3.588	17.018
250	H88	0.1	5.489	15.095
251	H89	-0.739	3.966	15.402
252	H90	6.72	2.125	14.954
253	H91	7.343	1.44	16.447
254	H92	7.02	3.895	17.406
255	H93	6.981	4.377	15.722
256	H94	9.806	9.474	16.692
257	H95	9.149	2.775	17.134
258	H96	9.196	2.335	10.676
259	H97	9.646	8.999	10.208
260	H98	7.263	7.863	11.682
261	H99	7.358	8.306	9.993
262	H0	7.584	10.189	12.39
263	H1	6.236	10.034	11.284
264	H2	7.614	10.9	9.415
265	H3	9.026	11.001	10.468
266	H4	7.804	12.574	11.976
267	H5	6.455	12.607	10.845
268	H6	7.017	19.287	15.033
269	H7	7	3.376	10.347
270	H8	6.986	3.907	12.014
271	H9	-2.779	20.205	12.157
272	H10	11.687	8.814	10.348
273	H11	12.957	9.924	15.556
274	H12	12.255	1.733	16.205
275	H13	11.213	8.344	19.436
276	H14	10.775	3.97	19.735
277	H15	11.255	2.299	10.844
278	H16	11.572	3.174	8.578
279	H17	11.856	7.588	8.26
280	H18	-5.412	10.005	7.365
281	H19	-5.55	10.574	11.731
282	H20	-5.669	3.782	12.629
283	H21	-3.846	3.461	7.433
284	H22	-3.512	5.831	16.567
285	H23	-3.284	10.171	15.846
286	H24	-2.493	20.117	14.35
287	H25	-2.763	20.287	9.948
288	H26	1.857	22.971	14.68
289	H27	1.765	23.038	8.719
290	H28	6.123	22.379	8.489
291	H29	9.627	19.792	9.221
292	H30	9.031	18.979	14.46
293	H31	7.037	21.275	14.168
294	H32	-3.431	8.137	3.949
295	H33	-3.444	3.799	4.87
296	H34	-2.533	4.146	13.899
297	H35	5.005	16.965	8.192
298	H36	5.776	14.44	9.51
299	H37	5.979	14.666	7.776
300	H38	7.489	16.565	8.104
301	H39	7.491	16.326	9.85
302	H40	8.276	14.484	10.731
303	H41	9.338	13.278	10.037
304	H42	7.443	12.886	8.256
305	H43	8.496	14.282	8.115
306	H3	8.336	5.84	11.8
307	H6	11.921	5.367	8.391
308	H20	9.942	19.901	11.423

309	H23	5.219	18.438	11.817
310	H36	8.772	6.088	15.311
311	H39	11.002	6.168	19.744
312	H43	13.033	9.862	13.34
313	H46	8.457	7.985	13.566
314	H50	12.397	1.501	14.005
315	H53	8.129	4.001	13.812
316	H64	-1.779	3.193	7.622
317	H66	-1.088	6.815	8.515
318	H69	-3.501	5.945	4.262
319	H83	3.282	18.046	9.568
320	H86	3.965	22.845	8.547
321	H93	2.05	19.113	11.824
322	H97	4.077	22.962	14.677
323	CH00	3.724	18.045	14.26
324	CH12	-0.808	9.168	9.841
325	CH15	-5.614	10.352	9.534
326	CH18	-1.583	7.181	11.817
327	CH21	-3.386	8.025	16.365
328	CH26	-5.586	3.387	10.443
329	CH29	-0.882	4.887	10.707
330	H1	5.056	16.779	9.944
331	C1	2.904	6.92	12.088
332	C2	4.237	6.453	12.029
333	C3	2.156	7.013	10.902
334	C4	2.72	6.668	9.673
335	C5	4.032	6.21	9.615
336	C6	4.784	6.101	10.784
337	C7	4.985	6.357	13.216
338	C8	4.429	6.726	14.441
339	C9	3.119	7.19	14.498
340	C10	2.359	7.282	13.331
341	H1	1.126	7.357	10.926
342	H2	6.009	5.995	13.194
343	H3	5.018	6.649	15.351
344	H4	2.683	7.474	15.452
345	H5	1.334	7.638	13.403
346	H6	5.808	5.744	10.712
347	H7	2.134	6.753	8.762
348	H8	4.471	5.937	8.659

Table S3. Cartesian coordinates of the structure of (anthracene)⊂**1** optimized by MacroModel Ver 9.1 using the MMFFs force field.

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	C1	10.529	4.192	9.84
2	C2	9.502	4.259	10.795
3	C02B	0.507	19.947	13.24
4	C3	8.991	5.527	11.134
5	C4	9.486	6.701	10.538
6	C5	10.501	6.572	9.574
7	C6	11.017	5.331	9.21
8	C18	6.773	18.721	10.403
9	C19	8.14	19.001	10.271
10	C20	8.939	19.231	11.389
11	C21	8.379	19.154	12.66
12	C22	7.021	18.87	12.846
13	C23	6.233	18.649	11.701
14	C35	9.603	7.408	16.852
15	C36	9.228	6.139	16.368
16	C37	9.466	4.962	17.109
17	C38	10.108	5.082	18.35
18	C39	10.51	6.322	18.842
19	C40	10.248	7.471	18.098
20	C41	9.902	8.778	14.703
21	C42	11.168	9.363	14.554
22	C43	11.745	9.532	13.298
23	C44	11.059	9.115	12.16
24	C45	9.791	8.519	12.247
25	C46	9.249	8.327	13.537
26	C48	9.704	3.161	15.319
27	C49	10.955	2.529	15.378
28	C50	11.605	2.091	14.226
29	C51	11.002	2.264	12.984
30	C52	9.743	2.869	12.868
31	C53	9.135	3.354	14.048
32	C64	-1.144	4.234	8.217
33	C65	-1.467	5.401	7.291
34	C66	-1.223	6.729	7.681
35	C67	-1.597	7.812	6.862
36	C68	-2.141	7.535	5.598
37	C69	-2.401	6.228	5.193
38	C70	-2.095	5.181	6.057
39	C82	2.354	20.128	9.226
40	C83	3.403	19.195	9.348
41	C84	4.748	19.535	9.105
42	C85	5.026	20.873	8.782
43	C86	4.016	21.833	8.708
44	C87	2.693	21.455	8.927
45	C88	0.311	19.997	10.786
46	C89	-1.017	20.428	10.932
47	C91	-0.826	20.371	13.33
48	C93	1.057	19.759	11.955
49	C95	2.765	20.158	14.463
50	C96	3.023	21.536	14.543
51	C97	4.323	22.034	14.53
52	C98	5.399	21.155	14.431
53	C99	5.204	19.766	14.358
54	C100	3.875	19.296	14.37
55	C111	-2.467	9.804	11.072
56	C112	-1.715	9.51	9.916

57	C113	-2.292	9.496	8.631
58	C114	-3.677	9.71	8.537
59	C115	-4.456	9.953	9.666
60	C116	-3.847	10.008	10.917
61	C117	-2.097	8.718	13.359
62	C118	-1.823	7.406	12.924
63	C119	-2.094	6.286	13.736
64	C120	-2.623	6.515	15.016
65	C121	-2.874	7.804	15.482
66	C122	-2.604	8.893	14.656
67	C124	-2.379	4.554	11.871
68	C125	-3.718	4.167	11.718
69	C126	-4.232	3.817	10.471
70	C127	-3.408	3.839	9.346
71	C128	-2.065	4.235	9.44
72	C129	-1.586	4.619	10.711
73	C1	6.178	17.311	14.595
74	C2	5.803	17.06	16.061
75	C3	6.174	15.65	16.536
76	C4	5.52	14.521	15.734
77	C5	6.005	13.153	16.227
78	C6	5.423	12.013	15.389
79	C7	5.851	10.62	15.864
80	C8	7.355	10.369	15.732
81	C9	7.722	8.929	16.124
82	C10	5.881	18.498	9.182
83	C11	0.555	18.257	8.992
84	C12	0.885	19.723	9.393
85	C13	0.831	17.964	7.509
86	C14	0.492	16.527	7.102
87	C15	1.424	15.487	7.729
88	C16	1.096	14.078	7.227
89	C17	1.682	11.589	7.479
90	C18	1.947	13.026	7.94
91	C19	0.214	11.174	7.602
92	C20	0.027	9.663	7.413
93	C21	-1.466	9.252	7.36
94	C22	-1.83	9.929	12.462
95	C23	-0.319	10.274	12.504
96	C24	-0.014	11.673	11.948
97	C25	1.482	11.992	11.908
98	C26	2.164	12.131	13.271
99	C27	1.599	13.223	14.184
100	C28	1.622	14.614	13.549
101	C29	1.301	15.699	14.577
102	C30	1.258	17.082	13.924
103	C31	1.112	18.185	14.984
104	C32	1.318	19.648	14.501
105	C33	-0.293	4.498	13.402
106	C34	0.38	4.117	8.505
107	C35	0.715	2.74	9.103
108	C36	1.975	2.743	9.967
109	C37	1.492	3.673	15.031
110	C38	3.01	2.651	16.836
111	C39	2.131	1.386	10.662
112	C40	4.391	2.975	16.259
113	C41	5.427	1.978	16.789
114	C42	3.187	1.38	11.764
115	C43	5.601	1.359	12.408
116	C44	7.07	1.436	11.996
117	C45	4.621	1.467	11.241
118	C46	1.926	3.676	16.501
119	C47	0.175	4.439	14.864

120	C48	6.852	2.183	16.266
121	C49	7.434	3.568	16.582
122	C50	9.257	8.686	16.088
123	C51	8.991	3.598	16.599
124	C52	9.043	2.995	11.515
125	C53	9.026	8.089	10.994
126	C54	7.479	8.238	11.05
127	C55	6.956	9.647	11.393
128	C56	7.5	10.763	10.498
129	C57	7.033	12.147	10.965
130	C58	6.388	18.807	14.238
131	C59	7.5	2.844	11.554
132	C60	-1.587	20.621	12.19
133	O1	11.71	9.343	10.977
134	O2	11.845	9.794	15.662
135	O3	11.547	2.33	16.596
136	O4	10.595	8.691	18.613
137	O5	10.314	3.963	19.111
138	O6	11.716	1.8	11.911
139	O7	11.11	2.973	9.586
140	O8	11.048	7.712	9.037
141	O9	-4.272	9.69	7.305
142	O10	-4.606	10.283	12.023
143	O11	-4.527	4.118	12.82
144	O12	-4.001	3.441	8.177
145	O13	-2.881	5.448	15.835
146	O14	-2.819	10.161	15.124
147	O15	-1.393	20.521	14.567
148	O16	-1.774	20.635	9.81
149	O17	1.972	22.407	14.647
150	O18	1.698	22.389	8.833
151	O19	6.319	21.239	8.523
152	O20	8.701	19.031	9.024
153	O21	9.217	19.39	13.713
154	O22	6.633	21.749	14.416
155	O23	-2.437	8.572	4.756
156	O24	-2.479	3.902	5.741
157	C61	-1.801	4.864	13.259
158	C62	7.746	13.277	10.21
159	C63	5.403	17.019	9.105
160	C64	6.031	14.577	8.825
161	C65	6.553	16.013	8.969
162	C66	7.168	13.548	8.815
163	H1	5.429	16.851	13.938
164	H2	7.119	16.782	14.389
165	H3	4.729	17.22	16.211
166	H4	6.324	17.778	16.706
167	H5	5.891	15.552	17.592
168	H6	7.265	15.541	16.496
169	H7	5.765	14.619	14.671
170	H8	4.43	14.587	15.824
171	H9	5.723	13.019	17.278
172	H10	7.099	13.13	16.178
173	H11	5.707	12.142	14.337
174	H12	4.33	12.064	15.432
175	H13	5.312	9.876	15.266
176	H14	5.541	10.477	16.906
177	H15	7.903	11.06	16.381
178	H16	7.668	10.574	14.703
179	H17	7.183	8.216	15.49
180	H18	7.359	8.755	17.146
181	H19	6.467	18.653	8.266
182	H20	-0.511	18.064	9.175

183	H21	1.093	17.556	9.638
184	H22	0.334	20.346	8.675
185	H23	1.877	18.164	7.255
186	H24	0.226	18.646	6.898
187	H25	0.56	16.454	6.01
188	H26	-0.549	16.305	7.369
189	H27	1.329	15.507	8.82
190	H28	2.467	15.729	7.488
191	H29	1.263	14.02	6.145
192	H30	0.032	13.884	7.404
193	H31	2.306	10.919	8.083
194	H32	2.006	11.472	6.438
195	H33	3.009	13.25	7.788
196	H34	1.765	13.09	9.018
197	H35	-0.376	11.704	6.845
198	H36	-0.167	11.48	8.581
199	H37	0.557	9.122	8.204
200	H38	0.51	9.373	6.47
201	H39	-1.899	9.922	6.605
202	H40	-2.322	10.803	12.91
203	H41	0.269	9.518	11.972
204	H42	0.021	10.241	13.548
205	H43	-0.549	12.43	12.532
206	H44	-0.395	11.758	10.926
207	H45	1.625	12.92	11.344
208	H46	1.999	11.212	11.334
209	H47	3.227	12.338	13.095
210	H48	2.126	11.178	13.807
211	H49	2.195	13.235	15.105
212	H50	0.576	12.97	14.487
213	H51	0.894	14.663	12.731
214	H52	2.612	14.807	13.117
215	H53	2.064	15.684	15.364
216	H54	0.336	15.489	15.056
217	H55	0.408	17.118	13.232
218	H56	2.158	17.225	13.32
219	H57	1.787	17.988	15.827
220	H58	0.095	18.099	15.393
221	H59	0.881	20.241	15.32
222	H60	-0.126	3.513	12.946
223	H61	0.341	5.211	12.86
224	H62	0.729	4.93	9.152
225	H63	0.943	4.226	7.568
226	H64	0.827	2.014	8.288
227	H65	-0.119	2.378	9.716
228	H66	1.9	3.534	10.722
229	H67	2.851	2.957	9.346
230	H68	1.353	2.64	14.689
231	H69	2.272	4.119	14.406
232	H70	3.091	2.6	17.93
233	H71	2.693	1.656	16.502
234	H72	2.355	0.611	9.92
235	H73	1.175	1.111	11.126
236	H74	4.673	3.994	16.546
237	H75	4.36	2.936	15.165
238	H76	5.111	0.96	16.527
239	H77	5.446	2.024	17.885
240	H78	3.075	0.449	12.334
241	H79	2.994	2.201	12.465
242	H80	5.44	0.4	12.917
243	H81	5.389	2.143	13.144
244	H82	7.275	0.717	11.194
245	H83	7.664	1.114	12.859

246	H84	4.807	0.655	10.529
247	H85	4.768	2.408	10.705
248	H86	2.258	4.682	16.786
249	H87	1.055	3.446	17.128
250	H88	0.29	5.458	15.253
251	H89	-0.59	3.942	15.473
252	H90	6.866	2.011	15.185
253	H91	7.484	1.406	16.715
254	H92	7.079	3.879	17.574
255	H93	7.028	4.302	15.875
256	H94	9.662	9.534	16.655
257	H95	9.25	2.839	17.349
258	H96	9.348	2.128	10.914
259	H97	9.303	8.786	10.196
260	H98	7.046	7.538	11.773
261	H99	7.068	7.95	10.073
262	H0	7.185	9.876	12.439
263	H1	5.862	9.636	11.321
264	H2	7.191	10.585	9.462
265	H3	8.594	10.758	10.516
266	H4	7.269	12.254	12.031
267	H5	5.945	12.239	10.869
268	H6	7.114	19.171	14.976
269	H7	7.098	3.028	10.549
270	H8	7.045	3.594	12.207
271	H9	-2.618	20.943	12.28
272	H10	11.356	8.751	10.278
273	H11	12.714	10.131	15.394
274	H12	12.417	1.921	16.463
275	H13	11.112	8.564	19.425
276	H14	10.861	4.191	19.879
277	H15	11.403	2.231	11.087
278	H16	11.667	3.059	8.79
279	H17	11.573	7.459	8.255
280	H18	-5.231	9.796	7.406
281	H19	-5.542	10.33	11.77
282	H20	-5.424	3.87	12.542
283	H21	-3.402	3.578	7.418
284	H22	-3.313	5.76	16.646
285	H23	-3.241	10.115	15.997
286	H24	-2.291	20.876	14.468
287	H25	-2.646	20.973	10.069
288	H26	2.311	23.316	14.638
289	H27	2.089	23.263	8.677
290	H28	6.361	22.196	8.372
291	H29	9.624	19.324	9.098
292	H30	9.084	18.678	14.362
293	H31	7.301	21.132	14.073
294	H32	-2.893	8.23	3.97
295	H33	-2.763	3.883	4.809
296	H34	-2.316	4.158	13.925
297	H35	4.738	16.902	8.239
298	H36	5.32	14.345	9.626
299	H37	5.481	14.5	7.879
300	H38	7.162	16.267	8.093
301	H39	7.206	16.082	9.845
302	H40	7.707	14.183	10.823
303	H41	8.81	13.026	10.11
304	H42	6.805	12.616	8.368
305	H43	7.97	13.913	8.161
306	H3	8.237	5.604	11.913
307	H6	11.83	5.261	8.495
308	H20	9.997	19.454	11.29

309	H23	5.173	18.428	11.817
310	H36	8.719	6.067	15.411
311	H39	10.994	6.395	19.809
312	H43	12.721	9.991	13.182
313	H46	8.281	7.845	13.632
314	H50	12.575	1.607	14.275
315	H53	8.183	3.869	13.98
316	H64	-1.364	3.296	7.689
317	H66	-0.783	6.923	8.657
318	H69	-2.868	6.033	4.234
319	H83	3.159	18.173	9.62
320	H86	4.257	22.862	8.463
321	H93	2.082	19.404	11.871
322	H97	4.52	23.099	14.592
323	CH00	3.707	18.229	14.308
324	CH12	-0.653	9.314	10.016
325	CH15	-5.524	10.119	9.569
326	CH18	-1.404	7.256	11.933
327	CH21	-3.264	7.959	16.482
328	CH26	-5.266	3.507	10.355
329	CH29	-0.559	4.954	10.813
330	H1	4.817	16.753	9.994
331	C1	4.832	5.2	8.553
332	C2	4.521	5.611	7.257
333	C3	3.765	6.761	7.058
334	C4	3.32	7.501	8.154
335	C5	3.614	7.095	9.466
336	C6	3.165	7.822	10.583
337	C7	3.478	7.416	11.892
338	C8	3.041	8.14	13.012
339	C9	3.372	7.732	14.305
340	C10	4.152	6.597	14.497
341	C11	4.589	5.86	13.396
342	C12	4.256	6.257	12.09
343	C13	4.691	5.529	10.974
344	C14	4.384	5.931	9.665
345	H1	5.428	4.3	8.689
346	H2	4.871	5.034	6.405
347	H3	3.525	7.088	6.049
348	H4	2.744	8.403	7.973
349	H5	2.439	9.034	12.885
350	H6	3.023	8.306	15.16
351	H7	4.414	6.283	15.503
352	H8	5.189	4.97	13.567
353	H9	5.287	4.635	11.125
354	H10	2.57	8.72	10.43

Table S4. Cartesian coordinates of the structure of (phenanthrene)⊂**1** optimized by MacroModel Ver 9.1 using the MMFFs force field.

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	C1	10.589	4.132	10.128
2	C2	9.534	4.219	11.05
3	C02B	0.561	20.2	13.361
4	C3	9.021	5.495	11.355
5	C4	9.543	6.658	10.758
6	C5	10.589	6.509	9.831
7	C6	11.107	5.26	9.5
8	C18	6.74	18.737	10.47
9	C19	8.079	19.135	10.338
10	C20	8.838	19.506	11.448
11	C21	8.263	19.446	12.714
12	C22	6.964	18.963	12.903
13	C23	6.206	18.631	11.766
14	C35	9.479	7.425	17.06
15	C36	9.116	6.148	16.587
16	C37	9.343	4.982	17.348
17	C38	9.964	5.121	18.598
18	C39	10.353	6.369	19.08
19	C40	10.1	7.507	18.317
20	C41	9.841	8.771	14.907
21	C42	11.111	9.357	14.793
22	C43	11.727	9.514	13.555
23	C44	11.079	9.088	12.399
24	C45	9.808	8.493	12.452
25	C46	9.227	8.309	13.725
26	C48	9.609	3.151	15.591
27	C49	10.851	2.506	15.684
28	C50	11.523	2.051	14.551
29	C51	10.952	2.222	13.293
30	C52	9.703	2.842	13.142
31	C53	9.072	3.34	14.305
32	C64	-1.172	4.301	8.418
33	C65	-1.484	5.445	7.459
34	C66	-1.274	6.784	7.831
35	C67	-1.645	7.846	6.982
36	C68	-2.146	7.537	5.708
37	C69	-2.366	6.218	5.318
38	C70	-2.068	5.191	6.21
39	C82	2.371	20.197	9.302
40	C83	3.398	19.238	9.437
41	C84	4.742	19.529	9.134
42	C85	5.043	20.84	8.729
43	C86	4.059	21.825	8.641
44	C87	2.735	21.497	8.926
45	C88	0.353	20.193	10.907
46	C89	-0.955	20.686	11.049
47	C91	-0.752	20.686	13.446
48	C93	1.098	19.96	12.078
49	C95	2.815	20.326	14.61
50	C96	3.135	21.683	14.766
51	C97	4.459	22.12	14.797
52	C98	5.495	21.199	14.664
53	C99	5.232	19.83	14.498
54	C100	3.884	19.423	14.467
55	C111	-2.594	9.885	11.157
56	C112	-1.822	9.607	10.01

57	C113	-2.393	9.535	8.724
58	C114	-3.787	9.677	8.622
59	C115	-4.583	9.903	9.743
60	C116	-3.983	10.013	10.994
61	C117	-2.183	8.877	13.478
62	C118	-1.899	7.56	13.064
63	C119	-2.134	6.453	13.905
64	C120	-2.631	6.702	15.195
65	C121	-2.882	7.998	15.642
66	C122	-2.653	9.071	14.786
67	C124	-2.424	4.699	12.059
68	C125	-3.767	4.329	11.905
69	C126	-4.279	3.966	10.66
70	C127	-3.448	3.959	9.54
71	C128	-2.1	4.337	9.636
72	C129	-1.623	4.735	10.903
73	C1	6.093	17.327	14.599
74	C2	5.709	17.044	16.058
75	C3	6.079	15.628	16.513
76	C4	5.433	14.509	15.691
77	C5	5.896	13.14	16.197
78	C6	5.344	11.995	15.346
79	C7	5.747	10.607	15.858
80	C8	7.256	10.361	15.818
81	C9	7.612	8.928	16.246
82	C10	5.858	18.474	9.249
83	C11	0.507	18.384	9.162
84	C12	0.894	19.846	9.518
85	C13	0.705	18.071	7.671
86	C14	0.31	16.642	7.292
87	C15	1.276	15.588	7.839
88	C16	0.9	14.19	7.341
89	C17	1.533	11.706	7.432
90	C18	1.829	13.126	7.925
91	C19	0.095	11.254	7.702
92	C20	-0.074	9.743	7.494
93	C21	-1.556	9.297	7.459
94	C22	-1.974	10.075	12.548
95	C23	-0.487	10.509	12.586
96	C24	-0.273	11.921	12.02
97	C25	1.203	12.302	11.884
98	C26	1.984	12.391	13.197
99	C27	1.481	13.447	14.187
100	C28	1.471	14.857	13.595
101	C29	1.223	15.92	14.665
102	C30	1.176	17.315	14.035
103	C31	1.092	18.412	15.106
104	C32	1.35	19.871	14.628
105	C33	-0.346	4.64	13.602
106	C34	0.349	4.183	8.716
107	C35	0.672	2.815	9.344
108	C36	1.946	2.815	10.188
109	C37	1.417	3.78	15.243
110	C38	2.889	2.708	17.062
111	C39	2.086	1.47	10.909
112	C40	4.273	2.993	16.474
113	C41	5.304	2.007	17.036
114	C42	3.155	1.462	11.999
115	C43	5.573	1.372	12.618
116	C44	7.04	1.429	12.197
117	C45	4.585	1.526	11.462
118	C46	1.827	3.755	16.719
119	C47	0.106	4.56	15.068

120	C48	6.734	2.196	16.516
121	C49	7.32	3.583	16.814
122	C50	9.149	8.692	16.27
123	C51	8.876	3.61	16.853
124	C52	9.04	2.967	11.769
125	C53	9.08	8.055	11.179
126	C54	7.534	8.219	11.185
127	C55	7.015	9.635	11.504
128	C56	7.563	10.739	10.596
129	C57	7.102	12.128	11.056
130	C58	6.365	18.828	14.304
131	C59	7.495	2.834	11.772
132	C60	-1.507	20.942	12.304
133	O1	11.766	9.302	11.235
134	O2	11.75	9.799	15.919
135	O3	11.413	2.31	16.916
136	O4	10.435	8.735	18.822
137	O5	10.16	4.014	19.378
138	O6	11.686	1.74	12.243
139	O7	11.165	2.906	9.904
140	O8	11.163	7.638	9.298
141	O9	-4.375	9.601	7.388
142	O10	-4.76	10.269	12.092
143	O11	-4.584	4.308	13.002
144	O12	-4.039	3.548	8.374
145	O13	-2.858	5.649	16.04
146	O14	-2.875	10.347	15.232
147	O15	-1.308	20.887	14.681
148	O16	-1.713	20.891	9.927
149	O17	2.124	22.595	14.905
150	O18	1.764	22.456	8.82
151	O19	6.333	21.159	8.403
152	O20	8.646	19.164	9.093
153	O21	8.947	19.916	13.805
154	O22	6.759	21.728	14.707
155	O23	-2.436	8.553	4.839
156	O24	-2.416	3.901	5.903
157	C61	-1.85	5.022	13.446
158	C62	7.776	13.251	10.256
159	C63	5.361	17	9.207
160	C64	5.981	14.548	8.966
161	C65	6.507	15.985	9.087
162	C66	7.118	13.52	8.898
163	H1	5.322	16.919	13.933
164	H2	7.013	16.772	14.367
165	H3	4.634	17.2	16.201
166	H4	6.221	17.75	16.723
167	H5	5.789	15.516	17.565
168	H6	7.171	15.522	16.478
169	H7	5.703	14.61	14.634
170	H8	4.341	14.584	15.758
171	H9	5.581	13.008	17.24
172	H10	6.991	13.116	16.184
173	H11	5.676	12.111	14.307
174	H12	4.249	12.052	15.336
175	H13	5.245	9.856	15.239
176	H14	5.377	10.474	16.882
177	H15	7.763	11.061	16.492
178	H16	7.628	10.56	14.808
179	H17	7.1	8.204	15.603
180	H18	7.212	8.768	17.257
181	H19	6.455	18.589	8.334
182	H20	-0.554	18.222	9.398

183	H21	1.057	17.675	9.791
184	H22	0.35	20.464	8.79
185	H23	1.742	18.245	7.365
186	H24	0.086	18.762	7.085
187	H25	0.291	16.571	6.198
188	H26	-0.709	16.433	7.64
189	H27	1.26	15.596	8.935
190	H28	2.299	15.825	7.526
191	H29	0.949	14.161	6.246
192	H30	-0.137	13.982	7.627
193	H31	2.235	11.024	7.925
194	H32	1.736	11.643	6.356
195	H33	2.868	13.37	7.672
196	H34	1.761	13.145	9.018
197	H35	-0.583	11.79	7.028
198	H36	-0.184	11.523	8.725
199	H37	0.479	9.2	8.267
200	H38	0.395	9.472	6.538
201	H39	-2.01	9.943	6.695
202	H40	-2.519	10.93	12.971
203	H41	0.142	9.783	12.059
204	H42	-0.141	10.504	13.628
205	H43	-0.796	12.652	12.648
206	H44	-0.725	12	11.027
207	H45	1.268	13.261	11.358
208	H46	1.697	11.575	11.23
209	H47	3.032	12.612	12.954
210	H48	1.991	11.416	13.697
211	H49	2.134	13.426	15.067
212	H50	0.477	13.187	14.542
213	H51	0.694	14.933	12.827
214	H52	2.433	15.056	13.106
215	H53	2.025	15.876	15.411
216	H54	0.279	15.718	15.186
217	H55	0.299	17.374	13.378
218	H56	2.053	17.448	13.397
219	H57	1.771	18.181	15.938
220	H58	0.079	18.365	15.531
221	H59	0.925	20.473	15.446
222	H60	-0.184	3.657	13.139
223	H61	0.299	5.352	13.072
224	H62	0.7	5.006	9.348
225	H63	0.917	4.268	7.78
226	H64	0.758	2.067	8.546
227	H65	-0.158	2.484	9.979
228	H66	1.898	3.624	10.926
229	H67	2.816	2.996	9.549
230	H68	1.276	2.755	14.88
231	H69	2.208	4.234	14.638
232	H70	2.972	2.667	18.156
233	H71	2.547	1.717	16.739
234	H72	2.286	0.676	10.18
235	H73	1.131	1.22	11.389
236	H74	4.566	4.02	16.717
237	H75	4.236	2.905	15.383
238	H76	4.986	0.984	16.798
239	H77	5.317	2.081	18.131
240	H78	3.035	0.539	12.58
241	H79	2.98	2.293	12.694
242	H80	5.397	0.405	13.106
243	H81	5.382	2.142	13.374
244	H82	7.228	0.718	11.383
245	H83	7.633	1.083	13.051

246	H84	4.746	0.724	10.733
247	H85	4.748	2.474	10.943
248	H86	2.174	4.751	17.021
249	H87	0.943	3.535	17.331
250	H88	0.225	5.572	15.472
251	H89	-0.668	4.06	15.662
252	H90	6.755	2.007	15.438
253	H91	7.359	1.424	16.982
254	H92	6.953	3.914	17.796
255	H93	6.928	4.306	16.089
256	H94	9.528	9.55	16.839
257	H95	9.122	2.863	17.619
258	H96	9.35	2.092	11.182
259	H97	9.388	8.742	10.383
260	H98	7.073	7.528	11.9
261	H99	7.149	7.926	10.199
262	H0	7.236	9.879	12.547
263	H1	5.922	9.626	11.424
264	H2	7.249	10.553	9.563
265	H3	8.658	10.728	10.61
266	H4	7.377	12.253	12.111
267	H5	6.011	12.209	10.999
268	H6	7.126	19.098	15.049
269	H7	7.111	3.035	10.764
270	H8	7.042	3.584	12.425
271	H9	-2.523	21.311	12.39
272	H10	11.437	8.698	10.534
273	H11	12.626	10.139	15.675
274	H12	12.282	1.892	16.807
275	H13	10.938	8.62	19.643
276	H14	10.692	4.254	20.153
277	H15	11.401	2.171	11.408
278	H16	11.746	2.978	9.124
279	H17	11.713	7.371	8.538
280	H18	-5.339	9.656	7.485
281	H19	-5.696	10.257	11.836
282	H20	-5.482	4.068	12.724
283	H21	-3.427	3.65	7.621
284	H22	-3.269	5.973	16.857
285	H23	-3.263	10.313	16.121
286	H24	-2.188	21.281	14.576
287	H25	-2.565	21.279	10.181
288	H26	2.506	23.486	14.956
289	H27	2.175	23.31	8.614
290	H28	6.391	22.104	8.192
291	H29	9.532	19.556	9.15
292	H30	9.867	20.093	13.543
293	H31	7.425	21.058	14.459
294	H32	-2.857	8.19	4.045
295	H33	-2.676	3.861	4.965
296	H34	-2.378	4.331	14.117
297	H35	4.693	16.873	8.345
298	H36	5.31	14.315	9.801
299	H37	5.386	14.471	8.048
300	H38	7.115	16.223	8.206
301	H39	7.161	16.068	9.96
302	H40	7.778	14.161	10.866
303	H41	8.831	12.994	10.095
304	H42	6.73	12.586	8.476
305	H43	7.88	13.882	8.197
306	H3	8.243	5.588	12.108
307	H6	11.941	5.174	8.812
308	H20	9.856	19.857	11.322

309	H23	5.174	18.311	11.891
310	H36	8.624	6.062	15.621
311	H39	10.82	6.457	20.055
312	H43	12.707	9.973	13.466
313	H46	8.257	7.825	13.792
314	H50	12.485	1.555	14.626
315	H53	8.128	3.866	14.213
316	H64	-1.397	3.351	7.915
317	H66	-0.865	7.004	8.815
318	H69	-2.798	5.997	4.349
319	H83	3.137	18.238	9.769
320	H86	4.318	22.832	8.334
321	H93	2.106	19.561	11.996
322	H97	4.704	23.17	14.925
323	CH00	3.67	18.37	14.333
324	CH12	-0.751	9.467	10.115
325	CH15	-5.657	10.012	9.639
326	CH18	-1.506	7.395	12.063
327	CH21	-3.247	8.168	16.649
328	CH26	-5.317	3.669	10.543
329	CH29	-0.592	5.059	11.007
330	H1	4.773	16.756	10.1
331	C1	2.849	8.678	10.278
332	C2	2.959	8.675	11.665
333	C3	4.845	5.561	13.729
334	C4	4.323	6.636	14.429
335	C5	3.685	7.657	13.734
336	C6	3.579	7.621	12.333
337	C7	4.105	6.534	11.592
338	C8	4.724	5.507	12.339
339	C9	4.371	5.553	7.925
340	C10	4.503	5.511	9.316
341	C11	3.997	6.535	10.156
342	C12	3.358	7.625	9.515
343	C13	3.237	7.658	8.114
344	C14	3.736	6.627	7.324
345	H1	5.341	4.753	14.258
346	H2	4.404	6.678	15.512
347	H3	3.274	8.492	14.297
348	H4	4.769	4.744	7.317
349	H5	2.754	8.498	7.621
350	H6	3.631	6.668	6.243
351	H7	2.365	9.526	9.801
352	H8	2.561	9.518	12.224
353	H9	5.134	4.636	11.841
354	H10	5.017	4.649	9.731

Table S5. Cartesian coordinates of the structure of (pyrene)⊂**1** optimized by MacroModel Ver 9.1 using the MMFFs force field.

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	C1	11.233	4.448	10.293
2	C2	10.101	4.611	11.107
3	C02B	0.601	19.968	13.166
4	C3	9.73	5.922	11.46
5	C4	10.452	7.044	11.007
6	C5	11.582	6.82	10.207
7	C6	11.969	5.537	9.83
8	C18	7.025	18.935	10.558
9	C19	8.33	19.449	10.525
10	C20	8.98	19.852	11.692
11	C21	8.33	19.707	12.915
12	C22	7.067	19.111	13.006
13	C23	6.418	18.748	11.813
14	C35	9.46	7.419	17.268
15	C36	9.12	6.186	16.674
16	C37	9.177	4.975	17.393
17	C38	9.611	5.022	18.727
18	C39	9.976	6.224	19.331
19	C40	9.886	7.41	18.605
20	C41	10.234	8.85	15.296
21	C42	11.554	9.296	15.451
22	C43	12.404	9.447	14.356
23	C44	11.94	9.163	13.074
24	C45	10.624	8.731	12.858
25	C46	9.804	8.541	13.992
26	C48	9.543	3.239	15.549
27	C49	10.728	2.508	15.715
28	C50	11.476	2.077	14.622
29	C51	11.048	2.37	13.33
30	C52	9.87	3.098	13.101
31	C53	9.151	3.55	14.233
32	C64	-1.758	4.218	8.6
33	C65	-2.223	5.362	7.702
34	C66	-2.041	6.698	8.092
35	C67	-2.474	7.769	7.287
36	C68	-3.063	7.47	6.051
37	C69	-3.291	6.151	5.659
38	C70	-2.894	5.114	6.5
39	C82	2.618	20.016	9.195
40	C83	3.721	19.151	9.363
41	C84	5.044	19.571	9.119
42	C85	5.241	20.91	8.74
43	C86	4.176	21.801	8.615
44	C87	2.879	21.349	8.842
45	C88	0.534	19.901	10.706
46	C89	-0.799	20.341	10.762
47	C91	-0.733	20.401	13.165
48	C93	1.22	19.721	11.922
49	C95	2.768	20.227	14.539
50	C96	3.02	21.59	14.766
51	C97	4.319	22.08	14.883
52	C98	5.399	21.209	14.766
53	C99	5.205	19.84	14.521
54	C100	3.879	19.379	14.396
55	C111	-3.37	9.726	11.488
56	C112	-2.593	9.492	10.333

57	C113	-3.154	9.461	9.041
58	C114	-4.545	9.631	8.937
59	C115	-5.347	9.82	10.061
60	C116	-4.757	9.867	11.322
61	C117	-2.916	8.616	13.767
62	C118	-2.623	7.316	13.297
63	C119	-2.734	6.179	14.13
64	C120	-3.153	6.382	15.456
65	C121	-3.439	7.654	15.947
66	C122	-3.309	8.757	15.107
67	C124	-2.977	4.418	12.266
68	C125	-4.27	3.9	12.135
69	C126	-4.758	3.485	10.895
70	C127	-3.952	3.58	9.76
71	C128	-2.657	4.114	9.834
72	C129	-2.21	4.558	11.095
73	C1	6.163	17.377	14.59
74	C2	5.685	17.031	16.007
75	C3	6.057	15.61	16.439
76	C4	5.548	14.511	15.502
77	C5	5.985	13.134	16.01
78	C6	5.636	12.023	15.019
79	C7	5.99	10.623	15.533
80	C8	7.489	10.423	15.782
81	C9	7.793	8.985	16.223
82	C10	6.252	18.629	9.275
83	C11	0.902	18.048	9.052
84	C12	1.169	19.546	9.358
85	C13	1.2	17.675	7.592
86	C14	0.681	16.287	7.206
87	C15	1.359	15.152	7.975
88	C16	0.841	13.787	7.513
89	C17	1.028	11.262	7.915
90	C18	1.475	12.664	8.331
91	C19	-0.482	11.024	8.041
92	C20	-0.801	9.537	7.851
93	C21	-2.316	9.212	7.778
94	C22	-2.756	9.865	12.886
95	C23	-1.28	10.334	12.935
96	C24	-1.055	11.754	12.399
97	C25	0.424	12.038	12.119
98	C26	1.336	12.086	13.348
99	C27	1.065	13.244	14.316
100	C28	1.211	14.619	13.659
101	C29	1.115	15.752	14.682
102	C30	1.202	17.118	13.993
103	C31	1.103	18.26	15.014
104	C32	1.327	19.708	14.484
105	C33	-0.872	4.435	13.734
106	C34	-0.226	4.314	8.862
107	C35	0.345	3.042	9.505
108	C36	1.681	3.294	10.214
109	C37	1.073	3.717	15.212
110	C38	2.744	2.678	16.868
111	C39	2.112	2.045	10.983
112	C40	4.094	3.075	16.255
113	C41	5.165	2.064	16.688
114	C42	3.277	2.278	11.943
115	C43	5.74	2.204	12.334
116	C44	7.167	2.091	11.796
117	C45	4.652	2.354	11.268
118	C46	1.604	3.675	16.648
119	C47	-0.314	4.379	15.162

120	C48	6.584	2.325	16.171
121	C49	7.168	3.681	16.59
122	C50	9.302	8.737	16.505
123	C51	8.715	3.656	16.767
124	C52	9.378	3.388	11.678
125	C53	10.092	8.465	11.451
126	C54	8.593	8.806	11.218
127	C55	8.208	10.274	11.473
128	C56	8.747	11.25	10.424
129	C57	8.45	12.704	10.818
130	C58	6.39	18.896	14.36
131	C59	7.832	3.449	11.515
132	C60	-1.432	20.6	11.976
133	O1	12.849	9.339	12.066
134	O2	12.015	9.6	16.703
135	O3	11.153	2.2	16.979
136	O4	10.186	8.594	19.222
137	O5	9.643	3.869	19.464
138	O6	11.848	1.888	12.329
139	O7	11.667	3.174	10.021
140	O8	12.363	7.895	9.858
141	O9	-5.126	9.616	7.698
142	O10	-5.54	10.075	12.425
143	O11	-5.057	3.779	13.246
144	O12	-4.514	3.113	8.601
145	O13	-3.266	5.304	16.293
146	O14	-3.548	10.01	15.604
147	O15	-1.368	20.607	14.361
148	O16	-1.5	20.489	9.594
149	O17	1.964	22.452	14.89
150	O18	1.83	22.217	8.699
151	O19	6.51	21.35	8.477
152	O20	8.971	19.565	9.322
153	O21	8.895	20.206	14.059
154	O22	6.633	21.788	14.908
155	O23	-3.426	8.494	5.22
156	O24	-3.217	3.817	6.193
157	C61	-2.394	4.767	13.644
158	C62	8.987	13.709	9.792
159	C63	5.922	17.114	9.152
160	C64	6.841	14.766	8.812
161	C65	7.184	16.246	9.025
162	C66	8.083	13.897	8.568
163	H1	5.461	16.96	13.858
164	H2	7.121	16.868	14.411
165	H3	4.598	17.153	16.077
166	H4	6.127	17.726	16.732
167	H5	5.661	15.438	17.447
168	H6	7.149	15.542	16.517
169	H7	5.947	14.661	14.492
170	H8	4.455	14.555	15.432
171	H9	5.509	12.932	16.977
172	H10	7.068	13.151	16.177
173	H11	6.151	12.201	14.067
174	H12	4.56	12.052	14.807
175	H13	5.649	9.892	14.79
176	H14	5.432	10.422	16.456
177	H15	7.834	11.106	16.566
178	H16	8.041	10.671	14.871
179	H17	7.408	8.281	15.478
180	H18	7.223	8.788	17.142
181	H19	6.889	18.84	8.406
182	H20	-0.157	17.829	9.246

183	H21	1.468	17.407	9.738
184	H22	0.615	20.089	8.579
185	H23	2.276	17.724	7.393
186	H24	0.723	18.407	6.929
187	H25	0.849	16.143	6.131
188	H26	-0.403	16.246	7.364
189	H27	1.167	15.26	9.048
190	H28	2.445	15.205	7.831
191	H29	1.067	13.644	6.449
192	H30	-0.248	13.765	7.623
193	H31	1.562	10.539	8.544
194	H32	1.341	11.072	6.881
195	H33	2.566	12.719	8.238
196	H34	1.246	12.813	9.391
197	H35	-1.014	11.61	7.283
198	H36	-0.828	11.364	9.022
199	H37	-0.312	8.961	8.644
200	H38	-0.331	9.211	6.912
201	H39	-2.711	9.896	7.016
202	H40	-3.319	10.685	13.352
203	H41	-0.65	9.636	12.382
204	H42	-0.925	10.305	13.973
205	H43	-1.466	12.487	13.102
206	H44	-1.599	11.894	11.459
207	H45	0.499	12.982	11.569
208	H46	0.807	11.267	11.438
209	H47	2.373	12.163	12.999
210	H48	1.273	11.14	13.898
211	H49	1.778	13.164	15.147
212	H50	0.065	13.144	14.753
213	H51	0.426	14.756	12.907
214	H52	2.175	14.68	13.14
215	H53	1.926	15.655	15.415
216	H54	0.168	15.676	15.231
217	H55	0.379	17.197	13.273
218	H56	2.132	17.174	13.421
219	H57	1.781	18.071	15.856
220	H58	0.089	18.215	15.437
221	H59	0.828	20.317	15.253
222	H60	-0.704	3.454	13.269
223	H61	-0.283	5.155	13.159
224	H62	0.007	5.188	9.478
225	H63	0.299	4.477	7.911
226	H64	0.472	2.272	8.735
227	H65	-0.363	2.633	10.234
228	H66	1.565	4.126	10.918
229	H67	2.449	3.58	9.487
230	H68	0.994	2.697	14.817
231	H69	1.776	4.258	14.569
232	H70	2.876	2.568	17.952
233	H71	2.445	1.692	16.493
234	H72	2.349	1.235	10.283
235	H73	1.262	1.697	11.585
236	H74	4.367	4.078	16.598
237	H75	4.022	3.103	15.163
238	H76	4.862	1.064	16.354
239	H77	5.2	2.025	17.784
240	H78	3.278	1.439	12.651
241	H79	3.105	3.183	12.539
242	H80	5.538	1.283	12.898
243	H81	5.667	3.027	13.055
244	H82	7.192	1.47	10.892
245	H83	7.745	1.545	12.55

246	H84	4.75	1.546	10.533
247	H85	4.764	3.303	10.734
248	H86	1.913	4.678	16.962
249	H87	0.785	3.381	17.317
250	H88	-0.254	5.391	15.578
251	H89	-0.998	3.803	15.796
252	H90	6.598	2.24	15.081
253	H91	7.218	1.514	16.551
254	H92	6.724	3.976	17.551
255	H93	6.859	4.446	15.868
256	H94	9.583	9.562	17.172
257	H95	8.869	2.857	17.504
258	H96	9.645	2.517	11.065
259	H97	10.606	9.162	10.781
260	H98	7.963	8.187	11.86
261	H99	8.318	8.544	10.187
262	H0	8.537	10.584	12.47
263	H1	7.113	10.342	11.478
264	H2	8.3	11.019	9.452
265	H3	9.831	11.134	10.318
266	H4	8.94	12.905	11.779
267	H5	7.376	12.844	10.978
268	H6	7.093	19.165	15.159
269	H7	7.578	3.753	10.491
270	H8	7.411	4.211	12.17
271	H9	-2.465	20.928	11.996
272	H10	12.576	8.831	11.272
273	H11	12.95	9.854	16.645
274	H12	12.001	1.731	16.924
275	H13	10.566	8.416	20.097
276	H14	10.055	4.046	20.324
277	H15	11.668	2.362	11.489
278	H16	12.328	3.221	9.305
279	H17	12.991	7.607	9.17
280	H18	-6.088	9.695	7.789
281	H19	-6.473	10.089	12.162
282	H20	-5.925	3.433	12.983
283	H21	-3.956	3.336	7.829
284	H22	-3.64	5.591	17.142
285	H23	-3.881	9.939	16.513
286	H24	-2.257	20.96	14.197
287	H25	-2.379	20.85	9.79
288	H26	2.304	23.355	15
289	H27	2.169	23.108	8.52
290	H28	6.491	22.299	8.279
291	H29	9.815	20.026	9.449
292	H30	9.816	20.459	13.866
293	H31	7.343	21.162	14.667
294	H32	-3.907	8.137	4.456
295	H33	-3.544	3.787	5.276
296	H34	-2.868	4.047	14.325
297	H35	5.3	16.955	8.261
298	H36	6.269	14.388	9.666
299	H37	6.189	14.68	7.934
300	H38	7.787	16.603	8.181
301	H39	7.793	16.355	9.928
302	H40	9.147	14.671	10.29
303	H41	9.976	13.38	9.452
304	H42	7.762	12.918	8.192
305	H43	8.675	14.353	7.765
306	H3	8.9	6.068	12.143
307	H6	12.864	5.384	9.237
308	H20	9.969	20.293	11.644

309	H23	5.411	18.339	11.86
310	H36	8.779	6.173	15.642
311	H39	10.294	6.24	20.367
312	H43	13.426	9.789	14.479
313	H46	8.795	8.169	13.849
314	H50	12.39	1.506	14.754
315	H53	8.25	4.137	14.093
316	H64	-1.866	3.267	8.061
317	H66	-1.579	6.912	9.053
318	H69	-3.791	5.937	4.72
319	H83	3.541	18.127	9.675
320	H86	4.354	22.831	8.327
321	H93	2.244	19.358	11.904
322	H97	4.511	23.132	15.069
323	CH00	3.712	18.329	14.191
324	CH12	-1.523	9.352	10.44
325	CH15	-6.419	9.945	9.954
326	CH18	-2.3	7.19	12.268
327	CH21	-3.744	7.786	16.98
328	CH26	-5.756	3.07	10.794
329	CH29	-1.222	4.998	11.182
330	H1	5.338	16.764	10.012
331	C1	1.071	7.505	11.77
332	C2	1.111	7.58	13.166
333	C3	4.691	6.859	15.234
334	C4	3.537	7.18	15.945
335	C5	2.347	7.428	15.265
336	C6	2.299	7.356	13.866
337	C7	3.468	7.044	13.142
338	C8	4.673	6.795	13.833
339	C9	4.558	6.621	9.599
340	C10	4.6	6.678	11
341	C11	3.43	6.98	11.725
342	C12	2.224	7.219	11.034
343	C13	2.208	7.159	9.632
344	C14	3.367	6.862	8.919
345	C15	5.823	6.493	13.097
346	C16	5.784	6.439	11.7
347	H1	5.606	6.662	15.787
348	H2	3.564	7.231	17.031
349	H3	1.453	7.668	15.837
350	H4	5.453	6.388	9.027
351	H5	1.29	7.338	9.08
352	H6	3.341	6.816	7.833
353	H7	6.763	6.3	13.607
354	H8	6.692	6.211	11.151
355	H9	0.126	7.673	11.261
356	H10	0.199	7.806	13.711

Table S6. Cartesian coordinates of the structure of (benz[*a*]anthracene)⊂**1** optimized by MacroModel Ver 9.1 using the MMFFs force field.

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	C1	10.542	4.443	10.118
2	C2	9.489	4.555	11.042
3	C02B	0.524	20.03	13.189
4	C3	9.097	5.843	11.448
5	C4	9.758	6.991	10.971
6	C5	10.808	6.819	10.054
7	C6	11.19	5.56	9.603
8	C18	6.798	18.973	10.352
9	C19	8.104	19.472	10.231
10	C20	8.825	19.895	11.348
11	C21	8.248	19.784	12.61
12	C22	6.988	19.202	12.788
13	C23	6.265	18.822	11.644
14	C35	9.117	7.254	17.38
15	C36	8.834	6.021	16.756
16	C37	8.882	4.804	17.468
17	C38	9.208	4.851	18.833
18	C39	9.493	6.055	19.472
19	C40	9.439	7.243	18.747
20	C41	9.881	8.633	15.355
21	C42	11.236	8.981	15.43
22	C43	12.012	9.123	14.282
23	C44	11.438	8.924	13.028
24	C45	10.087	8.57	12.894
25	C46	9.341	8.387	14.077
26	C48	9.335	3.178	15.533
27	C49	10.605	2.589	15.618
28	C50	11.322	2.241	14.476
29	C51	10.775	2.474	13.217
30	C52	9.514	3.074	13.07
31	C53	8.828	3.451	14.248
32	C64	-1.765	4.23	8.557
33	C65	-2.184	5.376	7.64
34	C66	-1.911	6.709	7.985
35	C67	-2.351	7.779	7.183
36	C68	-3.008	7.483	5.98
37	C69	-3.301	6.169	5.622
38	C70	-2.915	5.134	6.47
39	C82	2.347	20.108	9.13
40	C83	3.434	19.219	9.274
41	C84	4.76	19.603	8.987
42	C85	4.974	20.931	8.577
43	C86	3.926	21.845	8.474
44	C87	2.627	21.43	8.752
45	C88	0.331	20.003	10.735
46	C89	-1	20.433	10.869
47	C91	-0.811	20.451	13.266
48	C93	1.081	19.812	11.911
49	C95	2.753	20.284	14.463
50	C96	2.986	21.657	14.64
51	C97	4.279	22.175	14.694
52	C98	5.372	21.322	14.563
53	C99	5.196	19.942	14.376
54	C100	3.877	19.451	14.32
55	C111	-2.716	9.763	11.451
56	C112	-2.097	9.49	10.214

57	C113	-2.819	9.476	9.004
58	C114	-4.208	9.676	9.072
59	C115	-4.856	9.899	10.285
60	C116	-4.108	9.948	11.458
61	C117	-2.083	8.704	13.705
62	C118	-1.974	7.371	13.255
63	C119	-2.19	6.276	14.119
64	C120	-2.489	6.555	15.464
65	C121	-2.556	7.861	15.944
66	C122	-2.347	8.921	15.067
67	C124	-2.767	4.555	12.287
68	C125	-4.122	4.208	12.215
69	C126	-4.714	3.859	11.002
70	C127	-3.955	3.852	9.832
71	C128	-2.602	4.229	9.841
72	C129	-2.04	4.6	11.082
73	C1	6.219	17.5	14.472
74	C2	5.839	17.188	15.926
75	C3	6.246	15.779	16.372
76	C4	5.689	14.653	15.497
77	C5	6.083	13.283	16.059
78	C6	5.657	12.15	15.124
79	C7	5.887	10.753	15.706
80	C8	7.353	10.435	16.001
81	C9	7.529	8.97	16.434
82	C10	5.951	18.637	9.123
83	C11	0.578	18.193	9.004
84	C12	0.894	19.674	9.35
85	C13	0.769	17.885	7.51
86	C14	0.263	16.497	7.109
87	C15	1.105	15.359	7.685
88	C16	0.597	13.997	7.204
89	C17	1.038	11.468	7.316
90	C18	1.456	12.868	7.771
91	C19	-0.401	11.107	7.687
92	C20	-0.656	9.605	7.508
93	C21	-2.151	9.223	7.645
94	C22	-1.926	9.899	12.759
95	C23	-0.43	10.29	12.627
96	C24	-0.255	11.703	12.043
97	C25	1.205	12.084	11.795
98	C26	2.065	12.237	13.05
99	C27	1.615	13.316	14.038
100	C28	1.58	14.715	13.424
101	C29	1.343	15.785	14.49
102	C30	1.28	17.178	13.859
103	C31	1.143	18.267	14.933
104	C32	1.319	19.741	14.463
105	C33	-0.635	4.271	13.708
106	C34	-0.221	4.193	8.736
107	C35	0.242	2.854	9.33
108	C36	1.552	2.97	10.111
109	C37	1.099	3.134	15.203
110	C38	2.671	1.901	16.828
111	C39	1.855	1.643	10.81
112	C40	4.02	2.427	16.33
113	C41	5.157	1.5	16.767
114	C42	2.952	1.745	11.864
115	C43	5.378	1.81	12.422
116	C44	6.831	1.84	11.963
117	C45	4.36	1.898	11.287
118	C46	1.513	2.889	16.658
119	C47	-0.156	4.014	15.145

120	C48	6.549	1.909	16.27
121	C49	6.988	3.316	16.708
122	C50	9.021	8.58	16.622
123	C51	8.534	3.468	16.805
124	C52	8.897	3.302	11.684
125	C53	9.441	8.382	11.521
126	C54	7.934	8.739	11.412
127	C55	7.604	10.209	11.734
128	C56	8.124	11.198	10.686
129	C57	7.8	12.647	11.071
130	C58	6.393	19.017	14.184
131	C59	7.346	3.25	11.622
132	C60	-1.571	20.666	12.118
133	O1	12.282	9.109	11.965
134	O2	11.802	9.205	16.656
135	O3	11.143	2.335	16.85
136	O4	9.675	8.429	19.389
137	O5	9.218	3.691	19.56
138	O6	11.551	2.065	12.165
139	O7	11.001	3.189	9.797
140	O8	11.532	7.922	9.67
141	O9	-4.941	9.657	7.915
142	O10	-4.739	10.201	12.646
143	O11	-4.87	4.19	13.36
144	O12	-4.624	3.445	8.708
145	O13	-2.71	5.517	16.33
146	O14	-2.391	10.205	15.541
147	O15	-1.384	20.628	14.497
148	O16	-1.762	20.595	9.742
149	O17	1.918	22.503	14.778
150	O18	1.596	22.322	8.636
151	O19	6.242	21.337	8.26
152	O20	8.678	19.547	8.991
153	O21	8.886	20.3	13.708
154	O22	6.599	21.929	14.628
155	O23	-3.38	8.507	5.153
156	O24	-3.316	3.849	6.209
157	C61	-2.092	4.825	13.64
158	C62	8.429	13.658	10.104
159	C63	5.58	17.127	9.085
160	C64	6.434	14.738	8.884
161	C65	6.816	16.219	8.989
162	C66	7.664	13.825	8.785
163	H1	5.484	17.045	13.796
164	H2	7.176	17.007	14.25
165	H3	4.758	17.308	16.064
166	H4	6.324	17.903	16.601
167	H5	5.91	15.635	17.407
168	H6	7.341	15.715	16.388
169	H7	6.074	14.747	14.476
170	H8	4.597	14.73	15.443
171	H9	5.62	13.145	17.044
172	H10	7.169	13.253	16.202
173	H11	6.192	12.241	14.17
174	H12	4.59	12.252	14.897
175	H13	5.514	10.026	14.977
176	H14	5.29	10.63	16.617
177	H15	7.724	11.086	16.801
178	H16	7.95	10.651	15.11
179	H17	7.031	8.299	15.724
180	H18	6.999	8.836	17.387
181	H19	6.548	18.793	8.214
182	H20	-0.47	17.981	9.257

183	H21	1.174	17.512	9.622
184	H22	0.317	20.257	8.619
185	H23	1.823	17.982	7.227
186	H24	0.215	18.627	6.922
187	H25	0.279	16.431	6.013
188	H26	-0.783	16.382	7.416
189	H27	1.075	15.385	8.78
190	H28	2.152	15.489	7.386
191	H29	0.616	13.958	6.108
192	H30	-0.446	13.875	7.518
193	H31	1.721	10.744	7.774
194	H32	1.169	11.381	6.23
195	H33	2.497	13.031	7.469
196	H34	1.437	12.909	8.865
197	H35	-1.093	11.673	7.052
198	H36	-0.596	11.4	8.723
199	H37	-0.032	9.037	8.209
200	H38	-0.314	9.318	6.504
201	H39	-2.666	9.89	6.942
202	H40	-2.387	10.768	13.251
203	H41	0.12	9.554	12.03
204	H42	0.03	10.272	13.624
205	H43	-0.731	12.438	12.703
206	H44	-0.779	11.779	11.085
207	H45	1.231	13.019	11.225
208	H46	1.66	11.325	11.147
209	H47	3.093	12.455	12.735
210	H48	2.105	11.283	13.58
211	H49	2.312	13.311	14.885
212	H50	0.631	13.066	14.451
213	H51	0.785	14.773	12.672
214	H52	2.529	14.916	12.912
215	H53	2.156	15.75	15.226
216	H54	0.409	15.58	15.025
217	H55	0.419	17.217	13.182
218	H56	2.171	17.334	13.245
219	H57	1.833	18.068	15.763
220	H58	0.134	18.166	15.359
221	H59	0.851	20.311	15.279
222	H60	-0.594	3.316	13.167
223	H61	0.067	4.95	13.209
224	H62	0.13	5.036	9.341
225	H63	0.266	4.312	7.758
226	H64	0.355	2.121	8.521
227	H65	-0.525	2.449	10
228	H66	1.46	3.765	10.86
229	H67	2.371	3.246	9.437
230	H68	0.896	2.174	14.714
231	H69	1.911	3.613	14.651
232	H70	2.754	1.671	17.898
233	H71	2.431	0.958	16.322
234	H72	2.11	0.878	10.068
235	H73	0.948	1.294	11.32
236	H74	4.192	3.43	16.733
237	H75	4.006	2.502	15.238
238	H76	4.951	0.484	16.408
239	H77	5.178	1.445	17.863
240	H78	2.915	0.831	12.47
241	H79	2.738	2.578	12.545
242	H80	5.219	0.866	12.958
243	H81	5.2	2.612	13.148
244	H82	6.975	1.176	11.102
245	H83	7.427	1.41	12.776

246	H84	4.549	1.099	10.56
247	H85	4.456	2.85	10.757
248	H86	1.767	3.841	17.138
249	H87	0.65	2.486	17.204
250	H88	0.049	4.97	15.641
251	H89	-0.951	3.514	15.711
252	H90	6.576	1.839	15.179
253	H91	7.26	1.164	16.649
254	H92	6.563	3.524	17.699
255	H93	6.557	4.065	16.032
256	H94	9.422	9.373	17.266
257	H95	8.824	2.667	17.498
258	H96	9.184	2.435	11.073
259	H97	9.914	9.113	10.857
260	H98	7.332	8.098	12.066
261	H99	7.594	8.523	10.391
262	H0	7.998	10.48	12.719
263	H1	6.516	10.314	11.806
264	H2	7.688	10.958	9.711
265	H3	9.21	11.102	10.587
266	H4	8.207	12.838	12.072
267	H5	6.717	12.79	11.138
268	H6	7.13	19.33	14.935
269	H7	7.01	3.504	10.609
270	H8	6.897	3.998	12.283
271	H9	-2.604	20.986	12.198
272	H10	11.904	8.71	11.153
273	H11	12.747	9.393	16.539
274	H12	12.037	1.973	16.738
275	H13	9.97	8.252	20.297
276	H14	9.544	3.873	20.455
277	H15	11.233	2.46	11.326
278	H16	11.582	3.265	9.018
279	H17	12.081	7.677	8.902
280	H18	-5.883	9.748	8.127
281	H19	-5.698	10.231	12.504
282	H20	-5.787	3.963	13.135
283	H21	-4.064	3.539	7.913
284	H22	-2.971	5.868	17.196
285	H23	-2.653	10.194	16.476
286	H24	-2.282	20.98	14.386
287	H25	-2.634	20.942	9.99
288	H26	2.243	23.415	14.844
289	H27	1.95	23.202	8.431
290	H28	6.237	22.282	8.044
291	H29	9.529	20.007	9.056
292	H30	9.793	20.547	13.454
293	H31	7.308	21.308	14.37
294	H32	-3.895	8.153	4.411
295	H33	-3.677	3.814	5.305
296	H34	-2.657	4.2	14.344
297	H35	4.938	16.937	8.214
298	H36	5.808	14.446	9.734
299	H37	5.827	14.598	7.98
300	H38	7.409	16.504	8.112
301	H39	7.448	16.372	9.869
302	H40	8.517	14.623	10.613
303	H41	9.455	13.344	9.877
304	H42	7.352	12.844	8.409
305	H43	8.347	14.237	8.032
306	H3	8.315	5.951	12.196
307	H6	12.027	5.448	8.923
308	H20	9.814	20.323	11.231

309	H23	5.259	18.423	11.759
310	H36	8.56	6.011	15.705
311	H39	9.731	6.07	20.53
312	H43	13.06	9.399	14.34
313	H46	8.303	8.08	14
314	H50	12.3	1.775	14.544
315	H53	7.863	3.941	14.171
316	H64	-1.986	3.276	8.059
317	H66	-1.387	6.919	8.914
318	H69	-3.852	5.958	4.712
319	H83	3.239	18.204	9.606
320	H86	4.119	22.866	8.164
321	H93	2.107	19.462	11.836
322	H97	4.456	23.236	14.837
323	CH00	3.729	18.389	14.168
324	CH12	-1.027	9.308	10.187
325	CH15	-5.929	10.053	10.312
326	CH18	-1.739	7.19	12.209
327	CH21	-2.765	8.05	16.991
328	CH26	-5.759	3.57	10.949
329	CH29	-1	4.908	11.13
330	H1	5.001	16.839	9.971
331	C1	5.187	6.963	8.48
332	C2	4.98	6.2	9.624
333	C3	4.665	11.124	8.475
334	C4	5.086	10.477	7.325
335	C5	5.241	9.094	7.335
336	C6	4.983	8.345	8.496
337	C7	4.536	8.981	9.683
338	C8	4.384	10.389	9.629
339	C9	3.974	6.544	13.181
340	C10	3.668	7.912	13.248
341	C11	3.836	8.706	12.098
342	C12	4.297	8.186	10.861
343	C13	4.55	6.794	10.813
344	C14	4.391	6	11.96
345	C15	3.218	8.45	14.467
346	C16	3.098	7.654	15.605
347	C17	3.861	5.755	14.335
348	C18	3.428	6.307	15.54
349	H1	4.552	12.205	8.482
350	H2	5.3	11.045	6.424
351	H3	5.581	8.603	6.426
352	H4	4.064	10.953	10.501
353	H5	3.61	9.765	12.187
354	H6	4.605	4.935	11.907
355	H7	5.169	5.13	9.574
356	H8	5.528	6.464	7.575
357	H9	2.97	9.504	14.548
358	H10	3.345	5.687	16.427
359	H11	4.112	4.698	14.3
360	H12	2.755	8.088	16.54

Table S7. Cartesian coordinates of the structure of (biphenyl)⊂**1** optimized by MacroModel Ver 9.1 using the MMFFs force field.

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	C1	10.049	4.276	10.032
2	C2	9.051	4.393	11.013
3	C02B	0.389	19.951	13.205
4	C3	8.621	5.683	11.375
5	C4	9.176	6.831	10.782
6	C5	10.163	6.655	9.797
7	C6	10.593	5.391	9.404
8	C18	6.787	18.989	10.603
9	C19	8.099	19.481	10.528
10	C20	8.782	19.9	11.669
11	C21	8.159	19.795	12.91
12	C22	6.889	19.223	13.044
13	C23	6.207	18.839	11.875
14	C35	9.347	7.465	17.129
15	C36	8.931	6.214	16.629
16	C37	9.118	5.024	17.362
17	C38	9.747	5.111	18.614
18	C39	10.184	6.333	19.122
19	C40	9.974	7.496	18.384
20	C41	9.719	8.82	14.984
21	C42	11.026	9.308	14.848
22	C43	11.623	9.441	13.597
23	C44	10.916	9.089	12.451
24	C45	9.604	8.592	12.526
25	C46	9.041	8.43	13.81
26	C48	9.28	3.249	15.536
27	C49	10.517	2.589	15.565
28	C50	11.134	2.148	14.396
29	C51	10.513	2.348	13.167
30	C52	9.268	2.99	13.081
31	C53	8.694	3.474	14.277
32	C64	-1.767	4.273	8.58
33	C65	-2.073	5.438	7.644
34	C66	-1.73	6.756	7.991
35	C67	-2.051	7.841	7.153
36	C68	-2.66	7.57	5.919
37	C69	-3.029	6.274	5.562
38	C70	-2.762	5.229	6.443
39	C82	2.368	20.095	9.234
40	C83	3.464	19.229	9.424
41	C84	4.792	19.631	9.183
42	C85	5.001	20.963	8.79
43	C86	3.942	21.861	8.65
44	C87	2.639	21.422	8.87
45	C88	0.29	19.917	10.745
46	C89	-1.057	20.307	10.825
47	C91	-0.961	20.333	13.228
48	C93	0.998	19.745	11.95
49	C95	2.572	20.268	14.545
50	C96	2.78	21.649	14.689
51	C97	4.062	22.189	14.771
52	C98	5.171	21.35	14.701
53	C99	5.023	19.962	14.548
54	C100	3.713	19.449	14.466
55	C111	-2.676	9.976	11.328
56	C112	-1.971	9.607	10.165

57	C113	-2.574	9.612	8.891
58	C114	-3.942	9.926	8.819
59	C115	-4.679	10.245	9.957
60	C116	-4.042	10.276	11.195
61	C117	-2.338	8.91	13.629
62	C118	-2.142	7.575	13.223
63	C119	-2.466	6.491	14.065
64	C120	-2.975	6.779	15.342
65	C121	-3.153	8.091	15.776
66	C122	-2.828	9.143	14.923
67	C124	-2.871	4.717	12.264
68	C125	-4.226	4.376	12.161
69	C126	-4.791	4.014	10.939
70	C127	-4.003	3.982	9.789
71	C128	-2.645	4.33	9.832
72	C129	-2.112	4.723	11.08
73	C1	6.074	17.537	14.72
74	C2	5.68	17.244	16.176
75	C3	6.093	15.844	16.641
76	C4	5.457	14.703	15.843
77	C5	5.939	13.346	16.366
78	C6	5.335	12.189	15.57
79	C7	5.726	10.807	16.103
80	C8	7.224	10.513	15.994
81	C9	7.54	9.066	16.399
82	C10	5.981	18.667	9.345
83	C11	0.676	18.123	9.024
84	C12	0.921	19.616	9.383
85	C13	1.013	17.8	7.559
86	C14	0.641	16.372	7.151
87	C15	1.487	15.3	7.843
88	C16	1.108	13.903	7.343
89	C17	1.513	11.387	7.66
90	C18	1.866	12.812	8.102
91	C19	0.018	11.077	7.775
92	C20	-0.276	9.579	7.621
93	C21	-1.797	9.278	7.609
94	C22	-2.006	10.082	12.703
95	C23	-0.475	10.337	12.716
96	C24	-0.104	11.702	12.115
97	C25	1.402	11.97	12.108
98	C26	2.047	12.137	13.485
99	C27	1.48	13.264	14.353
100	C28	1.546	14.638	13.684
101	C29	1.194	15.751	14.673
102	C30	1.174	17.119	13.986
103	C31	0.971	18.243	15.015
104	C32	1.146	19.704	14.509
105	C33	-0.744	4.629	13.744
106	C34	-0.239	4.13	8.818
107	C35	0.106	2.773	9.448
108	C36	1.395	2.817	10.269
109	C37	1.076	3.85	15.364
110	C38	2.602	2.852	17.178
111	C39	1.604	1.478	10.98
112	C40	3.975	3.14	16.565
113	C41	5.009	2.142	17.096
114	C42	2.67	1.529	12.07
115	C43	5.085	1.604	12.69
116	C44	6.546	1.658	12.257
117	C45	4.092	1.691	11.533
118	C46	1.524	3.88	16.829
119	C47	-0.245	4.612	15.197

120	C48	6.425	2.32	16.538
121	C49	7.044	3.69	16.848
122	C50	9.062	8.76	16.366
123	C51	8.601	3.683	16.836
124	C52	8.548	3.15	11.741
125	C53	8.815	8.238	11.265
126	C54	7.284	8.498	11.314
127	C55	6.867	9.94	11.673
128	C56	7.537	11.026	10.828
129	C57	7.144	12.434	11.289
130	C58	6.239	19.051	14.417
131	C59	7	3.056	11.805
132	C60	-1.683	20.522	12.052
133	O1	11.59	9.276	11.274
134	O2	11.725	9.676	15.965
135	O3	11.126	2.362	16.769
136	O4	10.356	8.699	18.913
137	O5	9.904	3.98	19.367
138	O6	11.193	1.87	12.08
139	O7	10.553	3.029	9.753
140	O8	10.776	7.767	9.272
141	O9	-4.562	9.928	7.599
142	O10	-4.758	10.624	12.309
143	O11	-5.003	4.382	13.287
144	O12	-4.647	3.581	8.648
145	O13	-3.28	5.747	16.188
146	O14	-2.97	10.432	15.362
147	O15	-1.584	20.498	14.436
148	O16	-1.778	20.448	9.669
149	O17	1.696	22.482	14.765
150	O18	1.596	22.293	8.711
151	O19	6.274	21.389	8.526
152	O20	8.714	19.557	9.308
153	O21	8.762	20.309	14.028
154	O22	6.386	21.977	14.791
155	O23	-2.912	8.602	5.057
156	O24	-3.239	3.971	6.177
157	C61	-2.242	5.044	13.625
158	C62	7.979	13.52	10.596
159	C63	5.594	17.163	9.276
160	C64	6.379	14.768	9.036
161	C65	6.808	16.227	9.236
162	C66	7.561	13.799	9.148
163	H1	5.352	17.067	14.041
164	H2	7.037	17.047	14.518
165	H3	4.599	17.366	16.306
166	H4	6.163	17.969	16.843
167	H5	5.82	15.738	17.698
168	H6	7.186	15.76	16.591
169	H7	5.718	14.791	14.782
170	H8	4.365	14.766	15.917
171	H9	5.67	13.243	17.424
172	H10	7.032	13.311	16.304
173	H11	5.625	12.27	14.516
174	H12	4.243	12.266	15.607
175	H13	5.171	10.054	15.534
176	H14	5.406	10.712	17.148
177	H15	7.782	11.194	16.647
178	H16	7.558	10.703	14.97
179	H17	6.974	8.367	15.772
180	H18	7.169	8.914	17.423
181	H19	6.606	18.831	8.457
182	H20	-0.384	17.885	9.185

183	H21	1.231	17.468	9.704
184	H22	0.359	20.181	8.625
185	H23	2.077	17.961	7.357
186	H24	0.462	18.492	6.91
187	H25	0.772	16.281	6.065
188	H26	-0.422	16.198	7.355
189	H27	1.334	15.346	8.927
190	H28	2.551	15.484	7.655
191	H29	1.318	13.822	6.27
192	H30	0.028	13.77	7.475
193	H31	2.083	10.686	8.283
194	H32	1.84	11.23	6.625
195	H33	2.945	12.961	7.974
196	H34	1.66	12.911	9.173
197	H35	-0.526	11.626	6.997
198	H36	-0.351	11.435	8.74
199	H37	0.236	9.016	8.409
200	H38	0.161	9.239	6.672
201	H39	-2.196	9.959	6.845
202	H40	-2.433	10.994	13.142
203	H41	0.067	9.534	12.201
204	H42	-0.127	10.313	13.757
205	H43	-0.628	12.5	12.653
206	H44	-0.452	11.758	11.08
207	H45	1.592	12.874	11.517
208	H46	1.909	11.154	11.578
209	H47	3.119	12.314	13.335
210	H48	1.969	11.199	14.045
211	H49	2.051	13.29	15.289
212	H50	0.445	13.039	14.634
213	H51	0.852	14.675	12.836
214	H52	2.554	14.81	13.289
215	H53	1.931	15.755	15.485
216	H54	0.214	15.555	15.124
217	H55	0.357	17.133	13.256
218	H56	2.101	17.255	13.423
219	H57	1.626	18.082	15.88
220	H58	-0.055	18.138	15.398
221	H59	0.643	20.29	15.293
222	H60	-0.623	3.622	13.324
223	H61	-0.099	5.297	13.16
224	H62	0.143	4.954	9.428
225	H63	0.291	4.201	7.859
226	H64	0.195	2.02	8.655
227	H65	-0.707	2.434	10.1
228	H66	1.326	3.62	11.012
229	H67	2.247	3.043	9.618
230	H68	0.934	2.812	15.04
231	H69	1.848	4.289	14.724
232	H70	2.702	2.833	18.271
233	H71	2.265	1.851	16.88
234	H72	1.849	0.701	10.247
235	H73	0.664	1.174	11.457
236	H74	4.276	4.163	16.816
237	H75	3.917	3.067	15.474
238	H76	4.676	1.123	16.861
239	H77	5.051	2.21	18.191
240	H78	2.609	0.595	12.642
241	H79	2.442	2.34	12.773
242	H80	4.927	0.656	13.221
243	H81	4.885	2.403	13.413
244	H82	6.729	0.934	11.454
245	H83	7.145	1.326	13.111

246	H84	4.304	0.899	10.804
247	H85	4.196	2.648	11.014
248	H86	1.87	4.888	17.088
249	H87	0.658	3.674	17.471
250	H88	-0.118	5.641	15.555
251	H89	-0.999	4.137	15.835
252	H90	6.41	2.154	15.456
253	H91	7.05	1.528	16.969
254	H92	6.715	4.004	17.849
255	H93	6.643	4.438	16.153
256	H94	9.503	9.59	16.933
257	H95	8.857	2.904	17.567
258	H96	8.808	2.271	11.135
259	H97	9.145	8.93	10.481
260	H98	6.793	7.819	12.02
261	H99	6.861	8.259	10.329
262	H0	7.073	10.125	12.732
263	H1	5.78	10.023	11.559
264	H2	7.274	10.88	9.775
265	H3	8.626	10.943	10.906
266	H4	7.322	12.511	12.369
267	H5	6.073	12.602	11.131
268	H6	6.941	19.389	15.191
269	H7	6.584	3.253	10.809
270	H8	6.582	3.822	12.465
271	H9	-2.727	20.81	12.091
272	H10	11.184	8.739	10.561
273	H11	12.619	9.95	15.705
274	H12	11.985	1.937	16.616
275	H13	10.855	8.548	19.732
276	H14	10.443	4.183	20.147
277	H15	10.865	2.297	11.26
278	H16	11.092	3.089	8.942
279	H17	11.273	7.496	8.478
280	H18	-5.507	10.112	7.715
281	H19	-5.692	10.734	12.073
282	H20	-5.916	4.16	13.043
283	H21	-4.072	3.692	7.866
284	H22	-3.69	6.101	16.994
285	H23	-3.387	10.429	16.239
286	H24	-2.488	20.822	14.29
287	H25	-2.669	20.768	9.883
288	H26	2.005	23.401	14.814
289	H27	1.941	23.179	8.52
290	H28	6.264	22.336	8.315
291	H29	9.566	20.01	9.404
292	H30	9.678	20.551	13.806
293	H31	7.113	21.357	14.591
294	H32	-3.421	8.274	4.298
295	H33	-3.563	3.949	5.259
296	H34	-2.763	4.379	14.327
297	H35	4.991	16.991	8.374
298	H36	5.596	14.497	9.754
299	H37	5.939	14.67	8.036
300	H38	7.477	16.522	8.418
301	H39	7.375	16.326	10.166
302	H40	7.922	14.438	11.191
303	H41	9.034	13.218	10.607
304	H42	7.304	12.862	8.642
305	H43	8.417	14.218	8.604
306	H3	7.889	5.796	12.172
307	H6	11.385	5.281	8.672
308	H20	9.778	20.322	11.587

309	H23	5.197	18.445	11.956
310	H36	8.432	6.168	15.665
311	H39	10.657	6.381	20.097
312	H43	12.633	9.826	13.492
313	H46	8.038	8.02	13.894
314	H50	12.093	1.638	14.422
315	H53	7.753	4.012	14.233
316	H64	-2.029	3.333	8.076
317	H66	-1.246	6.945	8.946
318	H69	-3.544	6.088	4.627
319	H83	3.27	18.212	9.748
320	H86	4.13	22.887	8.353
321	H93	2.036	19.423	11.916
322	H97	4.219	23.256	14.89
323	CH00	3.585	18.381	14.344
324	CH12	-0.923	9.339	10.249
325	CH15	-5.733	10.486	9.878
326	CH18	-1.737	7.379	12.234
327	CH21	-3.529	8.291	16.774
328	CH26	-5.839	3.739	10.862
329	CH29	-1.071	5.022	11.144
330	H1	4.971	16.877	10.132
331	C1	3.741	6.781	11.559
332	C2	3.448	8.051	12.082
333	C3	3.567	8.312	13.45
334	C4	3.982	7.31	14.322
335	C5	4.273	6.044	13.826
336	C6	4.145	5.782	12.461
337	C7	3.479	5.978	7.346
338	C8	4.607	5.589	8.063
339	C9	4.691	5.853	9.432
340	C10	3.648	6.507	10.113
341	C11	2.521	6.893	9.369
342	C12	2.437	6.631	7.998
343	H1	3.144	8.86	11.422
344	H2	3.345	9.303	13.833
345	H3	4.076	7.516	15.384
346	H4	4.594	5.257	14.501
347	H5	4.358	4.779	12.102
348	H6	3.412	5.774	6.281
349	H7	5.426	5.084	7.557
350	H8	5.591	5.553	9.964
351	H9	1.686	7.391	9.857
352	H10	1.554	6.931	7.44

Table S8. Cartesian coordinates of the structure of (diphenylacetylene)⊂**1** optimized by MacroModel Ver 9.1 using the MMFFs force field.

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	C1	10.315	4.127	9.637
2	C2	9.314	4.213	10.616
3	C02B	0.383	19.517	13.239
4	C3	8.836	5.489	10.973
5	C4	9.338	6.654	10.365
6	C5	10.325	6.508	9.375
7	C6	10.81	5.258	8.998
8	C18	6.689	18.735	10.357
9	C19	8.038	19.087	10.214
10	C20	8.835	19.349	11.325
11	C21	8.292	19.233	12.601
12	C22	6.953	18.876	12.799
13	C23	6.166	18.623	11.66
14	C35	9.732	7.29	16.654
15	C36	9.27	6.04	16.197
16	C37	9.518	4.849	16.913
17	C38	10.258	4.937	18.101
18	C39	10.751	6.156	18.561
19	C40	10.478	7.319	17.843
20	C41	9.958	8.69	14.515
21	C42	11.219	9.27	14.318
22	C43	11.745	9.445	13.041
23	C44	11.009	9.045	11.929
24	C45	9.74	8.46	12.064
25	C46	9.252	8.257	13.373
26	C48	9.63	3.048	15.119
27	C49	10.848	2.352	15.135
28	C50	11.442	1.899	13.958
29	C51	10.815	2.122	12.737
30	C52	9.584	2.79	12.666
31	C53	9.037	3.29	13.867
32	C64	-1.273	4.19	8.095
33	C65	-1.55	5.366	7.167
34	C66	-1.256	6.682	7.561
35	C67	-1.566	7.779	6.735
36	C68	-2.101	7.525	5.463
37	C69	-2.41	6.23	5.054
38	C70	-2.164	5.17	5.922
39	C82	2.2	19.95	9.228
40	C83	3.293	19.064	9.332
41	C84	4.619	19.467	9.084
42	C85	4.832	20.819	8.773
43	C86	3.779	21.734	8.721
44	C87	2.476	21.294	8.946
45	C88	0.168	19.622	10.787
46	C89	-1.203	19.876	10.952
47	C91	-0.993	19.764	13.346
48	C93	0.946	19.441	11.947
49	C95	2.635	19.877	14.45
50	C96	2.802	21.269	14.528
51	C97	4.067	21.851	14.51
52	C98	5.198	21.045	14.404
53	C99	5.095	19.646	14.332
54	C100	3.8	19.091	14.354
55	C111	-2.298	9.763	10.97
56	C112	-1.574	9.455	9.8

57	C113	-2.171	9.475	8.523
58	C114	-3.55	9.733	8.453
59	C115	-4.304	9.991	9.596
60	C116	-3.674	10.015	10.838
61	C117	-1.961	8.668	13.257
62	C118	-1.759	7.343	12.822
63	C119	-2.077	6.24	13.639
64	C120	-2.579	6.497	14.925
65	C121	-2.76	7.798	15.39
66	C122	-2.446	8.87	14.558
67	C124	-2.458	4.539	11.768
68	C125	-3.82	4.245	11.618
69	C126	-4.363	3.943	10.37
70	C127	-3.546	3.925	9.241
71	C128	-2.18	4.232	9.329
72	C129	-1.668	4.564	10.603
73	C1	6.228	17.26	14.552
74	C2	5.914	16.99	16.03
75	C3	6.347	15.59	16.484
76	C4	5.648	14.447	15.742
77	C5	6.19	13.087	16.198
78	C6	5.527	11.937	15.438
79	C7	5.979	10.547	15.893
80	C8	7.469	10.286	15.665
81	C9	7.844	8.843	16.029
82	C10	5.797	18.479	9.143
83	C11	0.506	18.011	8.888
84	C12	0.754	19.465	9.38
85	C13	0.814	17.817	7.394
86	C14	0.558	16.387	6.913
87	C15	1.56	15.373	7.472
88	C16	1.235	13.959	6.984
89	C17	1.825	11.472	7.235
90	C18	2.125	12.914	7.661
91	C19	0.361	11.076	7.444
92	C20	0.131	9.572	7.257
93	C21	-1.376	9.21	7.237
94	C22	-1.637	9.857	12.351
95	C23	-0.107	10.111	12.376
96	C24	0.274	11.474	11.782
97	C25	1.784	11.721	11.761
98	C26	2.45	11.823	13.135
99	C27	1.856	12.877	14.075
100	C28	1.856	14.285	13.478
101	C29	1.464	15.33	14.522
102	C30	1.338	16.718	13.89
103	C31	1.125	17.794	14.965
104	C32	1.225	19.272	14.493
105	C33	-0.369	4.375	13.298
106	C34	0.248	4.032	8.363
107	C35	0.56	2.657	8.974
108	C36	1.795	2.676	9.871
109	C37	1.43	3.554	14.921
110	C38	2.956	2.51	16.708
111	C39	1.939	1.33	10.585
112	C40	4.333	2.918	16.173
113	C41	5.392	1.929	16.676
114	C42	2.996	1.338	11.683
115	C43	5.417	1.335	12.3
116	C44	6.875	1.422	11.863
117	C45	4.421	1.487	11.153
118	C46	1.827	3.494	16.399
119	C47	0.084	4.272	14.762

120	C48	6.804	2.141	16.127
121	C49	7.414	3.511	16.453
122	C50	9.372	8.585	15.925
123	C51	8.973	3.505	16.424
124	C52	8.844	2.956	11.339
125	C53	8.92	8.049	10.839
126	C54	7.379	8.232	10.953
127	C55	6.9	9.648	11.329
128	C56	7.442	10.764	10.431
129	C57	7.027	12.154	10.932
130	C58	6.339	18.767	14.197
131	C59	7.299	2.835	11.43
132	C60	-1.786	19.953	12.216
133	O1	11.612	9.277	10.721
134	O2	11.943	9.69	15.4
135	O3	11.46	2.098	16.332
136	O4	10.921	8.52	18.33
137	O5	10.476	3.807	18.842
138	O6	11.473	1.641	11.637
139	O7	10.863	2.898	9.364
140	O8	10.879	7.638	8.823
141	O9	-4.163	9.743	7.229
142	O10	-4.407	10.305	11.957
143	O11	-4.627	4.239	12.723
144	O12	-4.172	3.579	8.072
145	O13	-2.876	5.444	15.748
146	O14	-2.595	10.148	15.024
147	O15	-1.567	19.797	14.588
148	O16	-1.988	20.022	9.838
149	O17	1.696	22.068	14.635
150	O18	1.438	22.183	8.873
151	O19	6.104	21.246	8.502
152	O20	8.583	19.157	8.962
153	O21	9.13	19.503	13.647
154	O22	6.39	21.719	14.381
155	O23	-2.334	8.573	4.615
156	O24	-2.589	3.908	5.598
157	C61	-1.86	4.806	13.156
158	C62	7.783	13.277	10.207
159	C63	5.383	16.98	9.066
160	C64	6.096	14.566	8.776
161	C65	6.571	16.017	8.941
162	C66	7.261	13.569	8.794
163	H1	5.489	16.758	13.916
164	H2	7.192	16.785	14.318
165	H3	4.844	17.12	16.222
166	H4	6.44	17.72	16.658
167	H5	6.146	15.496	17.558
168	H6	7.433	15.497	16.361
169	H7	5.801	14.544	14.662
170	H8	4.569	14.497	15.925
171	H9	6.022	12.964	17.275
172	H10	7.274	13.067	16.033
173	H11	5.715	12.047	14.363
174	H12	4.444	11.997	15.582
175	H13	5.395	9.802	15.339
176	H14	5.739	10.414	16.954
177	H15	8.062	10.972	16.279
178	H16	7.718	10.491	14.619
179	H17	7.27	8.14	15.414
180	H18	7.524	8.662	17.065
181	H19	6.366	18.662	8.222
182	H20	-0.549	17.749	9.046

183	H21	1.073	17.303	9.502
184	H22	0.164	20.102	8.706
185	H23	1.848	18.089	7.162
186	H24	0.173	18.495	6.816
187	H25	0.617	16.375	5.817
188	H26	-0.464	16.09	7.177
189	H27	1.538	15.383	8.567
190	H28	2.577	15.645	7.166
191	H29	1.356	13.903	5.896
192	H30	0.183	13.753	7.208
193	H31	2.474	10.802	7.812
194	H32	2.089	11.34	6.179
195	H33	3.177	13.132	7.44
196	H34	2.011	12.991	8.749
197	H35	-0.264	11.62	6.725
198	H36	0.042	11.382	8.444
199	H37	0.668	9.01	8.029
200	H38	0.579	9.273	6.299
201	H39	-1.805	9.894	6.493
202	H40	-2.073	10.76	12.8
203	H41	0.436	9.307	11.865
204	H42	0.231	10.087	13.419
205	H43	-0.235	12.273	12.333
206	H44	-0.085	11.55	10.752
207	H45	1.977	12.643	11.202
208	H46	2.272	10.92	11.193
209	H47	3.513	12.046	12.98
210	H48	2.417	10.847	13.634
211	H49	2.437	12.878	15.003
212	H50	0.835	12.596	14.359
213	H51	1.156	14.335	12.637
214	H52	2.854	14.521	13.087
215	H53	2.222	15.348	15.314
216	H54	0.511	15.056	14.991
217	H55	0.486	16.711	13.198
218	H56	2.226	16.925	13.287
219	H57	1.82	17.636	15.8
220	H58	0.122	17.633	15.384
221	H59	0.752	19.831	15.315
222	H60	-0.239	3.39	12.828
223	H61	0.295	5.071	12.77
224	H62	0.628	4.845	8.992
225	H63	0.8	4.114	7.417
226	H64	0.699	1.928	8.165
227	H65	-0.291	2.295	9.562
228	H66	1.696	3.474	10.618
229	H67	2.685	2.893	9.271
230	H68	1.344	2.537	14.519
231	H69	2.206	4.071	14.344
232	H70	3.021	2.412	17.8
233	H71	2.69	1.518	16.322
234	H72	2.16	0.542	9.854
235	H73	0.981	1.066	11.052
236	H74	4.576	3.93	16.514
237	H75	4.32	2.932	15.079
238	H76	5.08	0.91	16.412
239	H77	5.429	1.968	17.772
240	H78	2.915	0.396	12.239
241	H79	2.782	2.143	12.397
242	H80	5.262	0.36	12.779
243	H81	5.218	2.095	13.064
244	H82	7.066	0.714	11.047
245	H83	7.485	1.087	12.709

246	H84	4.617	0.724	10.391
247	H85	4.543	2.465	10.676
248	H86	2.097	4.495	16.753
249	H87	0.955	3.182	16.988
250	H88	0.155	5.274	15.198
251	H89	-0.671	3.72	15.335
252	H90	6.79	1.989	15.043
253	H91	7.439	1.349	16.544
254	H92	7.095	3.81	17.462
255	H93	7.001	4.265	15.772
256	H94	9.808	9.42	16.49
257	H95	9.233	2.738	17.165
258	H96	9.107	2.09	10.716
259	H97	9.181	8.742	10.032
260	H98	6.953	7.532	11.68
261	H99	6.931	7.967	9.986
262	H0	7.169	9.857	12.37
263	H1	5.804	9.662	11.293
264	H2	7.092	10.608	9.405
265	H3	8.535	10.729	10.411
266	H4	7.265	12.226	12.001
267	H5	5.944	12.286	10.838
268	H6	7.048	19.179	14.927
269	H7	6.866	3.041	10.442
270	H8	6.873	3.581	12.108
271	H9	-2.85	20.138	12.318
272	H10	11.233	8.682	10.038
273	H11	12.793	10.045	15.096
274	H12	12.299	1.639	16.169
275	H13	11.51	8.366	19.085
276	H14	11.086	4.008	19.568
277	H15	11.165	2.11	10.832
278	H16	11.401	2.975	8.553
279	H17	11.385	7.374	8.032
280	H18	-5.117	9.873	7.346
281	H19	-5.344	10.38	11.719
282	H20	-5.541	4.067	12.446
283	H21	-3.564	3.662	7.314
284	H22	-3.266	5.776	16.571
285	H23	-3.049	10.127	15.882
286	H24	-2.51	20.013	14.501
287	H25	-2.903	20.199	10.111
288	H26	1.974	22.998	14.622
289	H27	1.787	23.074	8.713
290	H28	6.1	22.204	8.353
291	H29	9.487	19.504	9.028
292	H30	9.033	18.785	14.297
293	H31	7.092	21.15	14.025
294	H32	-2.778	8.25	3.815
295	H33	-2.861	3.901	4.663
296	H34	-2.409	4.124	13.82
297	H35	4.728	16.836	8.197
298	H36	5.368	14.31	9.554
299	H37	5.577	14.48	7.813
300	H38	7.185	16.298	8.077
301	H39	7.207	16.099	9.827
302	H40	7.739	14.181	10.823
303	H41	8.844	13.007	10.142
304	H42	6.945	12.639	8.309
305	H43	8.082	13.97	8.187
306	H3	8.104	5.577	11.772
307	H6	11.602	5.173	8.262
308	H20	9.878	19.628	11.218

309	H23	5.121	18.345	11.784
310	H36	8.688	5.994	15.281
311	H39	11.315	6.204	19.486
312	H43	12.72	9.896	12.888
313	H46	8.285	7.78	13.502
314	H50	12.388	1.366	13.972
315	H53	8.109	3.852	13.833
316	H64	-1.534	3.258	7.576
317	H66	-0.823	6.858	8.543
318	H69	-2.865	6.054	4.086
319	H83	3.095	18.029	9.592
320	H86	3.971	22.775	8.487
321	H93	2.005	19.221	11.851
322	H97	4.193	22.927	14.572
323	CH00	3.702	18.014	14.297
324	CH12	-0.517	9.221	9.88
325	CH15	-5.367	10.192	9.517
326	CH18	-1.356	7.172	11.827
327	CH21	-3.133	7.974	16.393
328	CH26	-5.416	3.703	10.257
329	CH29	-0.62	4.829	10.703
330	H1	4.804	16.691	9.952
331	C1	3.137	7.68	10.174
332	C2	3.653	6.788	11.116
333	C3	4.458	5.723	10.702
334	C4	4.755	5.558	9.348
335	C5	4.242	6.453	8.408
336	C6	3.433	7.513	8.82
337	C7	3.188	7.15	13.678
338	C8	3.384	6.979	12.506
339	C9	2.581	7.812	17.8
340	C10	1.566	8.107	16.89
341	C11	1.764	7.885	15.527
342	C12	2.98	7.368	15.075
343	C13	3.995	7.068	15.987
344	C14	3.795	7.292	17.35
345	H1	2.514	8.514	10.486
346	H2	4.864	5.026	11.429
347	H3	5.388	4.737	9.026
348	H4	4.476	6.33	7.355
349	H5	3.04	8.211	8.087
350	H6	2.427	7.986	18.861
351	H7	0.62	8.509	17.242
352	H8	0.964	8.112	14.826
353	H9	4.943	6.663	15.646
354	H10	4.584	7.059	18.059

Table S9. Cartesian coordinates of the structure of (octane)⊂**1** optimized by MacroModel Ver 9.1 using the MMFFs force field.

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	C1	10.247	4.338	9.827
2	C2	9.248	4.445	10.809
3	C02B	0.274	19.159	13.074
4	C3	8.836	5.732	11.201
5	C4	9.405	6.886	10.635
6	C5	10.393	6.721	9.649
7	C6	10.807	5.461	9.229
8	C18	6.714	18.92	10.443
9	C19	8.043	19.354	10.339
10	C20	8.788	19.668	11.473
11	C21	8.215	19.524	12.733
12	C22	6.893	19.092	12.891
13	C23	6.16	18.784	11.729
14	C35	9.583	7.353	16.99
15	C36	9.146	6.12	16.465
16	C37	9.318	4.911	17.172
17	C38	9.949	4.963	18.424
18	C39	10.405	6.166	18.957
19	C40	10.212	7.348	18.245
20	C41	9.975	8.757	14.877
21	C42	11.284	9.245	14.75
22	C43	11.875	9.414	13.501
23	C44	11.16	9.098	12.348
24	C45	9.848	8.603	12.414
25	C46	9.292	8.404	13.695
26	C48	9.464	3.182	15.301
27	C49	10.692	2.504	15.31
28	C50	11.299	2.084	14.129
29	C51	10.677	2.326	12.907
30	C52	9.443	2.989	12.84
31	C53	8.879	3.449	14.051
32	C64	-1.608	4.065	8.127
33	C65	-1.984	5.215	7.197
34	C66	-1.625	6.539	7.496
35	C67	-2.007	7.61	6.665
36	C68	-2.707	7.318	5.485
37	C69	-3.09	6.015	5.174
38	C70	-2.752	4.985	6.047
39	C82	2.18	19.788	9.136
40	C83	3.33	18.985	9.277
41	C84	4.632	19.493	9.103
42	C85	4.756	20.862	8.821
43	C86	3.64	21.695	8.729
44	C87	2.365	21.154	8.885
45	C88	0.131	19.31	10.621
46	C89	-1.249	19.534	10.748
47	C91	-1.109	19.374	13.145
48	C93	0.876	19.119	11.8
49	C95	2.439	19.674	14.369
50	C96	2.462	21.075	14.467
51	C97	3.66	21.783	14.495
52	C98	4.869	21.096	14.423
53	C99	4.91	19.694	14.347
54	C100	3.678	19.009	14.314
55	C111	-2.292	9.765	10.841
56	C112	-1.699	9.354	9.632

57	C113	-2.383	9.421	8.401
58	C114	-3.723	9.837	8.42
59	C115	-4.353	10.208	9.605
60	C116	-3.633	10.181	10.798
61	C117	-1.939	8.664	13.117
62	C118	-1.812	7.314	12.735
63	C119	-2.194	6.264	13.593
64	C120	-2.706	6.601	14.857
65	C121	-2.823	7.928	15.266
66	C122	-2.43	8.946	14.401
67	C124	-2.649	4.451	11.84
68	C125	-3.995	4.068	11.762
69	C126	-4.57	3.686	10.551
70	C127	-3.804	3.683	9.386
71	C128	-2.458	4.083	9.401
72	C129	-1.912	4.484	10.641
73	C1	6.27	17.447	14.653
74	C2	5.919	17.172	16.121
75	C3	6.359	15.778	16.586
76	C4	5.736	14.634	15.782
77	C5	6.213	13.272	16.296
78	C6	5.642	12.138	15.444
79	C7	6.002	10.739	15.946
80	C8	7.502	10.449	15.91
81	C9	7.798	8.99	16.288
82	C10	5.879	18.598	9.204
83	C11	0.628	17.734	8.731
84	C12	0.769	19.199	9.233
85	C13	1.007	17.561	7.252
86	C14	0.7	16.162	6.711
87	C15	1.552	15.061	7.348
88	C16	1.199	13.691	6.761
89	C17	1.6	11.163	6.972
90	C18	1.962	12.569	7.469
91	C19	0.109	10.849	7.119
92	C20	-0.193	9.352	6.97
93	C21	-1.712	9.054	7.07
94	C22	-1.528	9.794	12.17
95	C23	0.022	9.863	12.098
96	C24	0.527	11.164	11.457
97	C25	2.044	11.348	11.553
98	C26	2.605	11.485	12.972
99	C27	1.935	12.548	13.849
100	C28	2.018	13.963	13.271
101	C29	1.522	14.995	14.285
102	C30	1.456	16.402	13.682
103	C31	1.104	17.436	14.764
104	C32	1.095	18.933	14.345
105	C33	-0.525	4.349	13.329
106	C34	-0.07	3.982	8.33
107	C35	0.34	2.638	8.952
108	C36	1.565	2.759	9.857
109	C37	1.27	3.603	15.002
110	C38	2.781	2.671	16.863
111	C39	1.812	1.435	10.58
112	C40	4.162	3.006	16.293
113	C41	5.206	2.022	16.831
114	C42	2.829	1.544	11.711
115	C43	5.221	1.701	12.41
116	C44	6.691	1.742	12.009
117	C45	4.259	1.784	11.227
118	C46	1.68	3.66	16.478
119	C47	-0.042	4.368	14.789

120	C48	6.623	2.224	16.288
121	C49	7.233	3.592	16.63
122	C50	9.317	8.669	16.258
123	C51	8.791	3.587	16.614
124	C52	8.721	3.197	11.507
125	C53	9.052	8.284	11.148
126	C54	7.52	8.542	11.213
127	C55	7.104	9.979	11.586
128	C56	7.732	11.064	10.707
129	C57	7.331	12.473	11.159
130	C58	6.243	18.949	14.269
131	C59	7.171	3.136	11.574
132	C60	-1.872	19.571	11.995
133	O1	11.829	9.317	11.173
134	O2	11.988	9.578	15.874
135	O3	11.301	2.238	16.506
136	O4	10.615	8.534	18.798
137	O5	10.092	3.813	19.152
138	O6	11.347	1.864	11.806
139	O7	10.732	3.091	9.518
140	O8	11.018	7.838	9.15
141	O9	-4.422	9.892	7.244
142	O10	-4.242	10.585	11.955
143	O11	-4.753	4.052	12.901
144	O12	-4.459	3.253	8.263
145	O13	-3.07	5.602	15.719
146	O14	-2.503	10.248	14.819
147	O15	-1.721	19.373	14.369
148	O16	-2.002	19.693	9.614
149	O17	1.279	21.758	14.546
150	O18	1.268	21.964	8.777
151	O19	6.003	21.39	8.622
152	O20	8.622	19.452	9.104
153	O21	9.009	19.84	13.8
154	O22	5.988	21.884	14.437
155	O23	-3.03	8.336	4.629
156	O24	-3.229	3.717	5.827
157	C61	-2.012	4.8	13.192
158	C62	8.135	13.561	10.432
159	C63	5.578	17.073	9.12
160	C64	6.472	14.719	8.864
161	C65	6.835	16.198	9.051
162	C66	7.695	13.804	8.982
163	H1	5.612	16.866	13.994
164	H2	7.284	17.064	14.472
165	H3	4.842	17.282	16.283
166	H4	6.414	17.912	16.762
167	H5	6.092	15.665	17.644
168	H6	7.453	15.711	16.529
169	H7	6.007	14.725	14.724
170	H8	4.643	14.693	15.845
171	H9	5.906	13.143	17.34
172	H10	7.308	13.244	16.27
173	H11	5.976	12.25	14.405
174	H12	4.551	12.22	15.435
175	H13	5.481	10.012	15.311
176	H14	5.621	10.603	16.965
177	H15	8.025	11.108	16.611
178	H16	7.889	10.671	14.911
179	H17	7.232	8.31	15.641
180	H18	7.416	8.821	17.305
181	H19	6.461	18.822	8.299
182	H20	-0.416	17.414	8.85

183	H21	1.215	17.057	9.362
184	H22	0.16	19.797	8.54
185	H23	2.069	17.778	7.093
186	H24	0.443	18.288	6.654
187	H25	0.873	16.165	5.628
188	H26	-0.365	15.941	6.859
189	H27	1.385	15.035	8.43
190	H28	2.615	15.272	7.187
191	H29	1.427	13.673	5.689
192	H30	0.12	13.537	6.868
193	H31	2.188	10.439	7.548
194	H32	1.896	11.052	5.923
195	H33	3.04	12.721	7.336
196	H34	1.768	12.623	8.547
197	H35	-0.454	11.401	6.357
198	H36	-0.238	11.207	8.093
199	H37	0.373	8.779	7.711
200	H38	0.173	9.021	5.988
201	H39	-2.159	9.721	6.322
202	H40	-1.817	10.75	12.629
203	H41	0.439	8.998	11.568
204	H42	0.411	9.803	13.122
205	H43	0.018	12.025	11.904
206	H44	0.261	11.178	10.396
207	H45	2.321	12.24	10.978
208	H46	2.542	10.504	11.06
209	H47	3.676	11.708	12.897
210	H48	2.537	10.519	13.485
211	H49	2.415	12.532	14.834
212	H50	0.886	12.283	14.028
213	H51	1.417	14.03	12.357
214	H52	3.055	14.193	12.997
215	H53	2.192	14.994	15.153
216	H54	0.526	14.712	14.647
217	H55	0.692	16.406	12.896
218	H56	2.408	16.638	13.199
219	H57	1.769	17.309	15.629
220	H58	0.097	17.183	15.128
221	H59	0.552	19.415	15.173
222	H60	-0.429	3.326	12.941
223	H61	0.14	4.981	12.727
224	H62	0.297	4.825	8.927
225	H63	0.435	4.073	7.359
226	H64	0.541	1.917	8.149
227	H65	-0.484	2.217	9.537
228	H66	1.397	3.55	10.598
229	H67	2.441	3.046	9.265
230	H68	1.134	2.559	14.695
231	H69	2.061	4.029	14.376
232	H70	2.849	2.656	17.958
233	H71	2.489	1.659	16.555
234	H72	2.127	0.67	9.86
235	H73	0.87	1.083	11.019
236	H74	4.435	4.028	16.574
237	H75	4.136	2.959	15.2
238	H76	4.892	1	16.584
239	H77	5.233	2.083	17.926
240	H78	2.797	0.606	12.281
241	H79	2.533	2.34	12.403
242	H80	5.047	0.759	12.945
243	H81	5.007	2.509	13.119
244	H82	6.883	1.018	11.207
245	H83	7.268	1.398	12.874

246	H84	4.526	1.029	10.479
247	H85	4.338	2.766	10.747
248	H86	1.983	4.68	16.74
249	H87	0.803	3.428	17.098
250	H88	0.088	5.405	15.12
251	H89	-0.809	3.917	15.429
252	H90	6.617	2.079	15.203
253	H91	7.251	1.428	16.707
254	H92	6.905	3.881	17.638
255	H93	6.828	4.354	15.953
256	H94	9.764	9.481	16.845
257	H95	9.048	2.79	17.325
258	H96	8.962	2.328	10.879
259	H97	9.381	8.991	10.378
260	H98	7.033	7.857	11.917
261	H99	7.087	8.308	10.23
262	H0	7.354	10.172	12.634
263	H1	6.011	10.049	11.517
264	H2	7.438	10.9	9.664
265	H3	8.823	10.997	10.753
266	H4	7.535	12.567	12.233
267	H5	6.255	12.624	11.026
268	H6	6.88	19.445	15.013
269	H7	6.757	3.355	10.581
270	H8	6.765	3.902	12.244
271	H9	-2.942	19.732	12.068
272	H10	11.425	8.79	10.45
273	H11	12.882	9.854	15.619
274	H12	12.153	1.804	16.34
275	H13	11.112	8.358	19.613
276	H14	10.635	3.992	19.936
277	H15	11.023	2.315	10.998
278	H16	11.267	3.163	8.706
279	H17	11.516	7.579	8.352
280	H18	-5.341	10.146	7.424
281	H19	-5.176	10.781	11.78
282	H20	-5.664	3.805	12.672
283	H21	-3.911	3.389	7.463
284	H22	-3.474	5.991	16.512
285	H23	-2.939	10.284	15.685
286	H24	-2.66	19.594	14.26
287	H25	-2.92	19.884	9.863
288	H26	1.461	22.712	14.552
289	H27	1.556	22.883	8.655
290	H28	5.934	22.348	8.488
291	H29	9.504	19.847	9.198
292	H30	8.893	19.152	14.477
293	H31	6.743	21.398	14.066
294	H32	-3.586	7.993	3.912
295	H33	-3.6	3.679	4.927
296	H34	-2.548	4.171	13.914
297	H35	4.971	16.878	8.226
298	H36	5.703	14.419	9.586
299	H37	6.034	14.594	7.866
300	H38	7.47	16.524	8.219
301	H39	7.418	16.323	9.969
302	H40	8.067	14.489	11.009
303	H41	9.195	13.28	10.434
304	H42	7.478	12.85	8.49
305	H43	8.529	14.253	8.429
306	H3	8.104	5.834	11.998
307	H6	11.6	5.358	8.495
308	H20	9.816	20.007	11.397

309	H23	5.131	18.44	11.821
310	H36	8.644	6.102	15.501
311	H39	10.88	6.187	19.932
312	H43	12.885	9.798	13.402
313	H46	8.289	7.993	13.772
314	H50	12.25	1.56	14.138
315	H53	7.944	4	14.024
316	H64	-1.842	3.116	7.624
317	H66	-1.072	6.744	8.41
318	H69	-3.67	5.812	4.281
319	H83	3.197	17.934	9.513
320	H86	3.763	22.752	8.519
321	H93	1.943	18.924	11.734
322	H97	3.675	22.866	14.567
323	CH00	3.69	17.928	14.246
324	CH12	-0.672	9.001	9.642
325	CH15	-5.387	10.535	9.597
326	CH18	-1.406	7.084	11.753
327	CH21	-3.199	8.165	16.255
328	CH26	-5.608	3.375	10.494
329	CH29	-0.88	4.815	10.689
330	H1	4.985	16.748	9.984
331	C1	2.932	7.775	9.035
332	C2	3.17	6.592	9.959
333	C3	3.583	7.053	11.356
334	C4	3.826	5.86	12.281
335	C5	4.331	6.257	13.671
336	C6	3.342	7.13	14.447
337	C7	3.793	7.336	15.892
338	C8	2.845	8.259	16.642
339	H2	2.629	7.427	8.043
340	H3	2.14	8.422	9.426
341	H4	3.84	8.376	8.924
342	H5	3.947	5.95	9.53
343	H6	2.252	5.996	10.022
344	H7	2.794	7.693	11.766
345	H8	4.493	7.66	11.29
346	H9	4.569	5.195	11.824
347	H10	2.902	5.278	12.38
348	H11	5.29	6.782	13.579
349	H12	4.53	5.339	14.237
350	H13	2.349	6.666	14.437
351	H14	3.249	8.106	13.959
352	H15	3.84	6.373	16.41
353	H16	4.802	7.761	15.913
354	H17	2.801	9.245	16.168
355	H18	1.832	7.843	16.666
356	H19	3.183	8.392	17.674

Table S10. Cartesian coordinates of the structure of (decane)⊂**1** optimized by MacroModel Ver 9.1 using the MMFFs force field.

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	C1	10.255	4.341	9.834
2	C2	9.255	4.445	10.813
3	C02B	0.287	19.187	13.092
4	C3	8.837	5.731	11.204
5	C4	9.404	6.887	10.638
6	C5	10.394	6.724	9.654
7	C6	10.814	5.465	9.235
8	C18	6.716	18.919	10.433
9	C19	8.047	19.345	10.323
10	C20	8.799	19.655	11.454
11	C21	8.23	19.517	12.716
12	C22	6.905	19.094	12.88
13	C23	6.166	18.788	11.721
14	C35	9.573	7.365	16.993
15	C36	9.142	6.13	16.468
16	C37	9.317	4.923	17.175
17	C38	9.945	4.978	18.428
18	C39	10.396	6.183	18.962
19	C40	10.199	7.363	18.249
20	C41	9.961	8.769	14.879
21	C42	11.268	9.26	14.752
22	C43	11.86	9.429	13.504
23	C44	11.148	9.108	12.35
24	C45	9.838	8.609	12.416
25	C46	9.28	8.411	13.697
26	C48	9.47	3.191	15.307
27	C49	10.701	2.517	15.319
28	C50	11.31	2.097	14.139
29	C51	10.689	2.333	12.916
30	C52	9.452	2.992	12.847
31	C53	8.885	3.453	14.055
32	C64	-1.61	4.072	8.162
33	C65	-1.983	5.226	7.236
34	C66	-1.625	6.549	7.542
35	C67	-2.006	7.623	6.715
36	C68	-2.702	7.335	5.531
37	C69	-3.084	6.033	5.213
38	C70	-2.747	5	6.083
39	C82	2.18	19.803	9.145
40	C83	3.327	18.997	9.283
41	C84	4.63	19.499	9.102
42	C85	4.758	20.868	8.818
43	C86	3.645	21.705	8.729
44	C87	2.369	21.168	8.892
45	C88	0.135	19.335	10.639
46	C89	-1.244	19.565	10.771
47	C91	-1.095	19.408	13.168
48	C93	0.884	19.143	11.816
49	C95	2.459	19.697	14.376
50	C96	2.488	21.099	14.468
51	C97	3.689	21.802	14.488
52	C98	4.895	21.111	14.413
53	C99	4.931	19.708	14.342
54	C100	3.695	19.027	14.317
55	C111	-2.308	9.769	10.896
56	C112	-1.711	9.359	9.689

57	C113	-2.392	9.428	8.455
58	C114	-3.733	9.842	8.471
59	C115	-4.367	10.209	9.655
60	C116	-3.65	10.182	10.85
61	C117	-1.954	8.664	13.169
62	C118	-1.824	7.315	12.782
63	C119	-2.203	6.261	13.636
64	C120	-2.714	6.591	14.901
65	C121	-2.833	7.916	15.316
66	C122	-2.444	8.939	14.454
67	C124	-2.655	4.454	11.875
68	C125	-4	4.071	11.795
69	C126	-4.574	3.692	10.583
70	C127	-3.807	3.69	9.419
71	C128	-2.461	4.089	9.436
72	C129	-1.916	4.489	10.677
73	C1	6.283	17.457	14.649
74	C2	5.939	17.189	16.12
75	C3	6.375	15.795	16.588
76	C4	5.739	14.651	15.795
77	C5	6.217	13.289	16.309
78	C6	5.627	12.153	15.473
79	C7	5.99	10.756	15.979
80	C8	7.487	10.457	15.912
81	C9	7.783	8.999	16.292
82	C10	5.874	18.6	9.197
83	C11	0.621	17.753	8.752
84	C12	0.767	19.219	9.249
85	C13	0.995	17.574	7.273
86	C14	0.69	16.17	6.741
87	C15	1.545	15.075	7.383
88	C16	1.196	13.7	6.807
89	C17	1.597	11.175	7.044
90	C18	1.955	12.585	7.529
91	C19	0.105	10.863	7.178
92	C20	-0.195	9.365	7.036
93	C21	-1.714	9.065	7.126
94	C22	-1.547	9.798	12.226
95	C23	0.003	9.873	12.155
96	C24	0.504	11.174	11.512
97	C25	2.022	11.358	11.6
98	C26	2.588	11.501	13.015
99	C27	1.925	12.571	13.889
100	C28	2.009	13.982	13.303
101	C29	1.522	15.021	14.314
102	C30	1.46	16.426	13.705
103	C31	1.117	17.466	14.785
104	C32	1.112	18.961	14.36
105	C33	-0.529	4.353	13.36
106	C34	-0.072	3.986	8.368
107	C35	0.335	2.64	8.985
108	C36	1.57	2.753	9.879
109	C37	1.273	3.607	15.024
110	C38	2.789	2.667	16.876
111	C39	1.819	1.426	10.596
112	C40	4.167	3.01	16.302
113	C41	5.214	2.025	16.835
114	C42	2.842	1.53	11.722
115	C43	5.236	1.688	12.414
116	C44	6.705	1.733	12.01
117	C45	4.271	1.764	11.232
118	C46	1.682	3.653	16.5
119	C47	-0.042	4.367	14.819

120	C48	6.63	2.231	16.289
121	C49	7.237	3.599	16.632
122	C50	9.303	8.679	16.259
123	C51	8.795	3.596	16.619
124	C52	8.731	3.195	11.512
125	C53	9.046	8.284	11.149
126	C54	7.512	8.536	11.21
127	C55	7.09	9.973	11.58
128	C56	7.716	11.059	10.7
129	C57	7.311	12.467	11.15
130	C58	6.26	18.958	14.261
131	C59	7.181	3.129	11.577
132	C60	-1.861	19.606	12.02
133	O1	11.818	9.327	11.176
134	O2	11.97	9.599	15.877
135	O3	11.309	2.256	16.516
136	O4	10.596	8.551	18.803
137	O5	10.091	3.828	19.157
138	O6	11.361	1.871	11.816
139	O7	10.745	3.095	9.526
140	O8	11.017	7.842	9.155
141	O9	-4.427	9.898	7.293
142	O10	-4.263	10.584	12.006
143	O11	-4.759	4.053	12.934
144	O12	-4.461	3.262	8.294
145	O13	-3.074	5.588	15.76
146	O14	-2.521	10.239	14.877
147	O15	-1.702	19.411	14.395
148	O16	-2	19.725	9.64
149	O17	1.308	21.787	14.55
150	O18	1.274	21.982	8.787
151	O19	6.006	21.391	8.612
152	O20	8.622	19.436	9.085
153	O21	9.031	19.829	13.779
154	O22	6.017	21.895	14.419
155	O23	-3.024	8.356	4.679
156	O24	-3.224	3.733	5.857
157	C61	-2.017	4.8	13.228
158	C62	8.112	13.556	10.424
159	C63	5.567	17.076	9.115
160	C64	6.451	14.719	8.858
161	C65	6.821	16.196	9.041
162	C66	7.672	13.8	8.975
163	H1	5.619	16.877	13.996
164	H2	7.295	17.07	14.465
165	H3	4.863	17.304	16.288
166	H4	6.44	17.929	16.756
167	H5	6.117	15.688	17.648
168	H6	7.468	15.722	16.523
169	H7	6	14.736	14.734
170	H8	4.648	14.714	15.869
171	H9	5.925	13.167	17.359
172	H10	7.311	13.255	16.267
173	H11	5.943	12.257	14.428
174	H12	4.536	12.239	15.483
175	H13	5.45	10.026	15.364
176	H14	5.633	10.633	17.008
177	H15	8.028	11.118	16.598
178	H16	7.853	10.671	14.903
179	H17	7.215	8.318	15.648
180	H18	7.405	8.832	17.31
181	H19	6.453	18.821	8.29
182	H20	-0.424	17.437	8.874

183	H21	1.207	17.077	9.384
184	H22	0.158	19.817	8.556
185	H23	2.056	17.792	7.109
186	H24	0.428	18.296	6.673
187	H25	0.862	16.167	5.657
188	H26	-0.373	15.949	6.892
189	H27	1.379	15.057	8.466
190	H28	2.609	15.288	7.221
191	H29	1.429	13.674	5.736
192	H30	0.116	13.547	6.909
193	H31	2.179	10.458	7.635
194	H32	1.905	11.052	5.999
195	H33	3.034	12.737	7.402
196	H34	1.755	12.649	8.605
197	H35	-0.451	11.409	6.407
198	H36	-0.252	11.227	8.146
199	H37	0.365	8.799	7.788
200	H38	0.181	9.027	6.061
201	H39	-2.158	9.735	6.378
202	H40	-1.84	10.751	12.687
203	H41	0.424	9.009	11.628
204	H42	0.391	9.817	13.18
205	H43	-0.003	12.035	11.962
206	H44	0.232	11.189	10.452
207	H45	2.296	12.247	11.019
208	H46	2.516	10.511	11.108
209	H47	3.66	11.721	12.934
210	H48	2.521	10.538	13.534
211	H49	2.41	12.559	14.872
212	H50	0.877	12.309	14.073
213	H51	1.404	14.046	12.392
214	H52	3.046	14.207	13.022
215	H53	2.195	15.021	15.18
216	H54	0.526	14.744	14.681
217	H55	0.693	16.43	12.922
218	H56	2.411	16.656	13.218
219	H57	1.785	17.339	15.647
220	H58	0.111	17.219	15.154
221	H59	0.575	19.448	15.189
222	H60	-0.429	3.332	12.967
223	H61	0.133	4.991	12.761
224	H62	0.295	4.826	8.968
225	H63	0.435	4.079	7.398
226	H64	0.524	1.917	8.181
227	H65	-0.486	2.224	9.579
228	H66	1.411	3.542	10.623
229	H67	2.441	3.037	9.279
230	H68	1.142	2.566	14.707
231	H69	2.061	4.042	14.4
232	H70	2.861	2.646	17.971
233	H71	2.499	1.656	16.564
234	H72	2.128	0.662	9.872
235	H73	0.878	1.074	11.04
236	H74	4.437	4.032	16.586
237	H75	4.138	2.966	15.21
238	H76	4.901	1.003	16.587
239	H77	5.244	2.083	17.93
240	H78	2.808	0.592	12.292
241	H79	2.552	2.328	12.417
242	H80	5.066	0.746	12.951
243	H81	5.02	2.495	13.121
244	H82	6.899	1.011	11.207
245	H83	7.284	1.389	12.874

246	H84	4.535	1.002	10.49
247	H85	4.351	2.741	10.744
248	H86	1.98	4.672	16.772
249	H87	0.808	3.411	17.118
250	H88	0.084	5.403	15.155
251	H89	-0.807	3.909	15.458
252	H90	6.621	2.088	15.204
253	H91	7.26	1.435	16.705
254	H92	6.907	3.887	17.639
255	H93	6.832	4.36	15.954
256	H94	9.749	9.493	16.846
257	H95	9.052	2.801	17.33
258	H96	8.976	2.327	10.885
259	H97	9.373	8.991	10.379
260	H98	7.028	7.851	11.915
261	H99	7.083	8.299	10.227
262	H0	7.336	10.168	12.628
263	H1	5.997	10.039	11.507
264	H2	7.426	10.892	9.657
265	H3	8.808	10.995	10.75
266	H4	7.511	12.562	12.225
267	H5	6.234	12.614	11.014
268	H6	6.902	19.454	15.001
269	H7	6.767	3.347	10.584
270	H8	6.772	3.892	12.247
271	H9	-2.93	19.771	12.098
272	H10	11.417	8.797	10.454
273	H11	12.864	9.878	15.622
274	H12	12.163	1.824	16.351
275	H13	11.092	8.377	19.618
276	H14	10.631	4.01	19.943
277	H15	11.037	2.321	11.007
278	H16	11.282	3.168	8.716
279	H17	11.518	7.584	8.359
280	H18	-5.347	10.15	7.471
281	H19	-5.197	10.777	11.829
282	H20	-5.669	3.804	12.704
283	H21	-3.912	3.4	7.495
284	H22	-3.477	5.972	16.555
285	H23	-2.956	10.27	15.744
286	H24	-2.64	19.636	14.288
287	H25	-2.917	19.921	9.892
288	H26	1.494	22.739	14.55
289	H27	1.564	22.899	8.662
290	H28	5.94	22.349	8.477
291	H29	9.507	19.824	9.175
292	H30	8.911	19.144	14.459
293	H31	6.768	21.404	14.046
294	H32	-3.578	8.016	3.959
295	H33	-3.594	3.698	4.956
296	H34	-2.55	4.165	13.948
297	H35	4.955	16.883	8.225
298	H36	5.684	14.423	9.582
299	H37	6.01	14.593	7.861
300	H38	7.452	16.519	8.205
301	H39	7.409	16.321	9.956
302	H40	8.043	14.484	11.001
303	H41	9.174	13.277	10.426
304	H42	7.45	12.846	8.484
305	H43	8.507	14.245	8.419
306	H3	8.104	5.831	12
307	H6	11.608	5.363	8.503
308	H20	9.829	19.987	11.373

309	H23	5.135	18.452	11.818
310	H36	8.642	6.11	15.503
311	H39	10.869	6.206	19.938
312	H43	12.869	9.817	13.405
313	H46	8.279	7.998	13.774
314	H50	12.263	1.576	14.15
315	H53	7.949	4.002	14.027
316	H64	-1.845	3.125	7.658
317	H66	-1.075	6.751	8.458
318	H69	-3.661	5.833	4.317
319	H83	3.192	17.947	9.521
320	H86	3.77	22.761	8.517
321	H93	1.95	18.942	11.745
322	H97	3.708	22.885	14.556
323	CH00	3.703	17.947	14.253
324	CH12	-0.684	9.007	9.702
325	CH15	-5.401	10.534	9.645
326	CH18	-1.419	7.09	11.799
327	CH21	-3.209	8.148	16.306
328	CH26	-5.612	3.38	10.525
329	CH29	-0.884	4.819	10.726
330	H1	4.978	16.753	9.983
331	C1	3.182	7.591	8.793
332	C2	3.339	6.435	9.78
333	C3	3.667	6.943	11.184
334	C4	3.85	5.779	12.158
335	C5	4.294	6.215	13.557
336	C6	3.274	7.112	14.261
337	C7	3.653	7.341	15.724
338	C8	2.654	8.268	16.416
339	C9	3.005	8.467	17.881
340	C10	2.845	7.086	7.399
341	H2	2.39	8.267	9.136
342	H3	4.11	8.173	8.751
343	H4	4.133	5.762	9.434
344	H5	2.411	5.852	9.811
345	H6	2.857	7.598	11.525
346	H7	4.582	7.546	11.153
347	H8	4.606	5.092	11.76
348	H9	2.915	5.21	12.231
349	H10	5.259	6.732	13.494
350	H11	4.461	5.312	14.156
351	H12	2.279	6.656	14.208
352	H13	3.216	8.079	13.749
353	H14	3.687	6.38	16.249
354	H15	4.659	7.771	15.783
355	H16	2.64	9.242	15.913
356	H17	1.644	7.849	16.341
357	H18	2.284	9.14	18.355
358	H19	2.985	7.514	18.421
359	H20	4.002	8.903	17.991
360	H21	3.629	6.421	7.022
361	H22	1.899	6.537	7.399
362	H23	2.751	7.926	6.704

Table S11. Cartesian coordinates of the structure of (dodecane)⊂**1** optimized by MacroModel Ver 9.1 using the MMFFs force field.

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	C1	10.076	4.372	9.591
2	C2	9.124	4.462	10.619
3	C02B	0.308	19.131	13.166
4	C3	8.716	5.742	11.039
5	C4	9.246	6.906	10.454
6	C5	10.184	6.756	9.418
7	C6	10.593	5.503	8.97
8	C18	6.751	18.951	10.528
9	C19	8.077	19.393	10.429
10	C20	8.82	19.698	11.567
11	C21	8.248	19.536	12.825
12	C22	6.928	19.095	12.978
13	C23	6.197	18.796	11.813
14	C35	9.797	7.35	16.783
15	C36	9.32	6.124	16.277
16	C37	9.527	4.909	16.962
17	C38	10.241	4.945	18.169
18	C39	10.743	6.14	18.679
19	C40	10.511	7.33	17.991
20	C41	10.049	8.776	14.665
21	C42	11.342	9.279	14.461
22	C43	11.856	9.457	13.18
23	C44	11.078	9.133	12.071
24	C45	9.778	8.622	12.213
25	C46	9.3	8.416	13.525
26	C48	9.56	3.185	15.086
27	C49	10.783	2.498	15.04
28	C50	11.338	2.082	13.831
29	C51	10.666	2.332	12.639
30	C52	9.431	2.997	12.629
31	C53	8.923	3.458	13.863
32	C64	-1.6	4.074	8.189
33	C65	-1.923	5.232	7.249
34	C66	-1.529	6.545	7.553
35	C67	-1.861	7.624	6.712
36	C68	-2.541	7.348	5.515
37	C69	-2.958	6.057	5.2
38	C70	-2.674	5.021	6.085
39	C82	2.208	19.787	9.231
40	C83	3.367	18.998	9.368
41	C84	4.663	19.522	9.195
42	C85	4.772	20.894	8.924
43	C86	3.645	21.714	8.837
44	C87	2.377	21.157	8.989
45	C88	0.165	19.28	10.712
46	C89	-1.218	19.489	10.838
47	C91	-1.077	19.332	13.235
48	C93	0.911	19.097	11.891
49	C95	2.473	19.655	14.46
50	C96	2.492	21.056	14.556
51	C97	3.689	21.766	14.585
52	C98	4.9	21.082	14.515
53	C99	4.945	19.68	14.438
54	C100	3.714	18.992	14.407
55	C111	-2.179	9.801	10.881
56	C112	-1.571	9.377	9.684

57	C113	-2.237	9.437	8.443
58	C114	-3.576	9.857	8.44
59	C115	-4.222	10.237	9.615
60	C116	-3.519	10.218	10.817
61	C117	-1.847	8.719	13.17
62	C118	-1.74	7.367	12.789
63	C119	-2.129	6.324	13.652
64	C120	-2.619	6.669	14.922
65	C121	-2.715	7.998	15.33
66	C122	-2.321	9.01	14.457
67	C124	-2.627	4.526	11.898
68	C125	-3.986	4.195	11.821
69	C126	-4.577	3.834	10.611
70	C127	-3.811	3.795	9.446
71	C128	-2.45	4.138	9.46
72	C129	-1.89	4.525	10.698
73	C1	6.31	17.432	14.725
74	C2	5.973	17.145	16.194
75	C3	6.437	15.756	16.65
76	C4	5.801	14.603	15.87
77	C5	6.323	13.249	16.362
78	C6	5.71	12.1	15.56
79	C7	6.134	10.711	16.04
80	C8	7.628	10.438	15.871
81	C9	7.964	8.981	16.216
82	C10	5.918	18.637	9.285
83	C11	0.687	17.711	8.821
84	C12	0.805	19.178	9.324
85	C13	1.079	17.541	7.345
86	C14	0.805	16.135	6.804
87	C15	1.68	15.051	7.44
88	C16	1.358	13.675	6.85
89	C17	1.78	11.149	7.077
90	C18	2.127	12.562	7.566
91	C19	0.286	10.837	7.191
92	C20	-0.021	9.339	7.054
93	C21	-1.546	9.06	7.125
94	C22	-1.431	9.842	12.217
95	C23	0.119	9.912	12.159
96	C24	0.632	11.206	11.512
97	C25	2.151	11.376	11.603
98	C26	2.721	11.497	13.02
99	C27	2.051	12.543	13.916
100	C28	2.114	13.963	13.351
101	C29	1.603	14.98	14.373
102	C30	1.507	16.386	13.772
103	C31	1.146	17.413	14.856
104	C32	1.13	18.91	14.437
105	C33	-0.495	4.383	13.371
106	C34	-0.068	3.929	8.395
107	C35	0.285	2.577	9.032
108	C36	1.544	2.654	9.893
109	C37	1.338	3.666	15.014
110	C38	2.921	2.829	16.858
111	C39	1.765	1.331	10.626
112	C40	4.288	3.133	16.236
113	C41	5.327	2.137	16.765
114	C42	2.814	1.423	11.729
115	C43	5.223	1.611	12.362
116	C44	6.678	1.699	11.918
117	C45	4.226	1.686	11.209
118	C46	1.811	3.805	16.465
119	C47	0.004	4.398	14.824

120	C48	6.734	2.292	16.183
121	C49	7.393	3.641	16.504
122	C50	9.48	8.672	16.083
123	C51	8.949	3.597	16.427
124	C52	8.647	3.202	11.332
125	C53	8.912	8.298	10.994
126	C54	7.385	8.55	11.148
127	C55	6.986	9.981	11.561
128	C56	7.609	11.084	10.701
129	C57	7.236	12.485	11.197
130	C58	6.278	18.937	14.355
131	C59	7.103	3.109	11.471
132	C60	-1.841	19.52	12.085
133	O1	11.674	9.364	10.86
134	O2	12.108	9.619	15.542
135	O3	11.44	2.221	16.208
136	O4	10.958	8.508	18.526
137	O5	10.421	3.788	18.877
138	O6	11.286	1.877	11.506
139	O7	10.563	3.132	9.255
140	O8	10.77	7.881	8.891
141	O9	-4.258	9.906	7.255
142	O10	-4.142	10.631	11.964
143	O11	-4.744	4.213	12.96
144	O12	-4.482	3.389	8.322
145	O13	-2.983	5.675	15.791
146	O14	-2.376	10.313	14.872
147	O15	-1.689	19.326	14.46
148	O16	-1.972	19.639	9.704
149	O17	1.307	21.736	14.633
150	O18	1.269	21.954	8.884
151	O19	6.012	21.437	8.729
152	O20	8.655	19.509	9.195
153	O21	9.04	19.845	13.895
154	O22	6.017	21.874	14.53
155	O23	-2.812	8.372	4.649
156	O24	-3.191	3.769	5.863
157	C61	-1.975	4.858	13.247
158	C62	8.089	13.576	10.533
159	C63	5.627	17.113	9.181
160	C64	6.526	14.768	8.893
161	C65	6.886	16.243	9.113
162	C66	7.738	13.848	9.064
163	H1	5.649	16.854	14.068
164	H2	7.324	17.053	14.533
165	H3	4.896	17.24	16.364
166	H4	6.463	17.888	16.835
167	H5	6.201	15.644	17.715
168	H6	7.53	15.697	16.564
169	H7	6.026	14.699	14.802
170	H8	4.711	14.644	15.979
171	H9	6.085	13.125	17.425
172	H10	7.414	13.232	16.267
173	H11	5.96	12.213	14.498
174	H12	4.62	12.162	15.638
175	H13	5.57	9.969	15.463
176	H14	5.848	10.581	17.09
177	H15	8.204	11.101	16.526
178	H16	7.925	10.665	14.842
179	H17	7.36	8.3	15.605
180	H18	7.654	8.801	17.256
181	H19	6.498	18.877	8.384
182	H20	-0.354	17.377	8.933

183	H21	1.278	17.041	9.457
184	H22	0.19	19.767	8.629
185	H23	2.137	17.779	7.191
186	H24	0.504	18.255	6.742
187	H25	0.979	16.142	5.721
188	H26	-0.255	15.891	6.95
189	H27	1.512	15.022	8.522
190	H28	2.74	15.285	7.281
191	H29	1.597	13.661	5.78
192	H30	0.279	13.506	6.944
193	H31	2.355	10.431	7.674
194	H32	2.101	11.028	6.035
195	H33	3.205	12.724	7.439
196	H34	1.926	12.62	8.642
197	H35	-0.257	11.38	6.408
198	H36	-0.084	11.209	8.151
199	H37	0.528	8.771	7.814
200	H38	0.362	8.995	6.083
201	H39	-1.971	9.736	6.371
202	H40	-1.726	10.801	12.666
203	H41	0.543	9.041	11.644
204	H42	0.497	9.864	13.187
205	H43	0.132	12.071	11.961
206	H44	0.362	11.221	10.453
207	H45	2.433	12.271	11.035
208	H46	2.64	10.532	11.1
209	H47	3.791	11.727	12.941
210	H48	2.663	10.524	13.519
211	H49	2.543	12.522	14.895
212	H50	1.008	12.265	14.104
213	H51	1.513	14.031	12.437
214	H52	3.148	14.21	13.079
215	H53	2.278	14.99	15.237
216	H54	0.614	14.677	14.739
217	H55	0.736	16.377	12.993
218	H56	2.45	16.638	13.279
219	H57	1.811	17.29	15.721
220	H58	0.141	17.154	15.218
221	H59	0.585	19.391	15.264
222	H60	-0.416	3.358	12.985
223	H61	0.173	5.005	12.762
224	H62	0.334	4.762	8.983
225	H63	0.441	3.987	7.423
226	H64	0.42	1.83	8.24
227	H65	-0.54	2.214	9.655
228	H66	1.435	3.462	10.627
229	H67	2.409	2.893	9.266
230	H68	1.205	2.607	14.762
231	H69	2.094	4.071	14.333
232	H70	3.022	2.861	17.951
233	H71	2.616	1.807	16.604
234	H72	2.041	0.55	9.907
235	H73	0.824	1.011	11.091
236	H74	4.585	4.157	16.486
237	H75	4.227	3.065	15.146
238	H76	4.983	1.117	16.546
239	H77	5.384	2.216	17.858
240	H78	2.804	0.476	12.284
241	H79	2.531	2.206	12.443
242	H80	5.089	0.656	12.887
243	H81	5.009	2.402	13.089
244	H82	6.868	0.983	11.109
245	H83	7.291	1.373	12.765

246	H84	4.483	0.94	10.448
247	H85	4.28	2.672	10.735
248	H86	2.133	4.836	16.655
249	H87	0.961	3.617	17.134
250	H88	0.111	5.435	15.163
251	H89	-0.744	3.924	15.47
252	H90	6.693	2.143	15.099
253	H91	7.348	1.479	16.588
254	H92	7.113	3.933	17.526
255	H93	6.98	4.416	15.847
256	H94	9.958	9.481	16.651
257	H95	9.216	2.792	17.125
258	H96	8.873	2.342	10.687
259	H97	9.19	9.009	10.208
260	H98	6.942	7.857	11.871
261	H99	6.899	8.326	10.188
262	H0	7.254	10.145	12.61
263	H1	5.892	10.062	11.514
264	H2	7.295	10.951	9.66
265	H3	8.7	11.003	10.726
266	H4	7.413	12.536	12.279
267	H5	6.168	12.671	11.042
268	H6	6.914	19.429	15.103
269	H7	6.64	3.324	10.499
270	H8	6.71	3.861	12.163
271	H9	-2.912	19.67	12.158
272	H10	11.236	8.832	10.16
273	H11	12.983	9.905	15.235
274	H12	12.279	1.78	16.003
275	H13	11.508	8.322	19.303
276	H14	11.02	3.955	19.621
277	H15	10.932	2.341	10.717
278	H16	11.061	3.214	8.42
279	H17	11.226	7.631	8.066
280	H18	-5.179	10.163	7.42
281	H19	-5.074	10.825	11.775
282	H20	-5.663	4	12.733
283	H21	-3.925	3.494	7.525
284	H22	-3.367	6.07	16.59
285	H23	-2.795	10.355	15.746
286	H24	-2.63	19.536	14.349
287	H25	-2.892	19.821	9.952
288	H26	1.488	22.69	14.635
289	H27	1.546	22.876	8.768
290	H28	5.932	22.395	8.603
291	H29	9.534	19.908	9.293
292	H30	8.929	19.147	14.564
293	H31	6.776	21.387	14.168
294	H32	-3.362	8.044	3.921
295	H33	-3.55	3.739	4.957
296	H34	-2.517	4.235	13.97
297	H35	5.025	16.925	8.282
298	H36	5.721	14.463	9.572
299	H37	6.138	14.655	7.873
300	H38	7.532	16.584	8.295
301	H39	7.457	16.353	10.04
302	H40	7.998	14.496	11.121
303	H41	9.145	13.284	10.592
304	H42	7.55	12.905	8.541
305	H43	8.605	14.305	8.571
306	H3	8.022	5.832	11.871
307	H6	11.349	5.413	8.198
308	H20	9.847	20.043	11.494

309	H23	5.17	18.446	11.901
310	H36	8.756	6.118	15.348
311	H39	11.283	6.149	19.62
312	H43	12.854	9.853	13.022
313	H46	8.308	7.996	13.66
314	H50	12.286	1.554	13.798
315	H53	7.992	4.015	13.876
316	H64	-1.873	3.131	7.695
317	H66	-0.99	6.737	8.478
318	H69	-3.525	5.868	4.295
319	H83	3.246	17.945	9.598
320	H86	3.755	22.774	8.634
321	H93	1.98	18.912	11.825
322	H97	3.701	22.849	14.657
323	CH00	3.729	17.912	14.342
324	CH12	-0.546	9.021	9.712
325	CH15	-5.256	10.566	9.59
326	CH18	-1.348	7.129	11.804
327	CH21	-3.075	8.241	16.323
328	CH26	-5.627	3.564	10.555
329	CH29	-0.845	4.816	10.743
330	H1	5.031	16.774	10.039
331	C1	3.111	6.769	9.07
332	C2	3.846	6.162	10.267
333	C3	3.599	6.976	11.538
334	C4	4.274	6.333	12.752
335	C5	4.208	7.204	14.01
336	C6	2.779	7.47	14.486
337	C7	2.758	8.232	15.811
338	C8	1.325	8.507	16.269
339	C9	1.302	9.274	17.591
340	C10	3.388	5.98	7.792
341	C11	2.635	6.558	6.605
342	C12	-0.121	9.562	18.041
343	H2	2.033	6.783	9.27
344	H3	3.426	7.811	8.934
345	H4	4.922	6.123	10.06
346	H5	3.508	5.131	10.419
347	H6	2.519	7.051	11.709
348	H7	3.979	7.995	11.399
349	H8	5.329	6.14	12.523
350	H9	3.815	5.358	12.954
351	H10	4.717	8.157	13.821
352	H11	4.768	6.699	14.807
353	H12	2.251	6.519	14.604
354	H13	2.235	8.048	13.732
355	H14	3.287	7.653	16.578
356	H15	3.291	9.183	15.696
357	H16	0.799	9.086	15.502
358	H17	0.787	7.559	16.385
359	H18	1.814	8.693	18.366
360	H19	1.844	10.221	17.482
361	H20	4.463	5.989	7.576
362	H21	3.094	4.933	7.927
363	H22	2.863	5.989	5.698
364	H23	1.555	6.515	6.769
365	H24	2.916	7.602	6.431
366	H25	-0.116	10.098	18.995
367	H26	-0.645	10.183	17.307
368	H27	-0.687	8.635	18.174

References

[1] D. Shimoyama, R. Sekiya, H. Kudo, T. Haino, *Org. Lett.* **2020**, *22*, 352-356.

[2] F. Mohamadi, N. G. J. Richards, W. C. Guida, R. Liskamp, M. Lipton, C. Caufield, G. Chang, T. Hendrickson, W. C. Still, *J. Comput. Chem.* **1990**, *11*, 440-467.

[3] G. M. Sheldrick, *Acta Crystallogr., Sect. A: Found. Adv*., **2015**, *71*, 3–8.

[4] A. L. Spek, *Acta Crystallogr., Sect. C: Struct. Chem*., **2015**, *71*, 9–18.