Supplementary Information

Tuning Rotational Barriers through Substituent Modification in Catechol-Diyl Molecular Gyrotops

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1. Copies of NMR and HRMS Spectra for All New Compounds

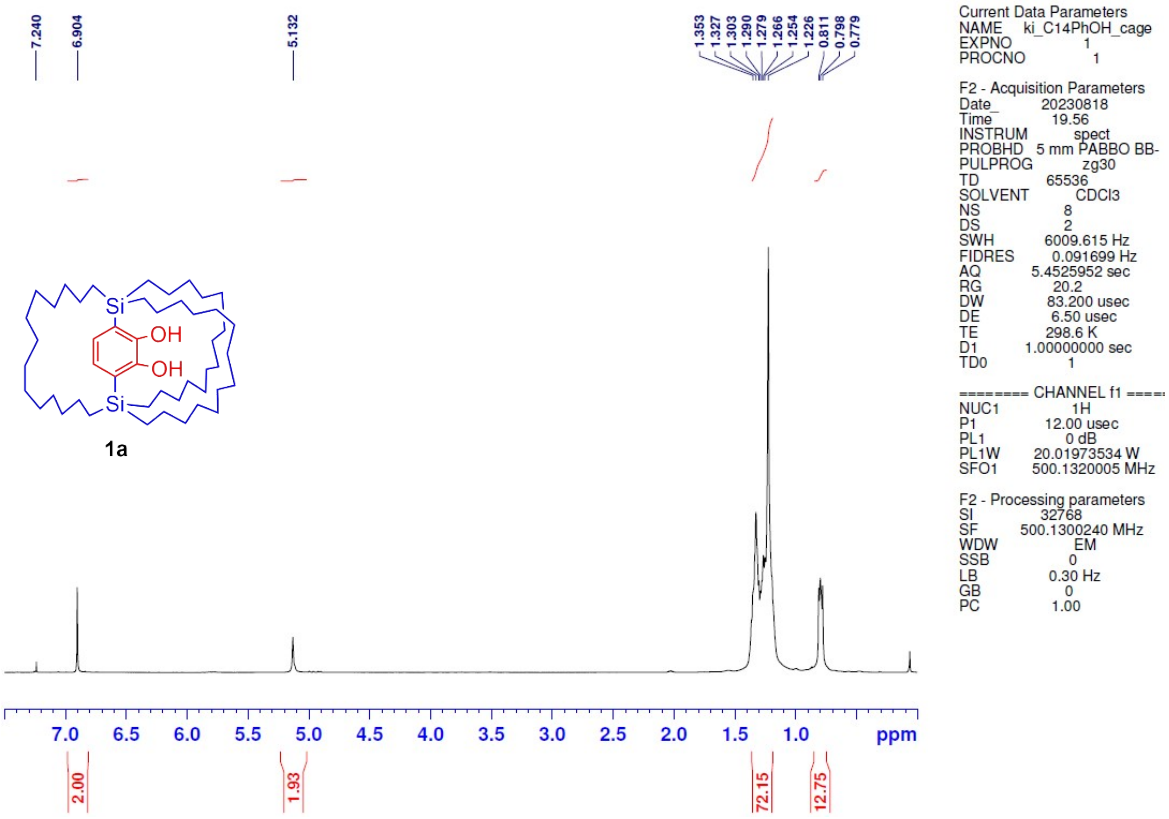


Fig. S1. ^{1}H NMR spectrum of **1a** in $CDCl_3$.

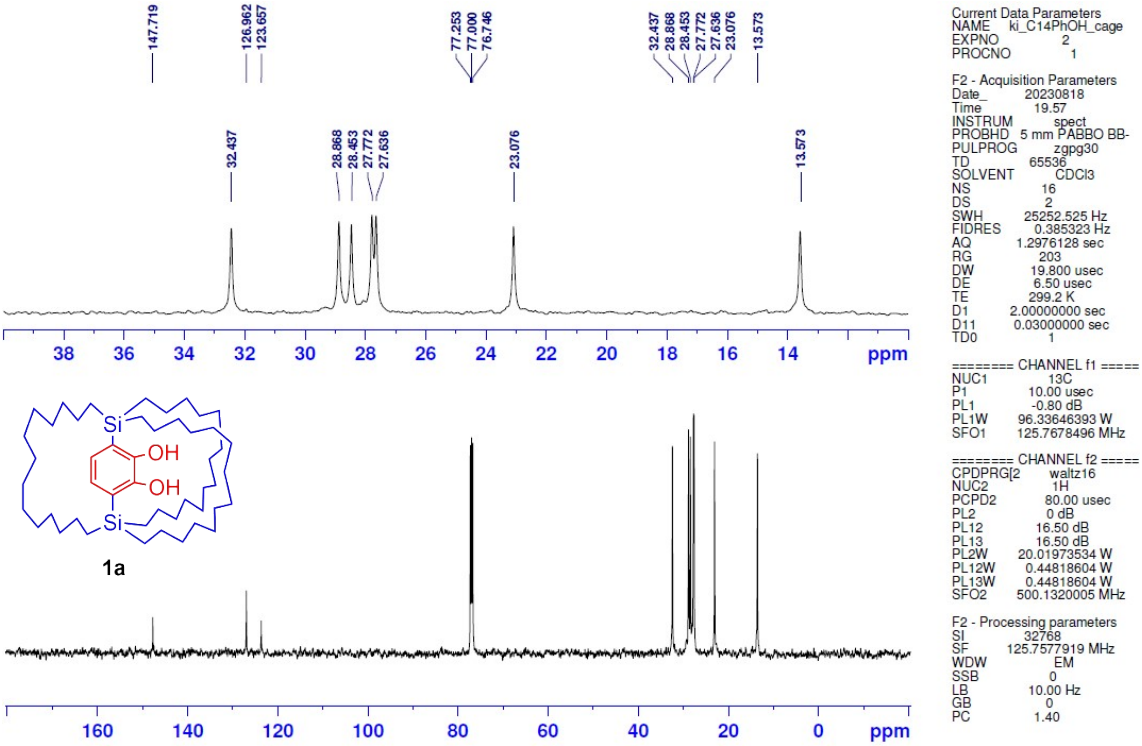


Fig. S2. ^{13}C NMR spectrum of **1a** in $CDCl_3$.

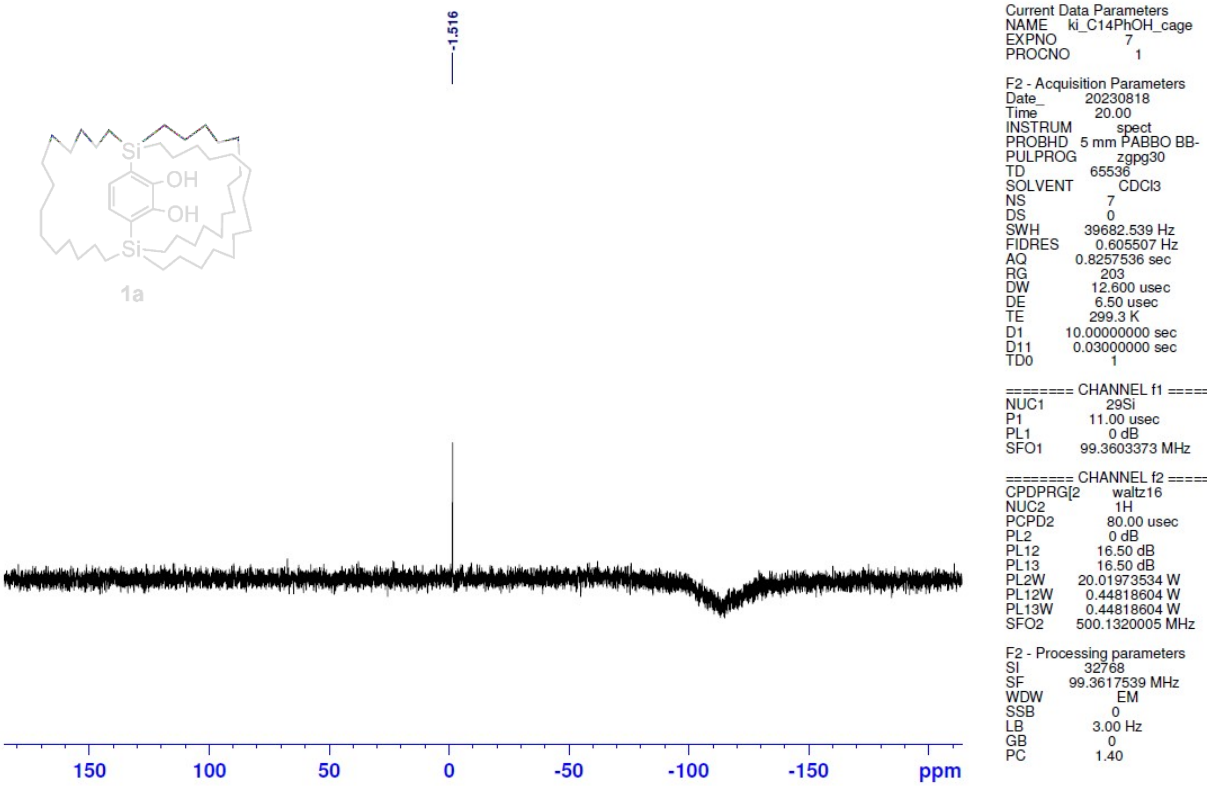


Fig. S3. ^{29}Si NMR spectrum of **1a** in $CDCl_3$.

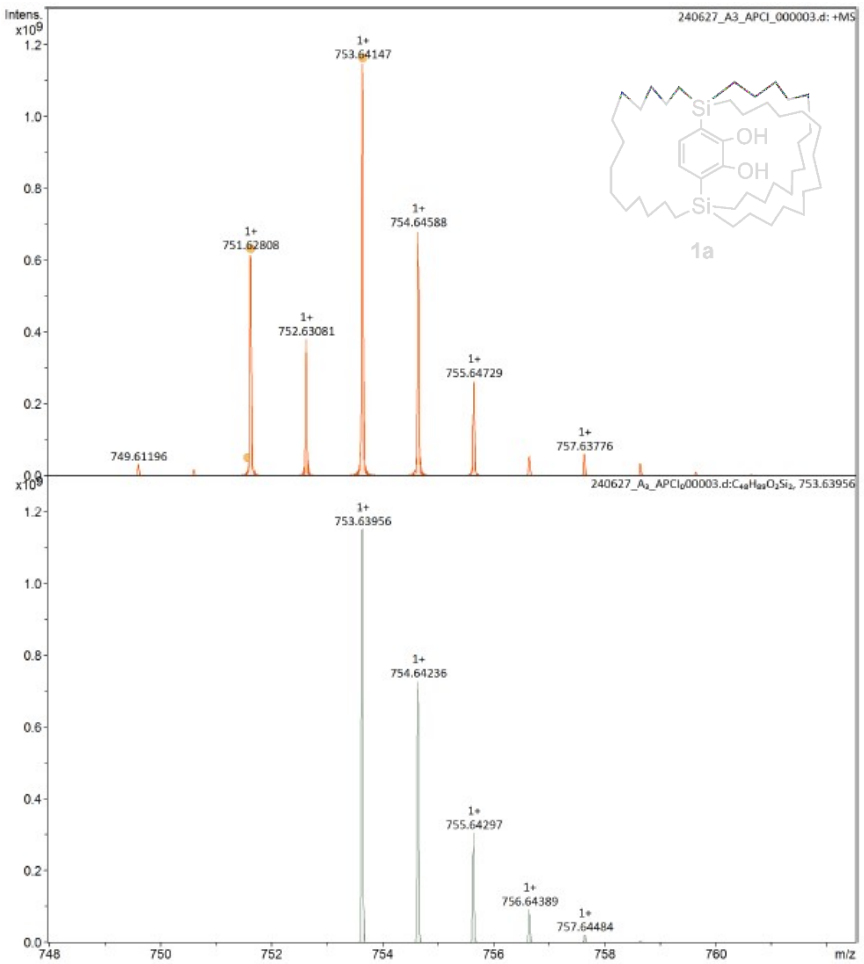


Fig. S4. HRMS spectrum of **1a** (APCI, positive). Top: obsd. Center and Bottom: sim.

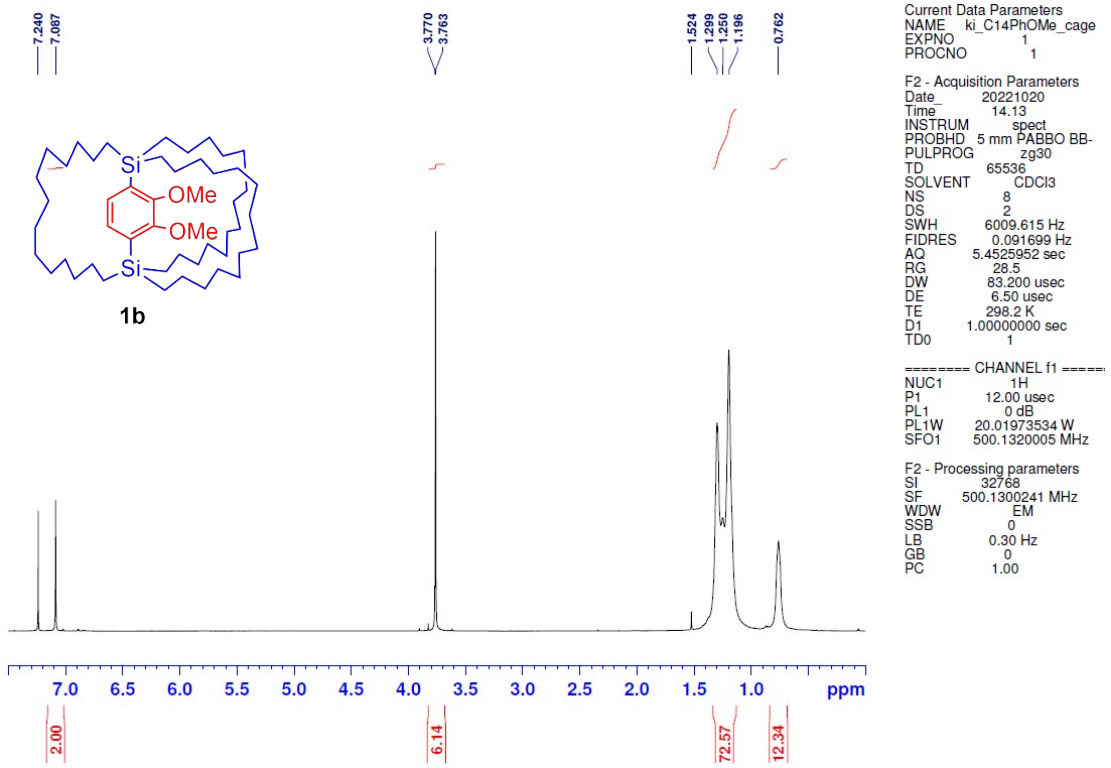


Fig. S5. ^{1}H NMR spectrum of **1b** in $CDCl_3$.

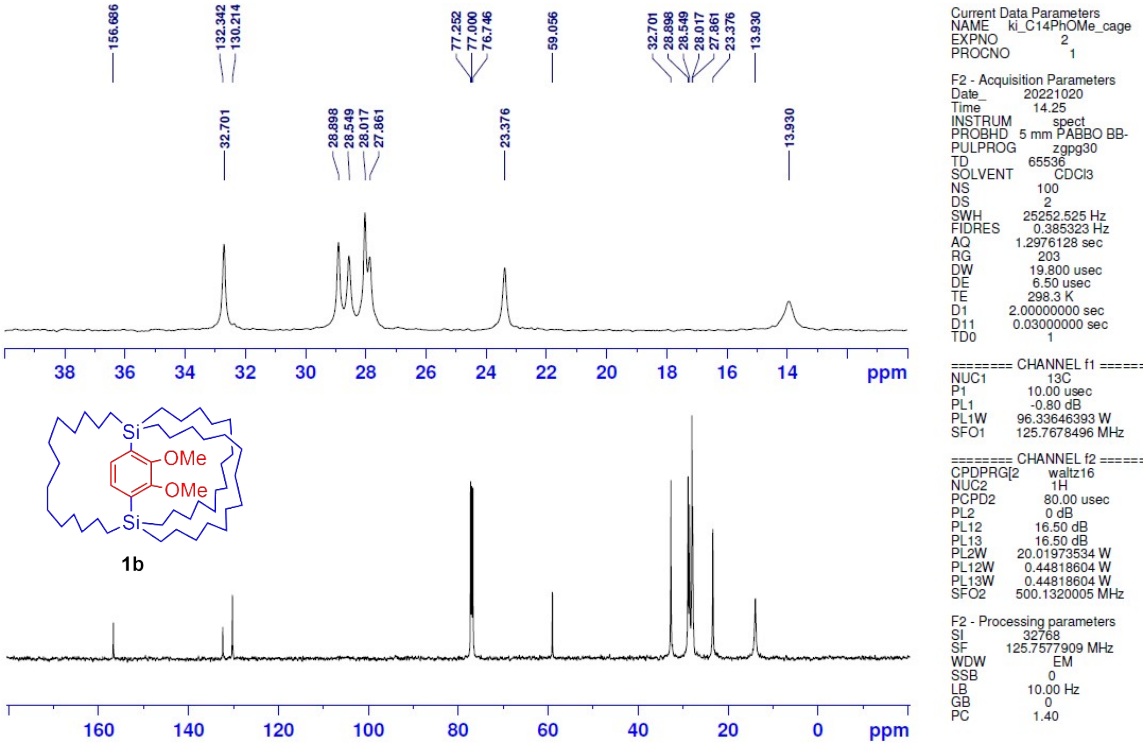


Fig. S6. ^{13}C NMR spectrum of **1b** in $CDCl_3$.

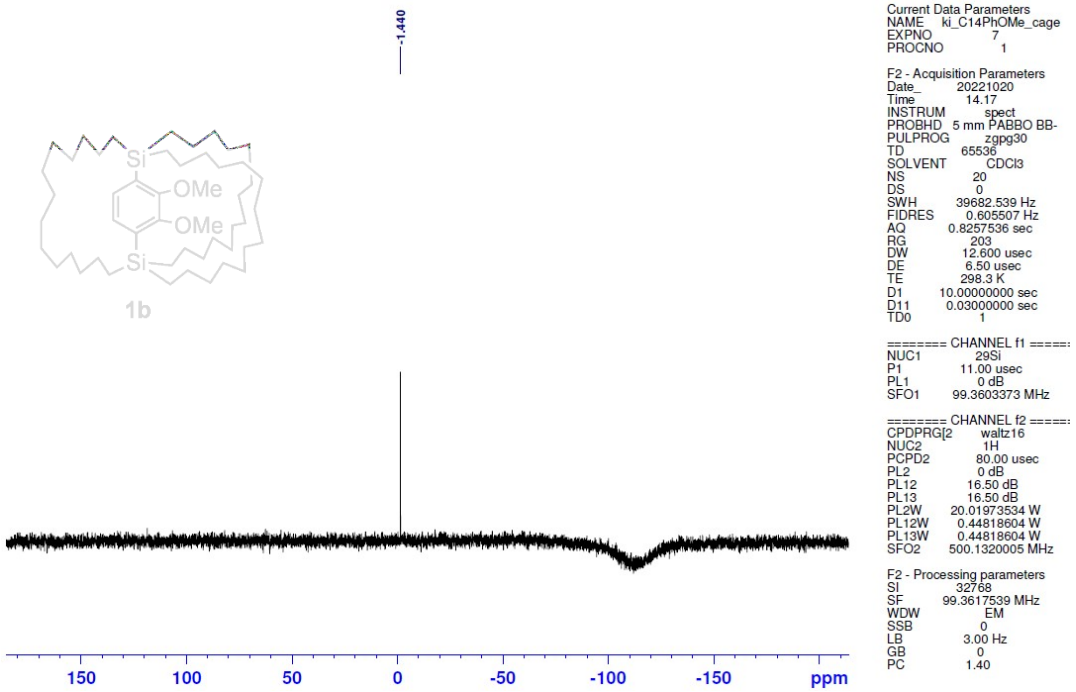


Fig. S7. ^{29}Si NMR spectrum of **1b** in $CDCl_3$.

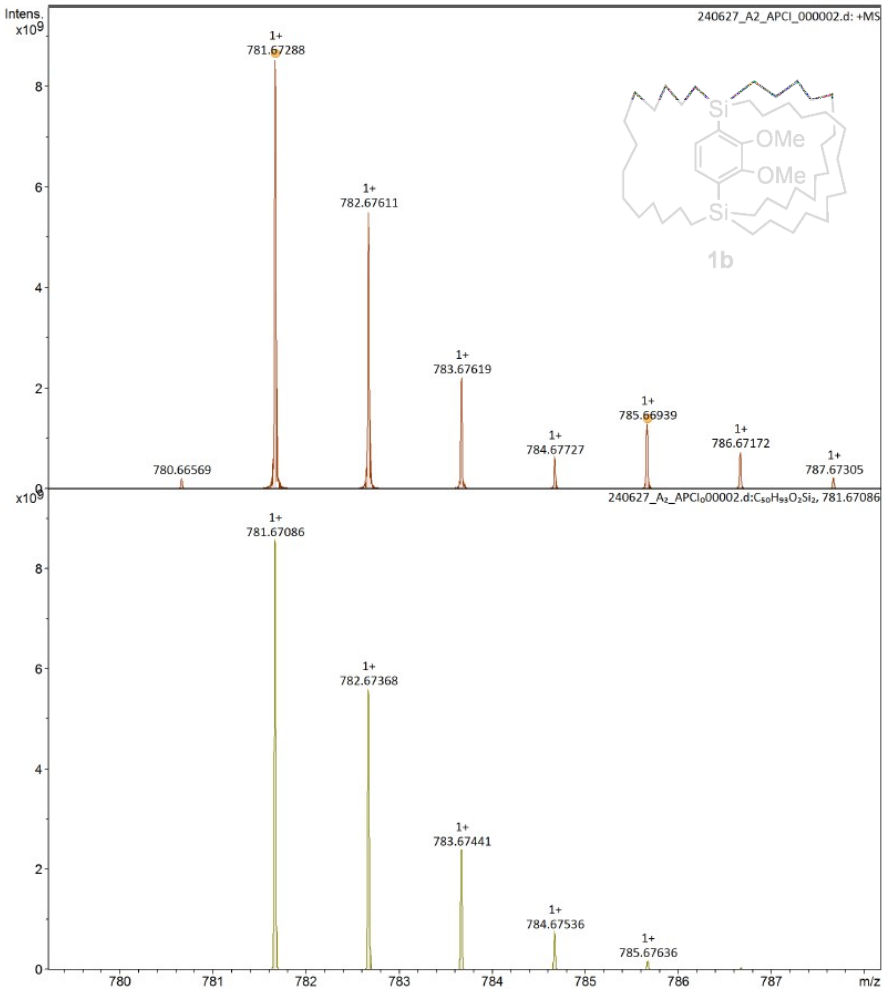


Fig. S8. HRMS spectrum of **1b** (APCI, positive). Top: obsd. Center and Bottom: sim.

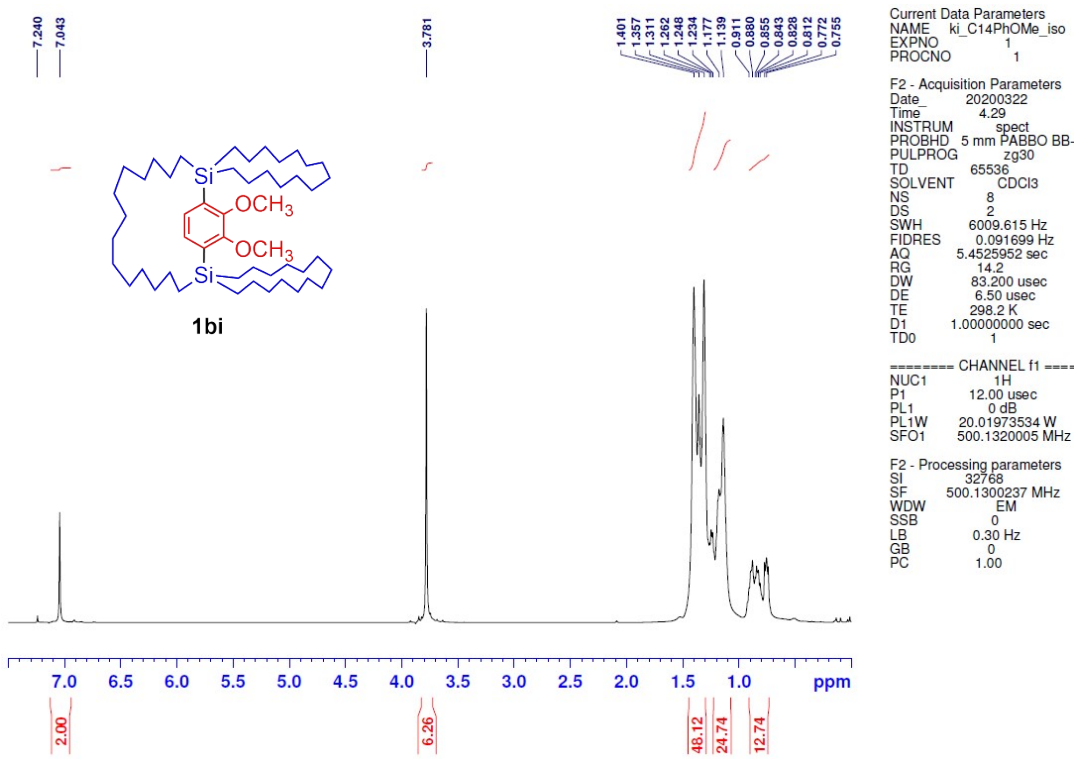


Fig. S9. ^{1}H NMR spectrum of **1bi** in $CDCl_3$.

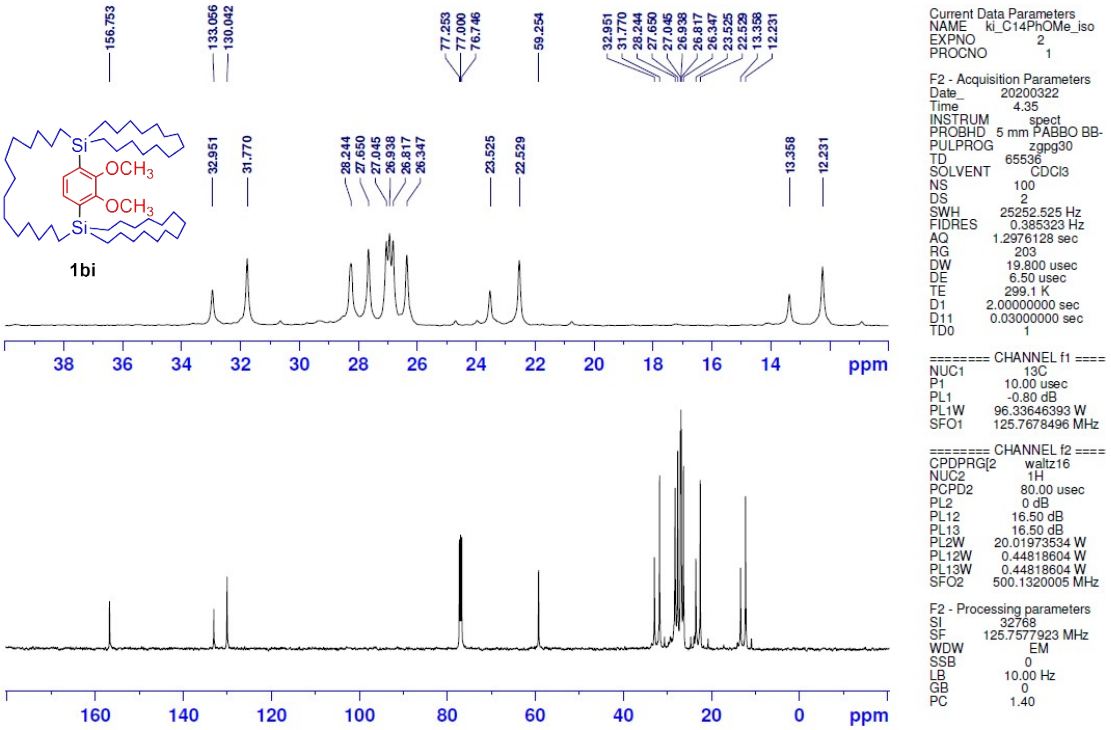


Fig. S10. ^{13}C NMR spectrum of **1bi** in $CDCl_3$.

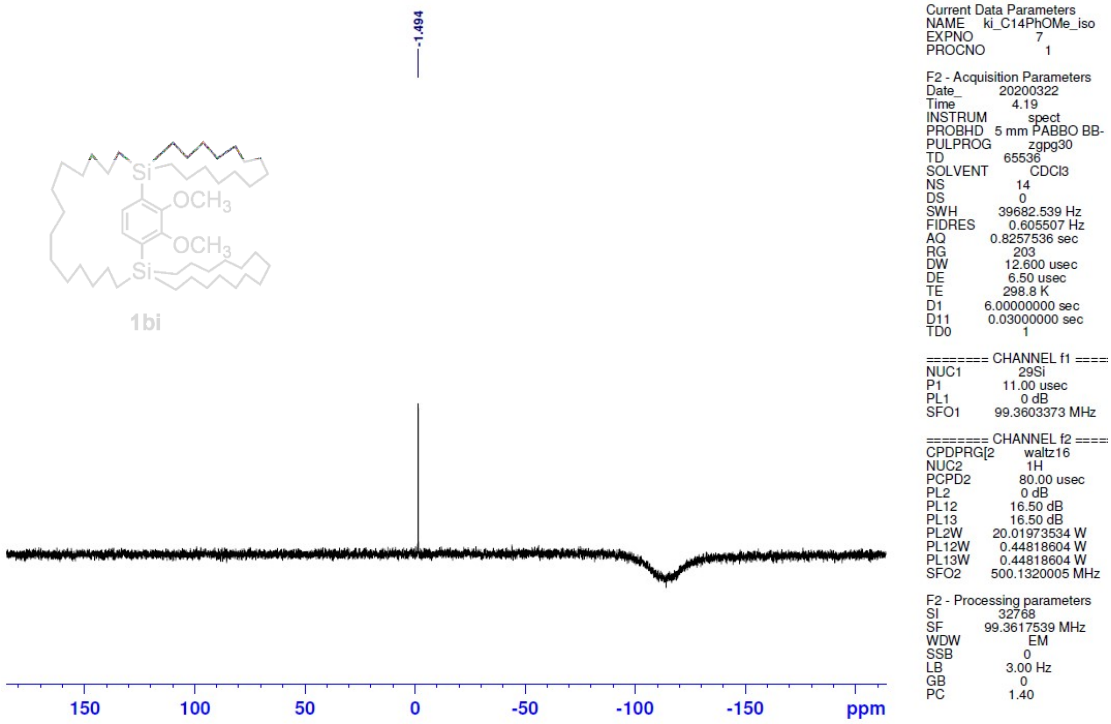


Fig. S11. ^{29}Si NMR spectrum of **1bi** in $CDCl_3$.

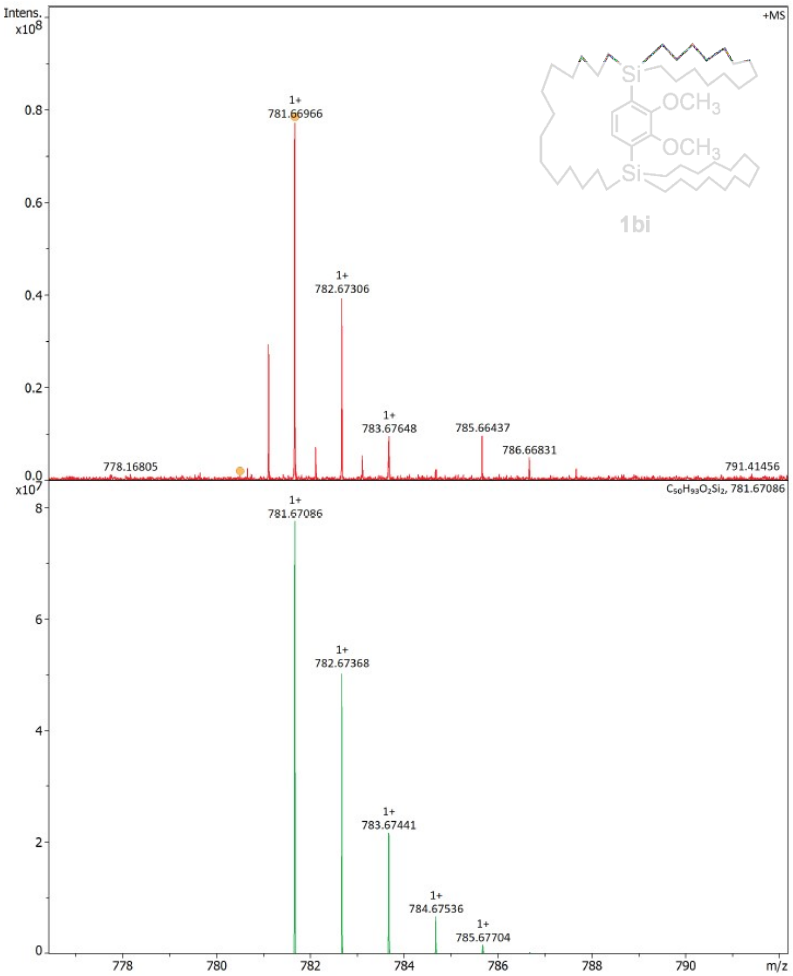


Fig. S12. HRMS spectrum of **1bi** (APCI, positive). Top: obsd. Center and Bottom: sim.

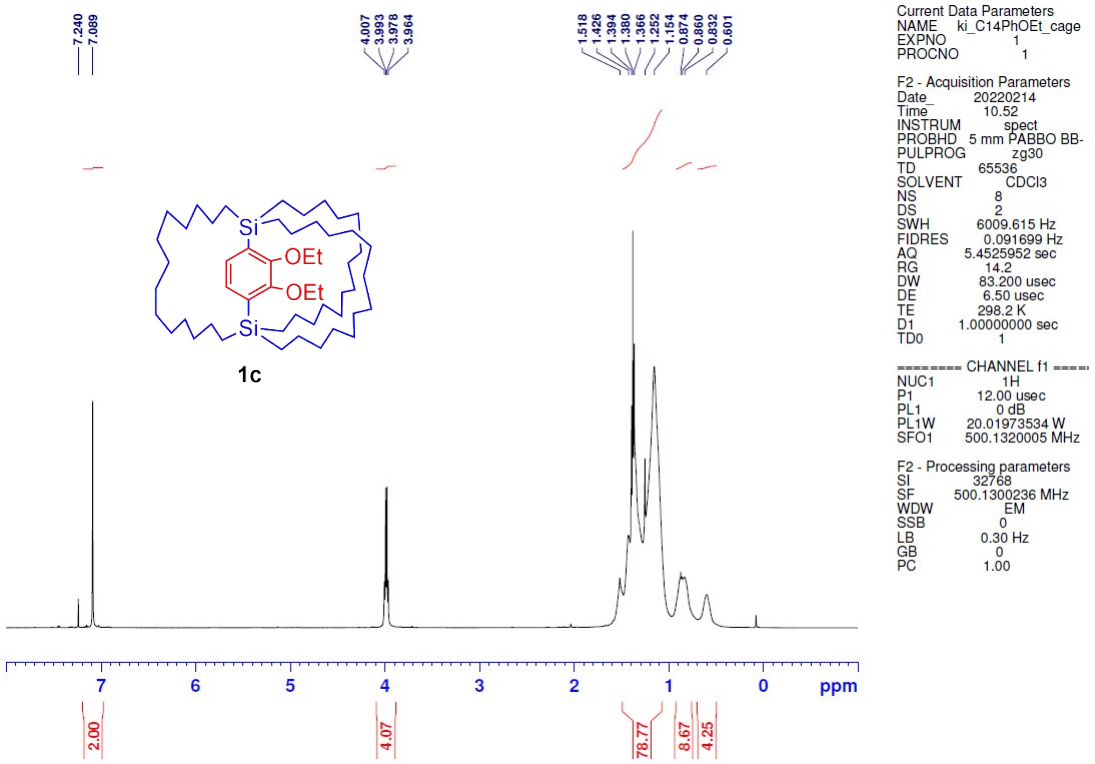


Fig. S13. ^{1}H NMR spectrum of **1c** in $CDCl_3$.

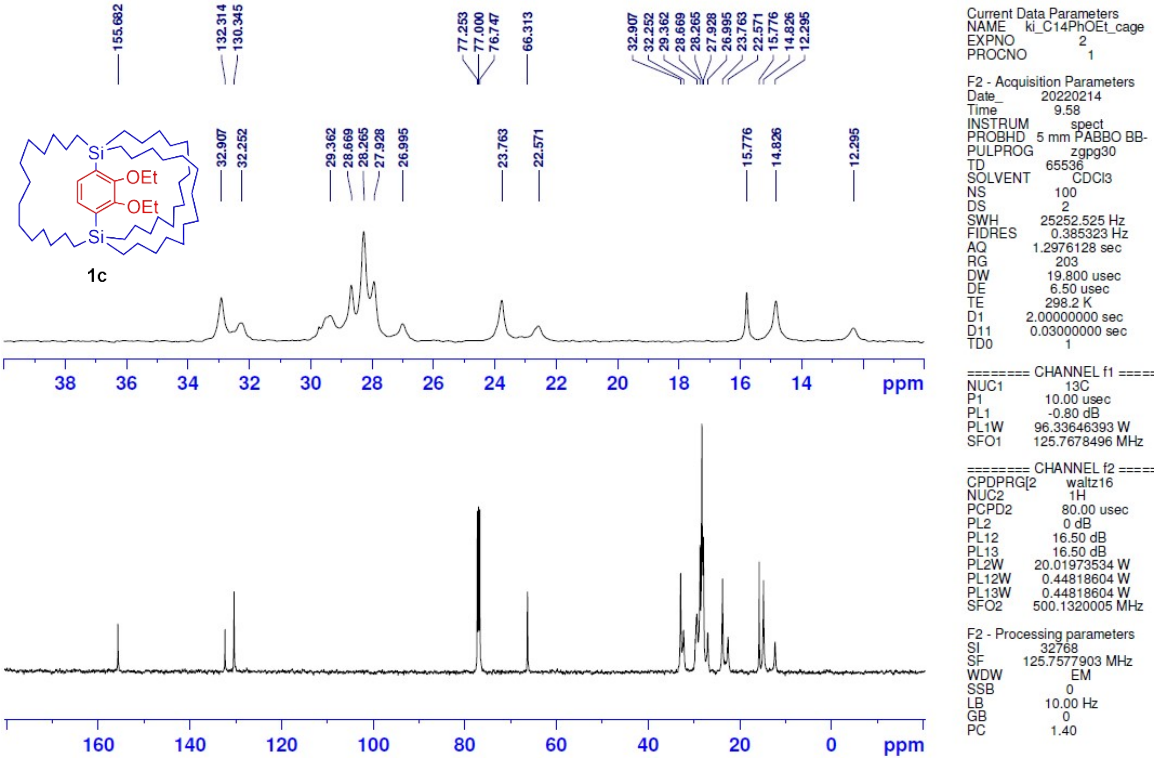


Fig. S14. ^{13}C NMR spectrum of **1c** in $CDCl_3$.

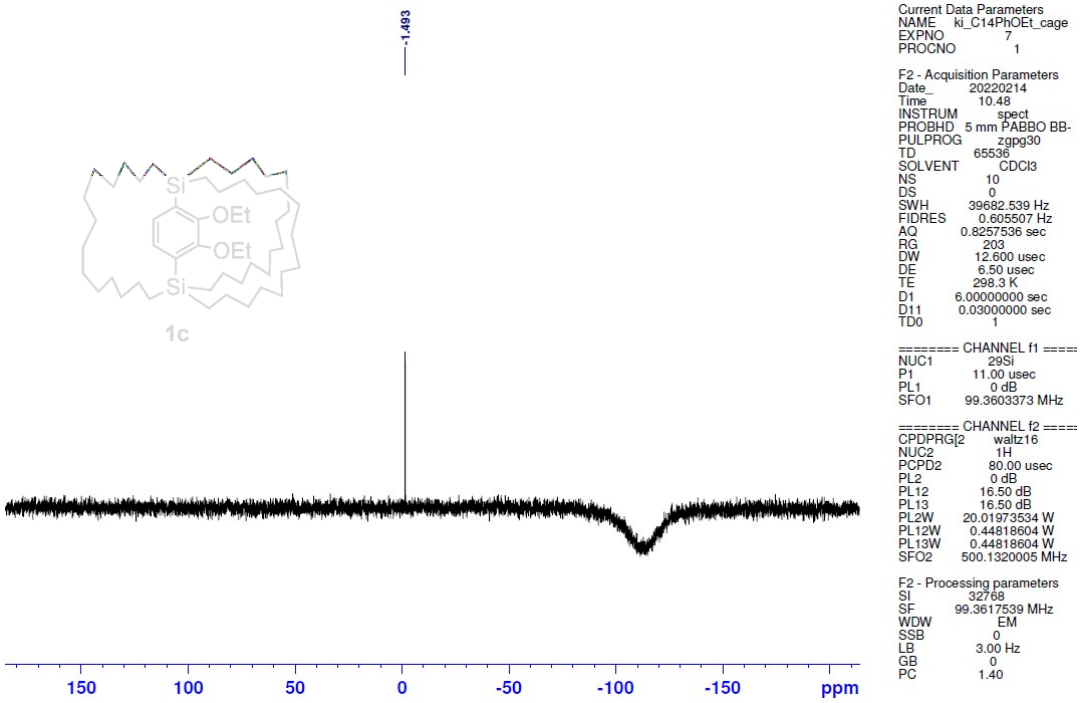


Fig. S15. ^{29}Si NMR spectrum of **1c** in $CDCl_3$.

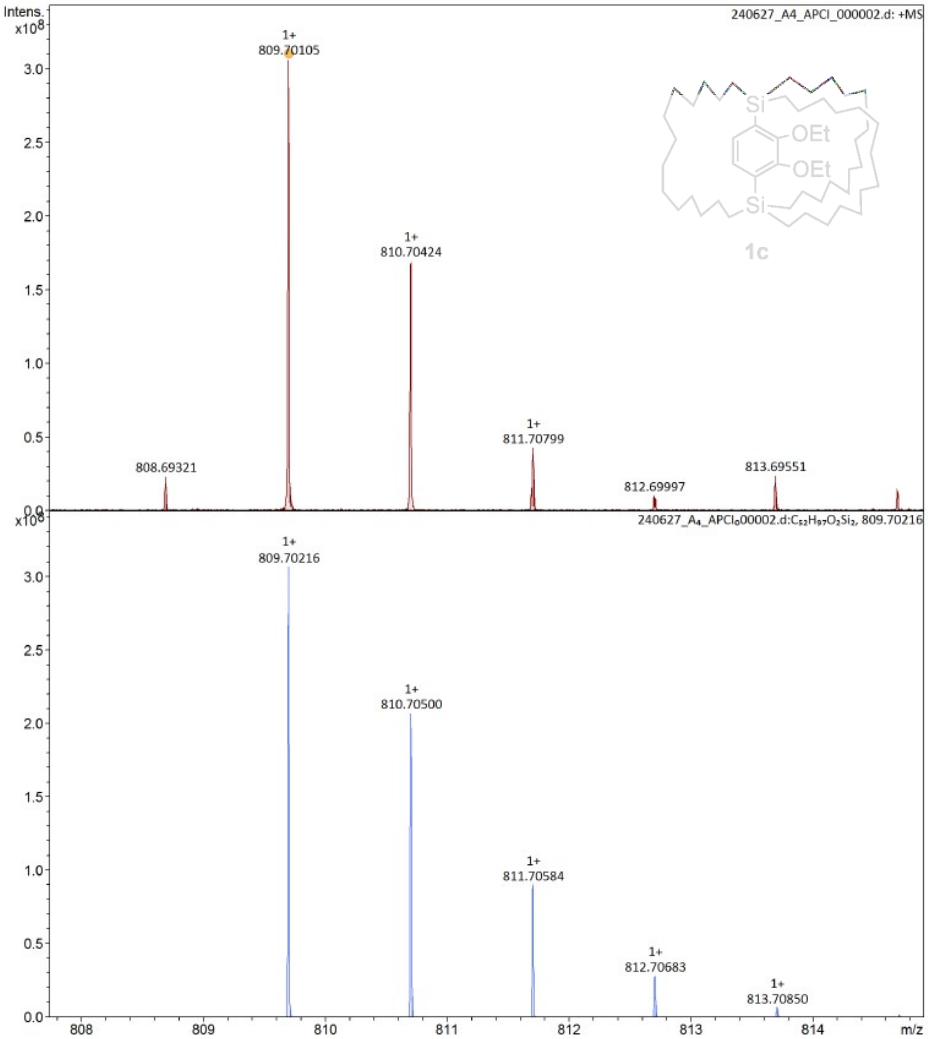
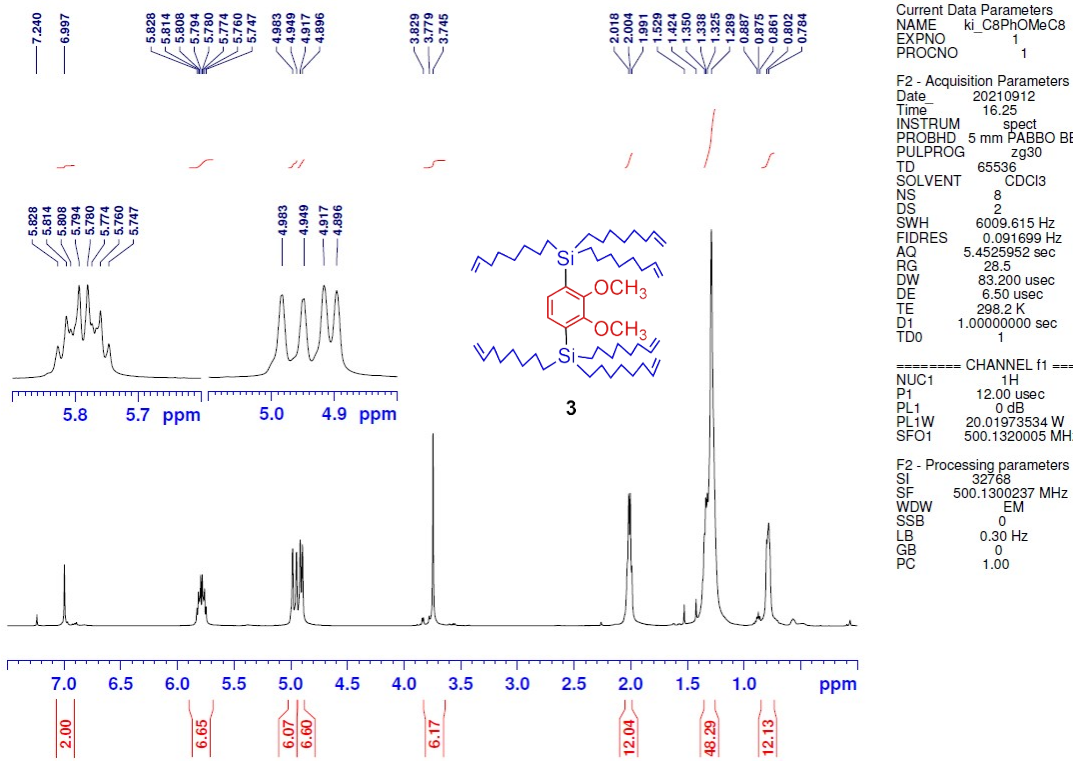


Fig. S16. HRMS spectrum of **1c** (APCI, positive). Top: obsd. Center and Bottom: sim.



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PROCNO 1

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SOLVENT CDCl3
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DS 2
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FIDRES 0.091699 Hz
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DW 83.200 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

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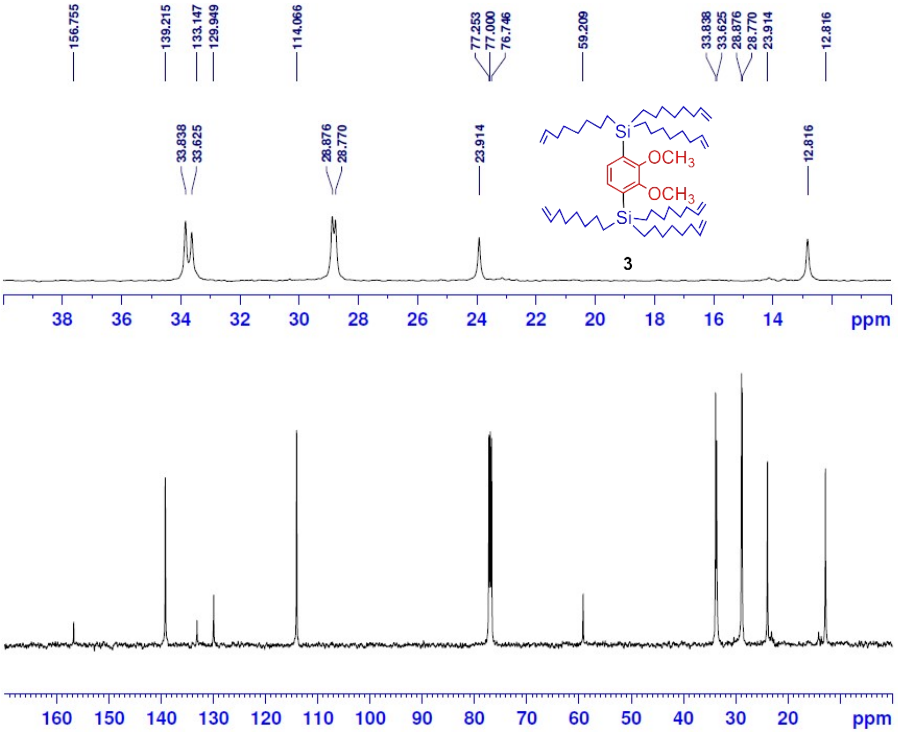
Fig. S17. ^{1}H NMR spectrum of **3** in $CDCl_3$.



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PROCNO 1

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RG 203
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DE 6.50 usec
TE 298.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

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F2 - Processing parameters
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SSB 0
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GB 0
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Fig. S18. ^{13}C NMR spectrum of **3** in $CDCl_3$.

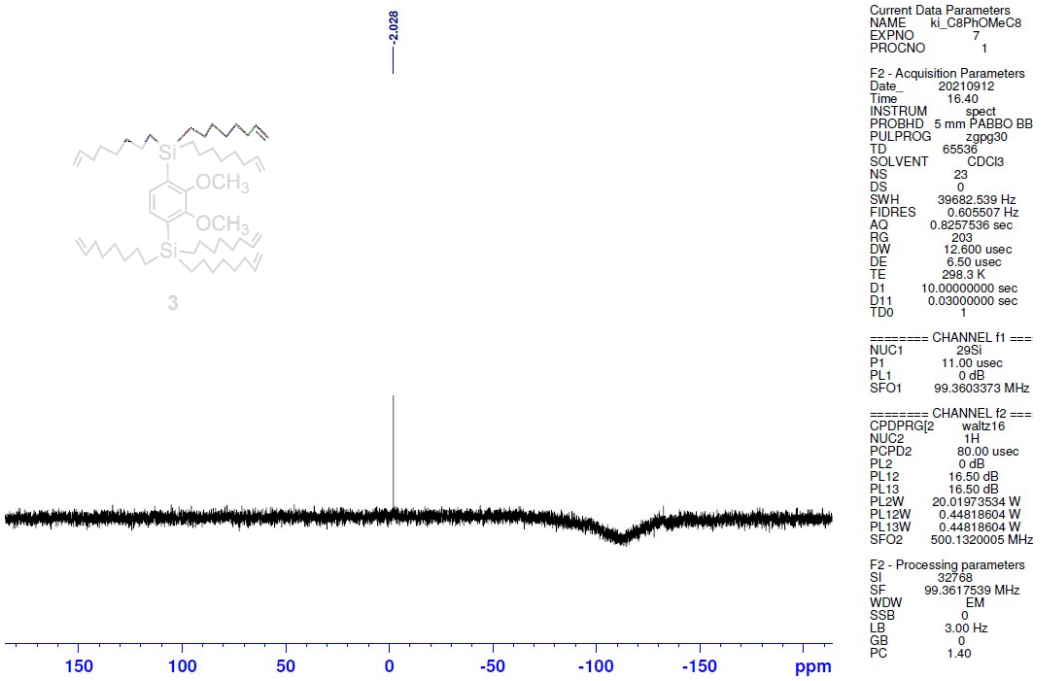


Fig. S19. ^{29}Si NMR spectrum of **3** in $CDCl_3$.

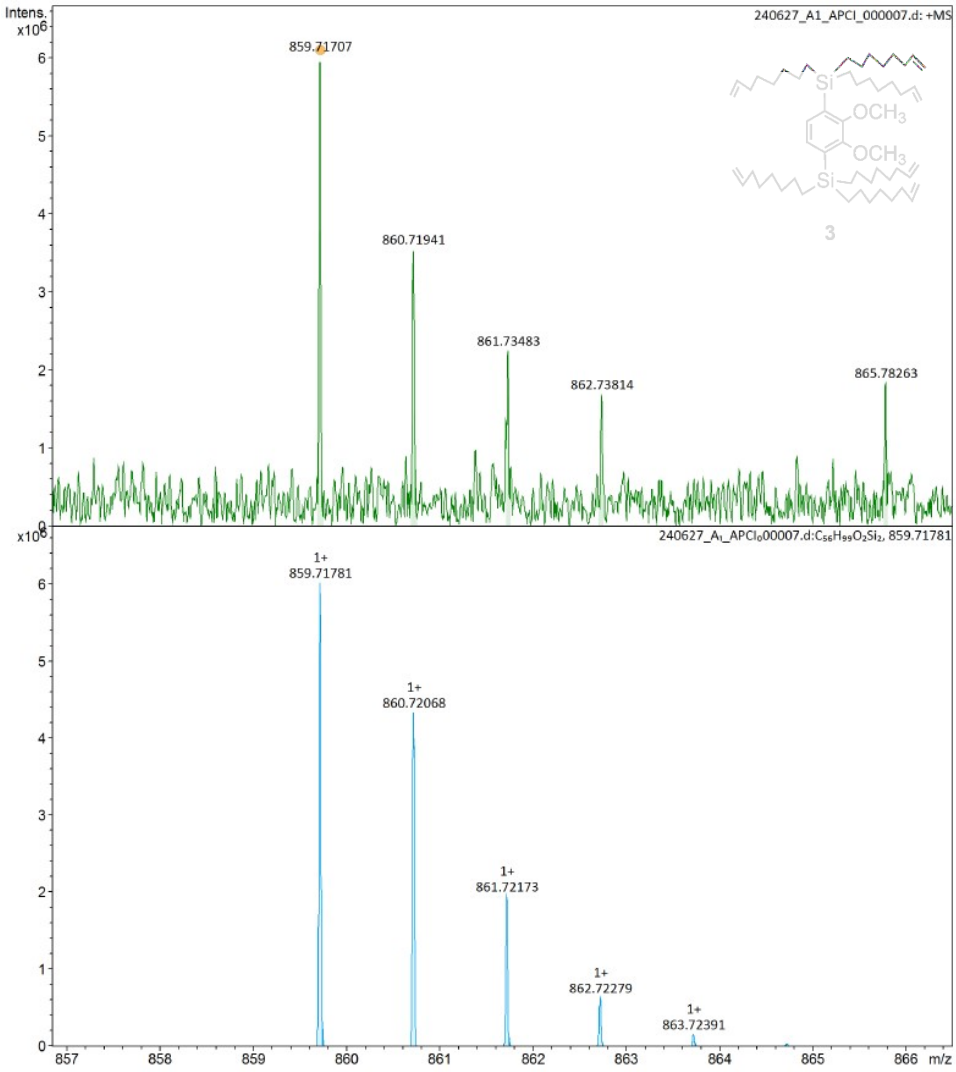


Fig. S20. HRMS spectrum of **3** (APCI, positive). Top: obsd. Center and Bottom: sim.

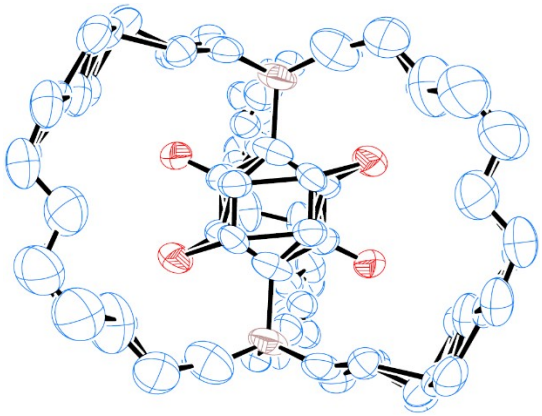
2. Details of X-ray Crystallography

Single-crystal X-ray crystallographic analyses were performed using a Bruker Venture diffractometer.

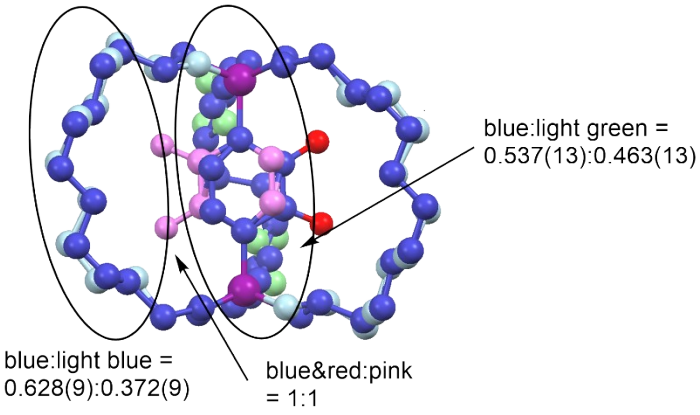
Table S1. Crystal Data

Compound		**1a**	**1b**	**1c**
CCDC #		2487573	2487574	2487575
Temperature		150(2) K	150(2) K	200(2) K
Empirical formula		C48 H88 O2 Si2	C50 H92 O2 Si2	C52 H96 O2 Si2
Formula weight / g mol^{-1}		753.36	781.41	809.46
Crystal shape		prism	plate	prism
Crystal color		colorless	colorless	colorless
Crystal size		0.130 x 0.060 x 0.040 mm^3	0.390 x 0.220 x 0.100 mm^3	0.250 x 0.070 x 0.070 mm^3
Crystal system		Monoclinic	Triclinic	Triclinic
Space group		*C* 2/*c*	*P* −1	*P* −1
Z		4	4	2
Calculated density		1.040 Mg/m^3	1.029 Mg/m^3	1.013 Mg/m^3
Cell parameter	*a*	25.0565(10) Å	11.9574(3) Å	12.0393(4) Å
	b	12.0044(5) Å	20.9583(6) Å	13.6446(5) Å
	c	18.4091(8) Å	23.0968(6) Å	19.0933(8) Å
	α	90°	114.7100(10)°	71.110(2)°
	β	119.657(2)°	90.6160(10)°	85.826(2)°
	γ	90°	104.5210(10)°	63.846(2)°
	V	4811.9(4) Å^3	5046.1(2) Å^3	2654.68(18) Å^3
F(000)		1680	1744	904
Absorption coefficient		0.908 mm^{-1}	0.880 mm^{-1}	0.850 mm^{-1}
***θ* range for collection (deg)**		4.205 to 72.566° (Cu)	2.124 to 78.360° (Cu)	3.817 to 72.645° (Cu)
Index ranges		-28<=h<=30, -14<=k<=14, -22<=l<=22	-12<=h<=14, -26<=k<=26, -27<=l<=29	-14<=h<=14, -16<=k<=16, -23<=l<=23
Reflections collected		35244	72665	37109
Independent reflections		4748 [R(int) = 0.0589]	20488 [R(int) = 0.0389]	10227 [R(int) = 0.0616]
Completeness		99.6 %	98.2 %	98.4 %
Goodness-of-fit on F^2		1.586	1.013	1.517
Final R indices [I>2sigma(I)]		R1 = 0.1201, wR2 = 0.3672	R1 = 0.0551, wR2 = 0.1409	R1 = 0.1344, wR2 = 0.3835
R indices (all data)		R1 = 0.1369, wR2 = 0.3871	R1 = 0.0637, wR2 = 0.1474	R1 = 0.1683, wR2 = 0.4120
Largest diff. peak and hole		0.756 and -0.565 e.Å^{-3}	1.092 and -0.446 e.Å^{-3}	0.704 and -0.468 e.Å^{-3}

(a)



(b)



(c)

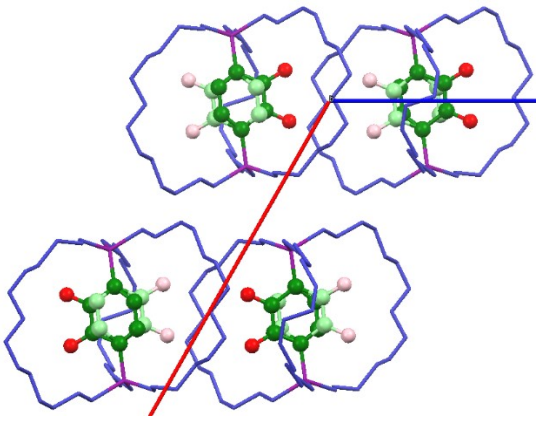
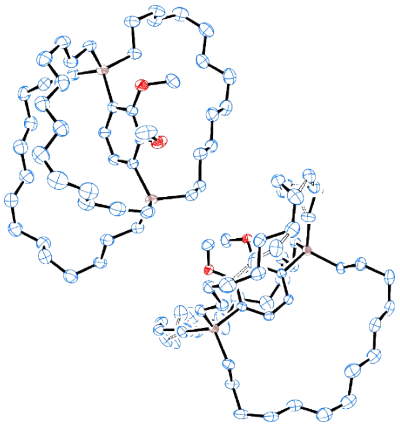


Fig. S21. X-ray crystal structure of **1a**: (a) ORTEP drawing showing 50% probability thermal ellipsoids; (b) occupancy ratios of the disordered sites; and (c) crystal packing structure.

(a)



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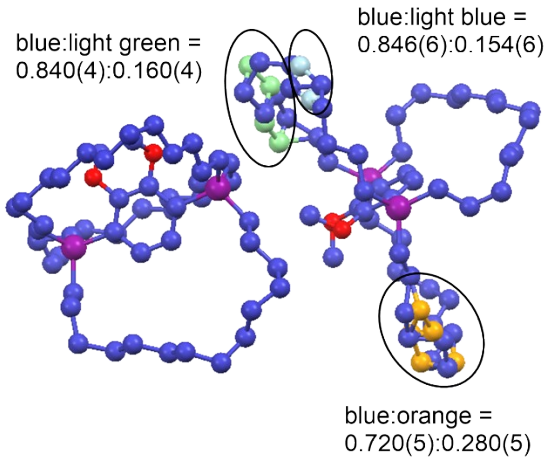

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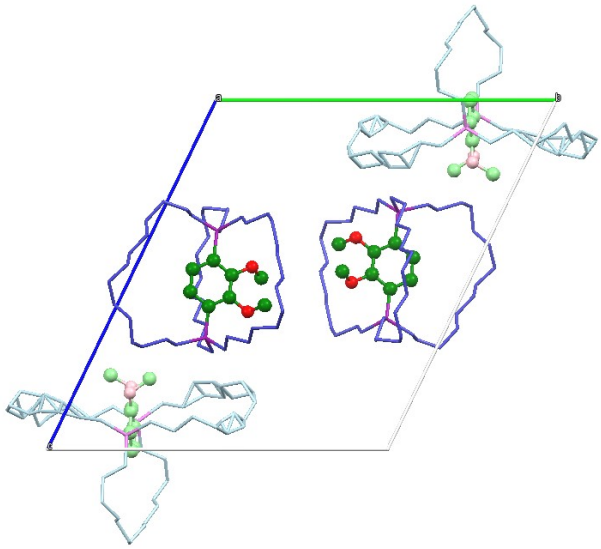
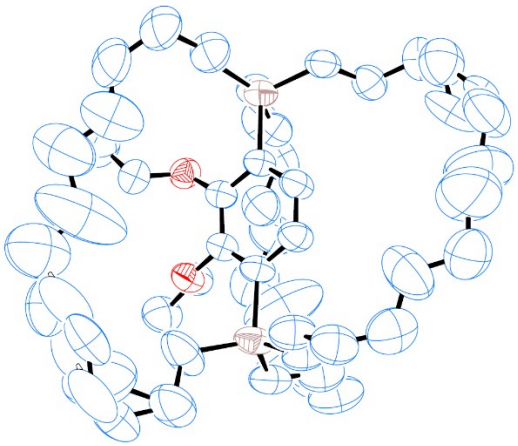


Fig. S22. X-ray crystal structure of **1b**: (a) ORTEP drawing showing 50% probability thermal ellipsoids; (b) occupancy ratios of the disordered sites; and (c) crystal packing structure.

(a)



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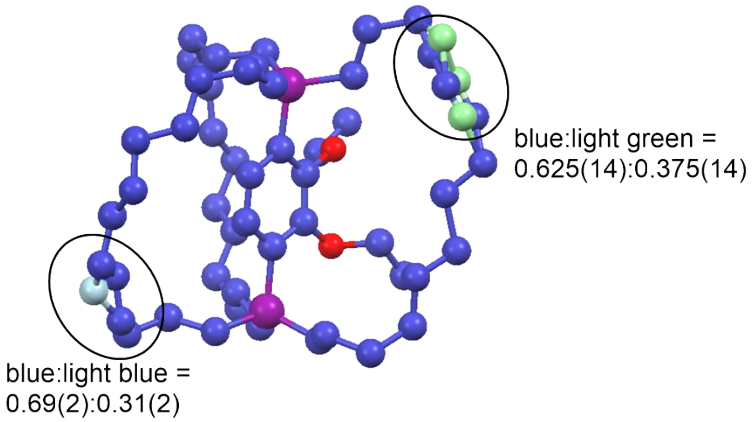

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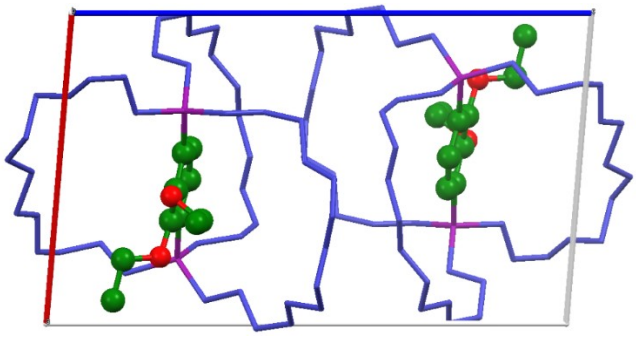


Fig. S23. X-ray crystal structure of **1c**: (a) ORTEP drawing showing 50% probability thermal ellipsoids; (b) occupancy ratios of the disordered sites; and (c) crystal packing structure.

3. Details of DFT Calculations

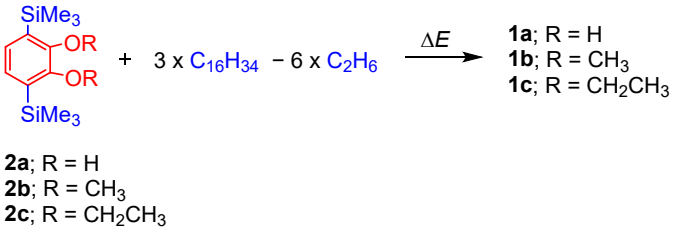


Fig. S24. Homodesmotic reactions.

Table S2. Strain Energies (ΔE) Calculated Using Homodesmotic Reactions

Cage	E_1 (**2** + 3x$C_{16}H_{34}$ − 6xC_2H_6) / au	E_2 (**1**) / au	ΔE (= $E_2 - E_1$) / kcal·mol^{-1}
1a	−2597.98447	−2598.0011755	−10.5
1b_i	−2676.206856	−2676.2002512	4.14
1b_ii	−2676.206856	−2676.2089044	−1.29
1c	−2754.430666	−2754.4341327	−2.18

Table S3. Optimized Structural Coordinate and its Total Energy of **1a** at B3LYP-D3/3-21G* level

HF=-2598.0011755 hartree, NImg=0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-0.143012	1.629351	-2.833962
2	14	0	-0.177711	-1.351147	3.056899
3	6	0	0.268977	3.472378	-2.675778
4	6	0	0.937239	0.681757	-4.059994
5	6	0	-1.963997	1.485420	-3.326579
6	6	0	1.893093	5.394581	-2.145595
7	6	0	3.229777	-0.447313	-4.460282
8	6	0	3.253681	5.780737	-1.517518
9	6	0	2.446360	0.640714	-3.688781
10	6	0	1.732184	3.869047	-2.341424
11	6	0	-4.418846	1.757916	-2.626653
12	6	0	-2.945502	1.865747	-2.182130
13	6	0	2.841761	-1.875204	-4.021656
14	6	0	-6.881231	1.955533	-1.978081
15	6	0	3.687277	-2.958820	-4.725078
16	6	0	3.321590	5.421480	-0.016260
17	6	0	-5.419842	2.059311	-1.491349
18	6	0	4.662984	5.816248	0.638035
19	6	0	3.263067	-4.397599	-4.349770
20	6	0	-7.930761	2.294986	-0.893409
21	6	0	4.681819	5.561289	2.163768
22	6	0	3.448147	-4.707694	-2.849052
23	6	0	-7.834228	1.414013	0.375317
24	6	0	-7.895726	-0.097026	0.066347
25	6	0	4.653304	4.062184	2.534393
26	6	0	3.078693	-6.164218	-2.495814
27	6	0	-8.026610	-0.972025	1.335066
28	6	0	4.592871	3.843657	4.062426
29	6	0	3.186050	-6.461246	-0.981679
30	6	0	2.111917	-5.726514	-0.149871
31	6	0	-5.483281	-0.948200	1.834115
32	6	0	-6.911891	-0.738141	2.381775
33	6	0	4.697336	2.357417	4.474017
34	6	0	3.538058	1.489463	3.938189
35	6	0	-2.982307	-1.017077	2.441199
36	6	0	-4.426714	-0.856740	2.955630
37	6	0	2.211766	-6.043512	1.358062
38	6	0	1.166569	-3.854543	2.256271
39	6	0	2.578542	-0.891225	3.764368
40	6	0	-1.942767	-0.932049	3.598819
41	6	0	3.626830	0.028451	4.432145
42	6	0	1.115509	-0.597970	4.213221
43	6	0	-0.042079	-3.241680	3.016565
44	6	0	1.075873	-5.395385	2.181363
45	1	0	1.769748	5.889266	-3.118028
46	1	0	-0.026846	3.966290	-3.615350
47	1	0	3.051883	-0.332126	-5.538533
48	1	0	0.820720	1.064141	-5.084633
49	1	0	-2.165436	2.120191	-4.203665
50	1	0	3.417602	6.861295	-1.626659
51	1	0	-4.595125	2.450740	-3.461597
52	1	0	4.306930	-0.309345	-4.288428
53	1	0	2.894930	1.619931	-3.892273
54	1	0	4.065653	5.271505	-2.055400
55	1	0	1.087325	5.759740	-1.492871
56	1	0	2.402657	3.542170	-3.144409
57	1	0	-0.393536	3.886871	-1.897826
58	1	0	3.597569	-2.827204	-5.812063
59	1	0	-7.017691	2.639135	-2.827337
60	1	0	-4.601412	0.742095	-3.005110
61	1	0	-2.154624	0.444277	-3.615918
62	1	0	0.529155	-0.337980	-4.043220
63	1	0	1.780038	-2.054746	-4.233081
64	1	0	-2.749321	2.890514	-1.835947
65	1	0	-7.057911	0.940574	-2.356453
66	1	0	4.845432	6.882840	0.448069
67	1	0	2.557683	0.453125	-2.611619
68	1	0	4.745771	-2.814652	-4.466245
69	1	0	2.057651	3.351811	-1.433277
70	1	0	-5.235641	3.067638	-1.094553
71	1	0	5.480474	5.256200	0.162944
72	1	0	2.504759	5.939241	0.506944
73	1	0	3.850524	-5.116653	-4.937110
74	1	0	2.207003	-4.543148	-4.617842
75	1	0	2.971001	-1.949410	-2.934443
76	1	0	-2.777593	1.197637	-1.327402
77	1	0	-8.934209	2.180890	-1.326290
78	1	0	3.155891	4.345539	0.109842
79	1	0	-5.248331	1.349482	-0.671567
80	1	0	-7.816946	3.349127	-0.605846
81	1	0	5.582859	6.013106	2.600379
82	1	0	3.815234	6.061675	2.619155
83	1	0	-6.996653	-0.393036	-0.486169
84	1	0	-8.754512	-0.292459	-0.590787
85	1	0	4.494283	-4.522802	-2.566297
86	1	0	2.828124	-4.022292	-2.261741
87	1	0	-8.659173	1.674513	1.052893
88	1	0	5.552680	3.574732	2.131828
89	1	0	3.786610	3.584659	2.064471
90	1	0	3.741135	-6.841826	-3.050884
91	1	0	-6.901899	1.640243	0.905188
92	1	0	2.051488	-6.368990	-2.829928
93	1	0	-8.017740	-2.030237	1.039816
94	1	0	-8.999676	-0.771962	1.804488
95	1	0	5.411842	4.405111	4.532830
96	1	0	-5.262219	-0.191306	1.070339
97	1	0	3.651110	4.260714	4.446324
98	1	0	2.208436	-4.645895	-0.304623
99	1	0	4.183678	-6.170046	-0.624292
100	1	0	3.551651	1.489461	2.840809
101	1	0	1.116854	-6.023388	-0.513075
102	1	0	-2.766803	-0.226678	1.711112
103	1	0	5.648604	1.947816	4.106263
104	1	0	-5.415093	-1.931532	1.347953
105	1	0	3.081270	-7.541356	-0.811674
106	1	0	-6.990674	0.279355	2.785484
107	1	0	1.235212	-3.436164	1.240825
108	1	0	2.664405	-0.776464	2.675387
109	1	0	2.584539	1.934503	4.252623
110	1	0	-2.880171	-1.967058	1.901342
111	1	0	-7.070822	-1.427272	3.222833
112	1	0	4.714785	2.286107	5.570268
113	1	0	0.949617	0.488363	4.247549
114	1	0	-4.520859	0.114423	3.462360
115	1	0	-1.976232	0.079701	4.030449
116	1	0	0.108320	-5.677783	1.740456
117	1	0	3.183330	-5.699973	1.739422
118	1	0	-0.976492	-3.633012	2.585204
119	1	0	2.102222	-3.573543	2.752291
120	1	0	2.176811	-7.133206	1.490846
121	1	0	4.632075	-0.353628	4.204586
122	1	0	-4.631943	-1.633581	3.706010
123	1	0	2.814692	-1.936879	3.996671
124	1	0	3.504280	-0.000225	5.523465
125	1	0	-2.239930	-1.626275	4.401553
126	1	0	0.970760	-0.961386	5.241281
127	1	0	-0.016008	-3.601467	4.056937
128	1	0	1.087396	-5.789078	3.206233
129	6	0	0.055315	0.790510	-1.159436
130	6	0	0.558736	1.395074	0.005796
131	1	0	0.916574	2.416441	-0.036432
132	6	0	0.586358	0.723704	1.228950
133	1	0	0.983321	1.232049	2.099994
134	6	0	0.075732	-0.586552	1.356306
135	6	0	-0.402704	-1.188944	0.193938
136	8	0	-1.028392	-2.472977	0.158887
137	6	0	-0.400829	-0.529190	-1.039372
138	8	0	-0.904129	-1.191463	-2.153101
139	1	0	-0.393761	-3.168485	0.473513
140	1	0	-1.247616	-2.066538	-1.808874

Table S4. Optimized Structural Coordinate and its Total Energy of **1b-i** at B3LYP-D3/3-21G* level

HF=-2676.2002512 hartree, NImg=0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-2.326265	1.636623	1.248058
2	14	0	1.580648	-2.361760	-2.235213
3	8	0	-1.381257	1.905472	-1.549051
4	8	0	0.502347	0.290410	-2.987166
5	6	0	-8.418628	0.231732	0.952118
6	6	0	-7.109588	0.810080	1.538741
7	6	0	-6.552596	2.014206	0.746959
8	6	0	-5.099223	2.354199	1.156049
9	6	0	-8.278945	-0.261772	-0.509904
10	6	0	-0.839609	0.950690	5.197540
11	6	0	-0.037219	5.254828	0.879037
12	6	0	-1.882586	3.464252	1.042339
13	6	0	-2.299460	1.169156	3.080930
14	6	0	-1.004198	1.622617	3.813296
15	6	0	-4.070593	1.333925	0.583992
16	6	0	1.480118	5.534851	0.978733
17	6	0	-0.359830	3.745083	0.954336
18	6	0	-7.103977	-1.241656	-0.714918
19	6	0	-0.342586	-0.512186	5.098811
20	6	0	-7.049354	-1.789683	-2.155567
21	6	0	2.284423	5.025720	-0.238510
22	6	0	1.146520	-0.603614	4.694494
23	6	0	3.802526	5.015782	0.037882
24	6	0	-1.081698	0.511761	0.389136
25	6	0	-2.205232	1.540228	-2.737643
26	6	0	-5.883693	-2.776660	-2.388040
27	6	0	1.691458	-2.048887	4.727505
28	6	0	-0.757069	0.787076	-0.944648
29	6	0	-0.486276	-0.613687	0.987039
30	6	0	-4.483738	-2.122325	-2.331125
31	6	0	4.629170	4.498686	-1.160417
32	6	0	3.235273	-2.089937	4.663568
33	6	0	0.148906	-0.008663	-1.648543
34	6	0	6.051921	4.074554	-0.734166
35	6	0	0.348116	-1.461368	0.253607
36	6	0	1.179828	1.610664	-3.128515
37	6	0	-3.375877	-3.128172	-2.712707
38	6	0	3.807606	-3.516711	4.846806
39	6	0	0.676636	-1.176777	-1.083069
40	6	0	-1.973398	-2.492523	-2.790168
41	6	0	6.929801	3.540816	-1.893171
42	6	0	3.703308	-4.400679	3.581274
43	6	0	6.240614	2.449458	-2.747746
44	6	0	-0.914968	-3.497204	-3.305886
45	6	0	5.667657	1.270168	-1.930708
46	6	0	4.730254	-3.997417	2.498675
47	6	0	3.956311	-0.658015	-2.036280

48	6	0	0.443025	-2.829790	-3.671475
49	6	0	4.889095	0.283548	-2.828147
50	6	0	2.009213	-3.922785	-1.254968
51	6	0	3.203446	-3.768953	-0.274418
52	6	0	3.117467	-1.555893	-2.986611
53	6	0	3.511699	-5.081320	0.477760
54	6	0	4.801193	-5.003434	1.326367
55	1	0	-9.207269	0.994805	0.999992
56	1	0	-7.284386	1.124083	2.576530
57	1	0	-7.206653	2.881073	0.911758
58	1	0	-8.741301	-0.611404	1.578082
59	1	0	-5.035983	2.380754	2.253094
60	1	0	-4.838158	3.356457	0.793488
61	1	0	-0.551602	5.765405	1.704777
62	1	0	-2.310369	4.025081	1.888505
63	1	0	-9.213775	-0.755374	-0.808564
64	1	0	-1.805355	0.982386	5.719342
65	1	0	-6.355330	0.016228	1.573544
66	1	0	-6.562825	1.797138	-0.328025
67	1	0	-3.167160	1.611249	3.593054
68	1	0	-8.144584	0.596038	-1.181114
69	1	0	-1.033370	2.712912	3.931649
70	1	0	-0.120824	1.518157	5.804896
71	1	0	1.657743	6.612224	1.096265
72	1	0	-2.360010	3.837833	0.126436
73	1	0	-0.435508	5.666340	-0.058779
74	1	0	0.154118	3.322004	1.827026
75	1	0	1.862165	5.044018	1.885735
76	1	0	-4.378238	0.308724	0.836578
77	1	0	-7.198482	-2.080542	-0.010620
78	1	0	-2.417287	0.078725	3.170854
79	1	0	-0.467088	-1.003685	6.073126
80	1	0	-4.075975	1.404952	-0.512355
81	1	0	-6.161899	-0.730605	-0.489799
82	1	0	-0.124162	1.397390	3.198640
83	1	0	-0.957874	-1.069391	4.379393
84	1	0	-8.000165	-2.292866	-2.378781
85	1	0	0.027312	3.240262	0.064838
86	1	0	1.730728	0.009349	5.395649
87	1	0	-6.954980	-0.948925	-2.857868
88	1	0	2.062368	5.651788	-1.113595
89	1	0	4.141340	6.022034	0.318771
90	1	0	-2.592189	2.486054	-3.117432
91	1	0	1.294481	-0.182329	3.692338
92	1	0	1.973469	4.001912	-0.483446
93	1	0	3.985766	4.361024	0.902072
94	1	0	-3.027949	0.884527	-2.435389
95	1	0	1.370649	-2.529491	5.662767
96	1	0	-0.700326	-0.849933	2.022565
97	1	0	-4.285889	-1.721112	-1.328925
98	1	0	-5.935745	-3.582099	-1.642085
99	1	0	3.623745	-1.444492	5.463111
100	1	0	-4.456043	-1.274858	-3.032380
101	1	0	-6.002707	-3.243437	-3.375611
102	1	0	-1.582137	1.038233	-3.479182
103	1	0	1.259617	-2.627053	3.899681
104	1	0	4.681647	5.267659	-1.942658
105	1	0	0.527563	2.402927	-2.756177
106	1	0	6.557387	4.930331	-0.266716
107	1	0	4.108201	3.634126	-1.591094
108	1	0	3.578920	-1.663644	3.712332
109	1	0	3.275964	-3.998231	5.678923
110	1	0	5.961662	3.299734	0.038287
111	1	0	-1.683882	-2.106679	-1.807513
112	1	0	-3.366541	-3.951666	-1.984925
113	1	0	0.743748	-2.353540	0.725746
114	1	0	2.125707	1.609882	-2.578648
115	1	0	4.865589	-3.453652	5.135800
116	1	0	1.366204	1.723118	-4.196844
117	1	0	-2.005310	-1.633862	-3.475577
118	1	0	-3.621745	-3.565620	-3.691111
119	1	0	7.204226	4.376955	-2.550477
120	1	0	2.685620	-4.346997	3.175530
121	1	0	4.980158	1.656824	-1.168430
122	1	0	5.418502	2.906619	-3.314239
123	1	0	7.860907	3.137885	-1.472639
124	1	0	3.284984	-0.045623	-1.419220
125	1	0	4.498597	-2.996081	2.117393
126	1	0	3.886322	-5.448293	3.857679
127	1	0	-0.768919	-4.287718	-2.556387
128	1	0	2.994632	-2.968252	0.446202
129	1	0	0.249043	-1.916930	-4.250961
130	1	0	5.721364	-3.938965	2.969699
131	1	0	1.121384	-4.264390	-0.700104
132	1	0	4.266263	0.862778	-3.525811
133	1	0	-1.323574	-3.985086	-4.202597
134	1	0	6.475565	0.747591	-1.402057
135	1	0	6.956380	2.063120	-3.485685
136	1	0	2.747316	-0.931579	-3.813055
137	1	0	2.655683	-5.344979	1.112100
138	1	0	4.544153	-1.277796	-1.348173
139	1	0	4.097137	-3.465967	-0.835839
140	1	0	1.015449	-3.509548	-4.323613
141	1	0	5.586397	-0.306311	-3.437548
142	1	0	2.245947	-4.723529	-1.973606
143	1	0	5.026890	-5.998081	1.735283
144	1	0	3.766638	-2.323489	-3.434568
145	1	0	5.634680	-4.727826	0.665247
146	1	0	3.621704	-5.885725	-0.262511

Table S5. Optimized Structural Coordinate and its Total Energy of **1b-ii** at B3LYP-D3/3-21G* level

HF=-2676.2089044 hartree, NImg=0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-0.835737	3.230089	0.996931
2	14	0	0.658021	-2.703291	-1.539854
3	8	0	-0.657245	2.368418	-1.880686
4	8	0	-0.168943	-0.242892	-2.932970
5	6	0	-3.026430	2.107499	4.529437
6	6	0	4.439823	3.878882	2.166809
7	6	0	3.209293	4.527701	1.488839
8	6	0	-1.976059	1.299816	5.327917
9	6	0	-2.661363	2.313375	3.037220
10	6	0	0.722662	4.294342	0.860601
11	6	0	-1.311177	3.053307	2.821416
12	6	0	-2.250941	4.004841	0.009585
13	6	0	1.943760	3.648634	1.570595
14	6	0	-4.251252	3.636421	-1.551403
15	6	0	4.925890	2.582445	1.474351
16	6	0	-3.345771	3.010904	-0.468725
17	6	0	-5.379288	2.686779	-2.012527
18	6	0	-1.723459	-0.105944	4.745797
19	6	0	5.452032	2.821825	0.043370
20	6	0	-0.576255	-0.852547	5.458524
21	6	0	-4.847161	1.414474	-2.708319
22	6	0	-0.395006	1.506484	0.359216
23	6	0	-5.972603	0.503283	-3.249308
24	6	0	0.471472	2.701452	-2.792300
25	6	0	-6.977836	0.042836	-2.163514
26	6	0	5.950772	1.524089	-0.625312
27	6	0	-0.044832	0.430698	1.196751
28	6	0	-0.370184	1.279504	-1.022230
29	6	0	-0.177296	-2.141389	4.710682
30	6	0	6.518273	1.779247	-2.038016
31	6	0	-6.321618	-0.647809	-0.945553
32	6	0	0.992556	-2.889205	5.385508
33	6	0	0.320291	-0.811448	0.671020
34	6	0	-0.096000	0.011622	-1.541774
35	6	0	-1.527551	-0.003959	-3.496984
36	6	0	7.071372	0.502925	-2.716093
37	6	0	-5.566762	-1.940599	-1.317692
38	6	0	0.286996	-1.049286	-0.714031
39	6	0	1.487566	-4.096626	4.554717
40	6	0	6.008074	-0.596910	-2.944302
41	6	0	2.248975	-3.670894	3.280296
42	6	0	4.894823	-0.175743	-3.929408
43	6	0	-5.005251	-2.670471	-0.078050
44	6	0	2.881325	-1.363790	-2.858162
45	6	0	3.808392	-1.264633	-4.090127
46	6	0	-2.085273	-3.399235	-1.031058
47	6	0	2.648503	-4.875330	2.404814
48	6	0	-4.486513	-4.092976	-0.398766
49	6	0	2.824164	-3.431485	0.250166
50	6	0	1.851289	-2.516748	-2.996600
51	6	0	-0.977955	-3.454887	-2.118785
52	6	0	-3.369938	-4.132241	-1.467387
53	6	0	1.412594	-3.856448	-0.240866
54	6	0	3.494749	-4.480188	1.172607
55	1	0	-3.152140	3.092664	4.999033
56	1	0	2.998085	5.491576	1.971727
57	1	0	4.185919	3.656511	3.212532
58	1	0	0.534142	5.291830	1.287635
59	1	0	5.268777	4.599976	2.179930
60	1	0	-3.994022	1.589543	4.588738
61	1	0	-1.374415	4.054965	3.274966
62	1	0	-2.718071	4.810268	0.597238
63	1	0	-2.307434	1.206147	6.370783
64	1	0	-3.462913	2.892713	2.562538
65	1	0	-4.689774	4.564920	-1.161118
66	1	0	-1.028026	1.852629	5.343970
67	1	0	1.708245	3.468896	2.629215
68	1	0	-3.623525	3.904215	-2.413128
69	1	0	3.430917	4.740511	0.435378
70	1	0	-1.803236	4.466025	-0.880559
71	1	0	0.963077	4.444817	-0.203133
72	1	0	-6.046518	3.214890	-2.707920
73	1	0	-0.507219	2.526334	3.354587
74	1	0	5.732538	2.138946	2.073996
75	1	0	-2.634627	1.343081	2.526587
76	1	0	-3.962585	2.688518	0.379835
77	1	0	2.139136	2.670586	1.115740
78	1	0	6.271362	3.553821	0.078460
79	1	0	-2.645162	-0.701210	4.799107
80	1	0	-5.978713	2.403425	-1.138066
81	1	0	4.111418	1.847931	1.441220
82	1	0	-0.866825	-1.091416	6.490454
83	1	0	0.300826	-0.191382	5.512306
84	1	0	-1.463865	-0.015687	3.685553
85	1	0	-2.865757	2.123820	-0.885750
86	1	0	4.657160	3.253534	-0.578359
87	1	0	-6.524384	1.044807	-4.029770
88	1	0	-4.197458	1.716449	-3.542067
89	1	0	-7.553366	0.909492	-1.816171
90	1	0	0.109053	3.528214	-3.403827
91	1	0	1.343189	3.015163	-2.208063
92	1	0	-0.036775	0.569775	2.270716
93	1	0	-4.222056	0.845836	-2.010631
94	1	0	6.729902	1.065588	0.000018
95	1	0	-7.693719	-0.654569	-2.619743
96	1	0	7.326275	2.519948	-1.963069

97	1	0	-5.523533	-0.377451	-3.725892
98	1	0	5.116095	0.813645	-0.680382
99	1	0	-1.044376	-2.812790	4.641694
100	1	0	-5.632489	0.046142	-0.447072
101	1	0	0.719679	1.835646	-3.409080
102	1	0	0.100428	-1.869809	3.684333
103	1	0	5.734944	2.224513	-2.664452
104	1	0	0.667547	-3.229093	6.377845
105	1	0	1.828616	-2.191990	5.538253
106	1	0	-1.824605	1.031496	-3.326347
107	1	0	-7.105723	-0.896872	-0.217449
108	1	0	0.611900	-1.606343	1.347674
109	1	0	7.878395	0.097357	-2.090384
110	1	0	-2.251793	-0.681611	-3.032140
111	1	0	-4.744104	-1.699241	-2.001814
112	1	0	-1.436982	-0.219842	-4.561803
113	1	0	7.514388	0.772725	-3.684761
114	1	0	4.415841	0.748441	-3.580823
115	1	0	-6.251280	-2.612993	-1.854871
116	1	0	5.563537	-0.879629	-1.983795
117	1	0	1.620294	-2.995827	2.690398
118	1	0	0.625887	-4.717981	4.271856
119	1	0	2.150820	-4.721291	5.167806
120	1	0	2.339207	-0.418358	-2.749966
121	1	0	3.148080	-3.107391	3.566711
122	1	0	-4.204230	-2.065784	0.365678
123	1	0	-5.800900	-2.750784	0.675379
124	1	0	-2.310188	-2.349533	-0.807501
125	1	0	5.354630	0.042744	-4.902954
126	1	0	2.758741	-2.468237	0.770158
127	1	0	3.483654	-1.505861	-1.953468
128	1	0	6.500952	-1.494013	-3.343423
129	1	0	-3.734201	-3.691887	-2.404462
130	1	0	0.729904	-3.944442	0.616912
131	1	0	-1.327515	-2.927957	-3.018176
132	1	0	3.188166	-1.046177	-4.969972
133	1	0	1.738427	-5.392917	2.075756
134	1	0	-1.719379	-3.851525	-0.098070
135	1	0	-5.334136	-4.700405	-0.745157
136	1	0	1.258119	-2.339070	-3.903666
137	1	0	3.219695	-5.588477	3.014902
138	1	0	3.477056	-3.273788	-0.617398
139	1	0	4.290815	-2.236768	-4.264990
140	1	0	4.460123	-4.083261	1.516767
141	1	0	-4.109091	-4.555954	0.523448
142	1	0	2.390746	-3.467189	-3.136815
143	1	0	-3.118331	-5.179459	-1.684188
144	1	0	1.479891	-4.863596	-0.683566
145	1	0	-0.808174	-4.503499	-2.410859
146	1	0	3.703326	-5.382645	0.581740

Table S5. Optimized Structural Coordinate and its Total Energy of **1c** at B3LYP-D3/3-21G* level

HF=-2754.4341327 hartree, NImg=0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-0.818186	2.509418	2.441123
2	14	0	1.642760	-2.019391	-1.747361
3	8	0	-2.114939	-0.081661	1.457206
4	8	0	-1.033932	-2.049611	-0.304564
5	6	0	0.093258	6.117672	0.282134
6	6	0	1.811262	1.051096	5.512851
7	6	0	-2.703980	2.634724	2.524759
8	6	0	-0.060490	4.190585	2.016909
9	6	0	-0.214335	1.927923	4.138822
10	6	0	1.637432	6.073163	0.204623
11	6	0	-5.019708	2.444576	1.466967
12	6	0	-0.554955	4.761693	0.658398
13	6	0	1.330347	1.800009	4.241899
14	6	0	1.144721	-0.334483	5.702429
15	6	0	-3.505537	2.595037	1.196088
16	6	0	-5.879115	2.416025	0.183890
17	6	0	2.160971	5.008023	-0.779444
18	6	0	-3.827823	-1.284172	2.629215
19	6	0	3.700244	4.910598	-0.792240
20	6	0	-5.535494	1.240408	-0.757999
21	6	0	1.249630	-1.242798	4.458838
22	6	0	-6.502304	1.168542	-1.961902
23	6	0	-0.126473	1.243933	1.212249
24	6	0	-2.339438	-1.286319	2.304751
25	6	0	0.364607	-2.503328	4.566099
26	6	0	4.189597	3.705016	-1.619893
27	6	0	-0.822929	0.064314	0.915190
28	6	0	1.156590	1.393689	0.650103
29	6	0	-6.070337	0.148333	-3.041430
30	6	0	5.725903	3.556010	-1.614292
31	6	0	0.343647	-3.293475	3.240672
32	6	0	1.718361	0.403289	-0.157449
33	6	0	-0.279305	-0.908552	0.061882
34	6	0	-4.778890	0.579916	-3.768152
35	6	0	-2.316808	-1.716343	-1.010173
36	6	0	1.008331	-0.769875	-0.478018
37	6	0	6.200906	2.271058	-2.332233
38	6	0	-0.819853	-4.304712	3.139034
39	6	0	-2.871329	-3.040016	-1.514630
40	6	0	5.858412	0.989666	-1.541986
41	6	0	-4.372946	-0.380679	-4.906938
42	6	0	-0.835007	-4.996728	1.753804
43	6	0	-2.981439	-0.046497	-5.501037
44	6	0	-1.863465	-0.293966	-4.469076
45	6	0	6.229858	-0.293676	-2.310207
46	6	0	4.496451	-1.730276	-1.009128
47	6	0	0.611723	-0.295037	-3.862124
48	6	0	1.388726	-3.845465	-1.328729
49	6	0	0.204926	-6.143530	1.686333
50	6	0	3.454234	-1.637694	-2.157478
51	6	0	5.958408	-1.583666	-1.502582
52	6	0	-0.428933	-0.089542	-4.993318
53	6	0	0.636437	-1.752260	-3.328057
54	6	0	0.632064	-6.534678	0.242791
55	6	0	2.163153	-4.465624	-0.138857
56	6	0	2.045564	-6.009238	-0.104665
57	1	0	-0.206344	6.869951	1.024524
58	1	0	1.601115	1.668265	6.396718
59	1	0	-0.586888	2.590164	4.935006
60	1	0	-0.306948	4.903490	2.819441
61	1	0	-2.957851	3.555349	3.075559
62	1	0	-5.353687	3.268728	2.112336
63	1	0	2.012975	7.060440	-0.096284
64	1	0	-1.642153	4.898817	0.703806
65	1	0	1.776507	2.803393	4.231697
66	1	0	-0.302654	6.440397	-0.691055
67	1	0	-3.042641	1.794354	3.147054
68	1	0	2.047376	5.866935	1.201676
69	1	0	2.900874	0.922813	5.452602
70	1	0	-5.178170	1.509841	2.023091
71	1	0	-6.940881	2.351043	0.460180
72	1	0	1.597079	-0.840780	6.565308
73	1	0	-0.679540	0.945333	4.305683
74	1	0	1.035218	4.105020	2.009076
75	1	0	0.083334	-0.189913	5.942216
76	1	0	-3.327848	3.507625	0.613730
77	1	0	-4.095158	-0.359853	3.148246
78	1	0	-5.744063	3.358675	-0.365202
79	1	0	-0.365686	4.029511	-0.136041
80	1	0	1.711881	1.276821	3.357696
81	1	0	4.060285	4.800121	0.240940
82	1	0	4.132175	5.839047	-1.189655
83	1	0	1.794679	5.227001	-1.791880
84	1	0	-3.165977	1.738439	0.612914
85	1	0	-4.411248	-1.338213	1.705004
86	1	0	-4.077262	-2.141244	3.263247
87	1	0	-7.505918	0.918059	-1.593087
88	1	0	1.758845	4.027618	-0.499793
89	1	0	-5.577966	0.295148	-0.196931
90	1	0	2.296107	-1.529955	4.290156
91	1	0	-6.567853	2.163100	-2.426007
92	1	0	0.923750	-0.687217	3.571335
93	1	0	-1.727548	-1.194946	3.206305
94	1	0	-0.660165	-2.184877	4.808434
95	1	0	0.702699	-3.145298	5.389765
96	1	0	1.730282	2.289816	0.855007
97	1	0	-4.506805	1.356460	-1.114579
98	1	0	3.727473	2.797664	-1.210293
99	1	0	3.839521	3.802909	-2.656903
100	1	0	-2.039360	-2.172663	1.747139
101	1	0	6.167730	4.437238	-2.098159
102	1	0	6.084960	3.540747	-0.575406
103	1	0	-6.875788	0.032874	-3.779288
104	1	0	-5.910755	-0.835049	-2.575156
105	1	0	-2.986675	-1.214020	-0.312601
106	1	0	-4.915649	1.588814	-4.182053
107	1	0	-3.967479	0.640359	-3.036131
108	1	0	1.302198	-3.809861	3.107890
109	1	0	0.251742	-2.583961	2.407314
110	1	0	-1.763818	-3.769195	3.303745
111	1	0	2.709299	0.560459	-0.566803
112	1	0	-2.088099	-1.037250	-1.833985
113	1	0	4.784981	0.975188	-1.325790
114	1	0	-0.736925	-5.058338	3.934251
115	1	0	-3.820794	-2.872117	-2.034848
116	1	0	-3.033528	-3.722650	-0.675236
117	1	0	5.733416	2.219344	-3.325901
118	1	0	6.382762	1.007788	-0.576221
119	1	0	7.287523	2.311182	-2.485799
120	1	0	-2.006020	0.371641	-3.608543
121	1	0	-5.137590	-0.345298	-5.694000
122	1	0	4.283349	-0.969218	-0.250337
123	1	0	-4.351315	-1.410136	-4.519612
124	1	0	0.374944	0.394172	-3.039923
125	1	0	-0.636875	-4.240316	0.984015
126	1	0	-2.961158	1.001278	-5.830244
127	1	0	-2.160259	-3.501700	-2.206260
128	1	0	-1.969743	-1.321915	-4.102223
129	1	0	0.312291	-3.988115	-1.179415
130	1	0	-1.830722	-5.410727	1.543916
131	1	0	1.100887	-5.846671	2.246265
132	1	0	3.496695	-0.635989	-2.611225
133	1	0	1.660609	-4.396208	-2.245859
134	1	0	6.629042	-1.605857	-0.632181
135	1	0	5.663901	-0.321680	-3.250051
136	1	0	-0.384670	-2.083924	-3.101445
137	1	0	-0.335160	0.927308	-5.398744
138	1	0	-2.798778	-0.673758	-6.383740
139	1	0	-0.096338	-6.146734	-0.480029
140	1	0	4.404437	-2.700203	-0.510068
141	1	0	7.294601	-0.257426	-2.578257
142	1	0	1.611536	-0.028129	-4.228889
143	1	0	-0.213190	-7.012961	2.209029
144	1	0	0.635690	-7.626737	0.137268
145	1	0	3.747850	-2.340104	-2.955409

146	1	0	6.204659	-2.452630	-2.128215
147	1	0	-0.228676	-0.794534	-5.811658
148	1	0	1.012850	-2.421725	-4.117325
149	1	0	1.800234	-4.037830	0.802428
150	1	0	2.352914	-6.400078	-1.084919
151	1	0	3.225203	-4.209911	-0.217215
152	1	0	2.749848	-6.409029	0.638905

Table S6. Optimized Structural Coordinate and its Total Energy of **2a** at B3LYP-D3/3-21G* level

HF=-1193.8203949 hartree, NImg=0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.709162	1.069498	-0.001072
2	6	0	0.709159	1.069502	-0.001151
3	6	0	1.425719	-0.129552	-0.001691
4	6	0	0.690784	-1.342205	-0.002247
5	6	0	-0.690793	-1.342205	-0.002121
6	6	0	-1.425721	-0.129548	-0.001524
7	14	0	3.295150	-0.324127	0.000348
8	14	0	-3.295146	-0.324126	0.000338
9	8	0	-1.278387	2.333218	-0.000113
10	8	0	1.278371	2.333220	-0.000276
11	6	0	-3.787922	-1.299512	-1.538160
12	6	0	-4.251043	1.316933	-0.004246
13	6	0	-3.785233	-1.290083	1.545584
14	6	0	3.788010	-1.300882	-1.537247
15	6	0	3.785161	-1.288696	1.546492
16	6	0	4.251048	1.316930	-0.005720
17	1	0	1.223803	-2.288274	-0.002635
18	1	0	-1.223819	-2.288272	-0.002451
19	1	0	-2.262870	2.261354	-0.002859
20	1	0	2.262855	2.261368	-0.002614
21	1	0	-4.865954	-1.510159	-1.547397
22	1	0	-3.255088	-2.258365	-1.581278
23	1	0	-3.539810	-0.740785	-2.449968
24	1	0	-5.325040	1.082704	-0.005113
25	1	0	-4.065190	1.923220	-0.902575
26	1	0	-4.067390	1.926982	0.891965
27	1	0	-4.863197	-1.500872	1.558293
28	1	0	-3.535319	-0.725847	2.453504
29	1	0	-3.251996	-2.248508	1.593302
30	1	0	4.866077	-1.511354	-1.546283
31	1	0	3.539814	-0.743026	-2.449566
32	1	0	3.255355	-2.259870	-1.579508
33	1	0	4.863092	-1.499638	1.559425
34	1	0	3.251763	-2.246993	1.595059
35	1	0	3.535297	-0.723598	2.453889
36	1	0	5.325044	1.082697	-0.007225
37	1	0	4.068103	1.927417	0.890350
38	1	0	4.064494	1.922774	-0.904190

Table S7. Optimized Structural Coordinate and its Total Energy of **2b** at B3LYP-D3/3-21G* level

HF=-1272.0427814 hartree, NImg=0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.699241	0.538704	0.008172
2	6	0	0.699187	0.538759	-0.008567
3	6	0	1.424632	-0.659896	0.019185
4	6	0	0.697881	-1.863122	0.021889
5	6	0	-0.697836	-1.863165	-0.022402
6	6	0	-1.424616	-0.659962	-0.019589
7	14	0	3.305768	-0.574449	0.088294
8	14	0	-3.305730	-0.574459	-0.088280
9	8	0	-1.431326	1.752369	0.021924
10	8	0	1.431175	1.752472	-0.022028
11	6	0	-1.163651	2.583348	1.229795
12	6	0	1.163517	2.583866	-1.229614
13	6	0	-3.964778	-2.344407	-0.181106
14	6	0	-3.817108	0.398404	-1.620122
15	6	0	-3.986786	0.261934	1.461571
16	6	0	3.816789	0.398456	1.620252
17	6	0	3.987474	0.261759	-1.461350
18	6	0	3.964576	-2.344472	0.181488
19	1	0	1.229062	-2.807999	0.044550
20	1	0	-1.228976	-2.808062	-0.045159
21	1	0	-0.094867	2.789189	1.306226
22	1	0	-1.516844	2.064469	2.126246
23	1	0	-1.731775	3.501427	1.076227
24	1	0	0.094711	2.789509	-1.306152
25	1	0	1.516970	2.065410	-2.126212
26	1	0	1.731440	3.501992	-1.075591
27	1	0	-5.061352	-2.340326	-0.243170
28	1	0	-3.683253	-2.926763	0.706467
29	1	0	-3.582506	-2.867756	-1.067565
30	1	0	-4.903165	0.557227	-1.656346
31	1	0	-3.516468	-0.120673	-2.539516
32	1	0	-3.316647	1.373137	-1.593455
33	1	0	-5.082351	0.189144	1.495491
34	1	0	-3.713882	1.322933	1.467103
35	1	0	-3.587848	-0.202155	2.373011
36	1	0	4.902670	0.558580	1.655939
37	1	0	3.517266	-0.121305	2.539625
38	1	0	3.315199	1.372620	1.594157
39	1	0	5.083243	0.191051	-1.493372
40	1	0	3.712577	1.322223	-1.468292
41	1	0	3.590961	-0.203988	-2.372995
42	1	0	5.061039	-2.340548	0.245469
43	1	0	3.684487	-2.926474	-0.706766
44	1	0	3.580740	-2.868105	1.067113

Table S8. Optimized Structural Coordinate and its Total Energy of **2c** at B3LYP-D3/3-21G* level

HF=-1350.2665915 hartree, NImg=0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.699031	0.148874	0.012790
2	6	0	0.699068	0.148842	-0.012580
3	6	0	1.423313	-1.050192	-0.056923
4	6	0	0.697243	-2.253661	-0.039432
5	6	0	-0.697301	-2.253635	0.039491
6	6	0	-1.423323	-1.050139	0.057050
7	14	0	3.301109	-0.955936	-0.172399
8	14	0	-3.301136	-0.955870	0.172314
9	8	0	-1.429165	1.361010	0.025713
10	8	0	1.429287	1.360952	-0.025581
11	6	0	-1.208943	2.219042	-1.181145
12	6	0	1.209065	2.219148	1.181190
13	6	0	-1.972603	3.507259	-0.901911
14	6	0	1.972794	3.507287	0.901813
15	6	0	-4.017145	-0.101901	-1.352840
16	6	0	-3.771687	0.010533	1.721592
17	6	0	-3.967952	-2.722835	0.267464
18	6	0	4.017103	-0.101716	1.352632
19	6	0	3.771429	0.010191	-1.721898
20	6	0	3.967966	-2.722908	-0.267164
21	1	0	1.227923	-3.198529	-0.074375
22	1	0	-1.228017	-3.198486	0.074342
23	1	0	-1.602581	1.695198	-2.058403
24	1	0	-0.136876	2.385451	-1.297618
25	1	0	1.602665	1.695387	2.058512
26	1	0	0.137009	2.385630	1.297622
27	1	0	-1.886776	4.193851	-1.750224
28	1	0	-1.569916	3.990925	-0.007102
29	1	0	-3.028951	3.280892	-0.728960
30	1	0	1.886690	4.194142	1.749887
31	1	0	3.029201	3.280926	0.729227
32	1	0	1.570334	3.990652	0.006738
33	1	0	-5.112457	-0.184386	-1.368452
34	1	0	-3.630167	-0.547009	-2.278700
35	1	0	-3.754381	0.961665	-1.346426
36	1	0	-4.855720	0.175353	1.783560
37	1	0	-3.266146	0.982370	1.687630
38	1	0	-3.452969	-0.514857	2.631225
39	1	0	-5.062515	-2.714135	0.357818
40	1	0	-3.565416	-3.255273	1.139447
41	1	0	-3.711871	-3.299158	-0.631682
42	1	0	5.112378	-0.184412	1.368702
43	1	0	3.629653	-0.546538	2.278443
44	1	0	3.754486	0.961878	1.345866
45	1	0	4.855637	0.173481	-1.784925
46	1	0	3.267255	0.982715	-1.687212
47	1	0	3.451033	-0.514504	-2.631336
48	1	0	5.062604	-2.714206	-0.356613
49	1	0	3.566135	-3.255381	-1.139445
50	1	0	3.711164	-3.299194	0.631803

Table S9. Optimized Structural Coordinate and its Total Energy of **C16H34** at B3LYP-D3/3-21G* level

HF=-626.8596176 hartree, NImg=0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-7.320846	-0.440031	0.000107
2	6	0	-5.971847	-1.189552	-0.000113
3	6	0	-4.770154	-0.220709	0.000105
4	6	0	-3.413433	-0.955847	-0.000113
5	6	0	-2.213365	0.014247	0.000106
6	6	0	-0.856439	-0.720533	-0.000112
7	6	0	0.343544	0.249621	0.000108
8	6	0	1.700516	-0.485077	-0.000110
9	6	0	2.900489	0.485077	0.000110
10	6	0	4.257462	-0.249621	-0.000108
11	6	0	5.457444	0.720533	0.000112
12	6	0	6.814371	-0.014247	-0.000106
13	6	0	8.014439	0.955847	0.000113
14	6	0	9.371160	0.220709	-0.000105
15	6	0	10.572852	1.189552	0.000113
16	6	0	11.921852	0.440031	-0.000107
17	1	0	-8.164329	-1.139408	-0.000051
18	1	0	-7.403403	0.198508	0.887719
19	1	0	-7.403442	0.198957	-0.887179
20	1	0	-5.909078	-1.838453	-0.883937
21	1	0	-5.909038	-1.838900	0.883380
22	1	0	-4.830027	0.429181	0.884535

23	1	0	-4.830067	0.429629	-0.883994
24	1	0	-3.353549	-1.605403	-0.884690
25	1	0	-3.353509	-1.605853	0.884132
26	1	0	-2.273127	0.663813	0.884642
27	1	0	-2.273168	0.664263	-0.884096
28	1	0	-0.796639	-1.370097	-0.884655
29	1	0	-0.796599	-1.370548	0.884097
30	1	0	0.283743	0.899189	0.884650
31	1	0	0.283703	0.899640	-0.884099
32	1	0	1.760323	-1.134646	-0.884651
33	1	0	1.760363	-1.135097	0.884097
34	1	0	2.840683	1.134646	0.884651
35	1	0	2.840643	1.135097	-0.884097
36	1	0	4.317263	-0.899189	-0.884650
37	1	0	4.317303	-0.899640	0.884099
38	1	0	5.397644	1.370097	0.884655
39	1	0	5.397604	1.370548	-0.884097
40	1	0	6.874133	-0.663813	-0.884642
41	1	0	6.874173	-0.664263	0.884096
42	1	0	7.954554	1.605403	0.884690
43	1	0	7.954514	1.605853	-0.884132
44	1	0	9.431032	-0.429181	-0.884535
45	1	0	9.431073	-0.429629	0.883994
46	1	0	10.510083	1.838453	0.883937
47	1	0	10.510043	1.838900	-0.883380
48	1	0	12.765334	1.139408	0.000051
49	1	0	12.004408	-0.198508	-0.887719
50	1	0	12.004448	-0.198957	0.887179

Table S10. Optimized Structural Coordinate and its Total Energy of **C2H4** at B3LYP-D3/3-21G* level

HF=-79.402463 hartree, NImg=0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.000000	-0.000000	-0.002561
2	6	0	-0.000000	-0.000000	1.542561
3	1	0	1.024219	0.000000	-0.392021
4	1	0	-1.024219	-0.000000	1.932021
5	1	0	-0.512110	-0.887000	-0.392021
6	1	0	0.512110	-0.887000	1.932021
7	1	0	-0.512110	0.887000	-0.392021
8	1	0	0.512110	0.887000	1.932021

4. Details of Temperature-Dependent NMR Study

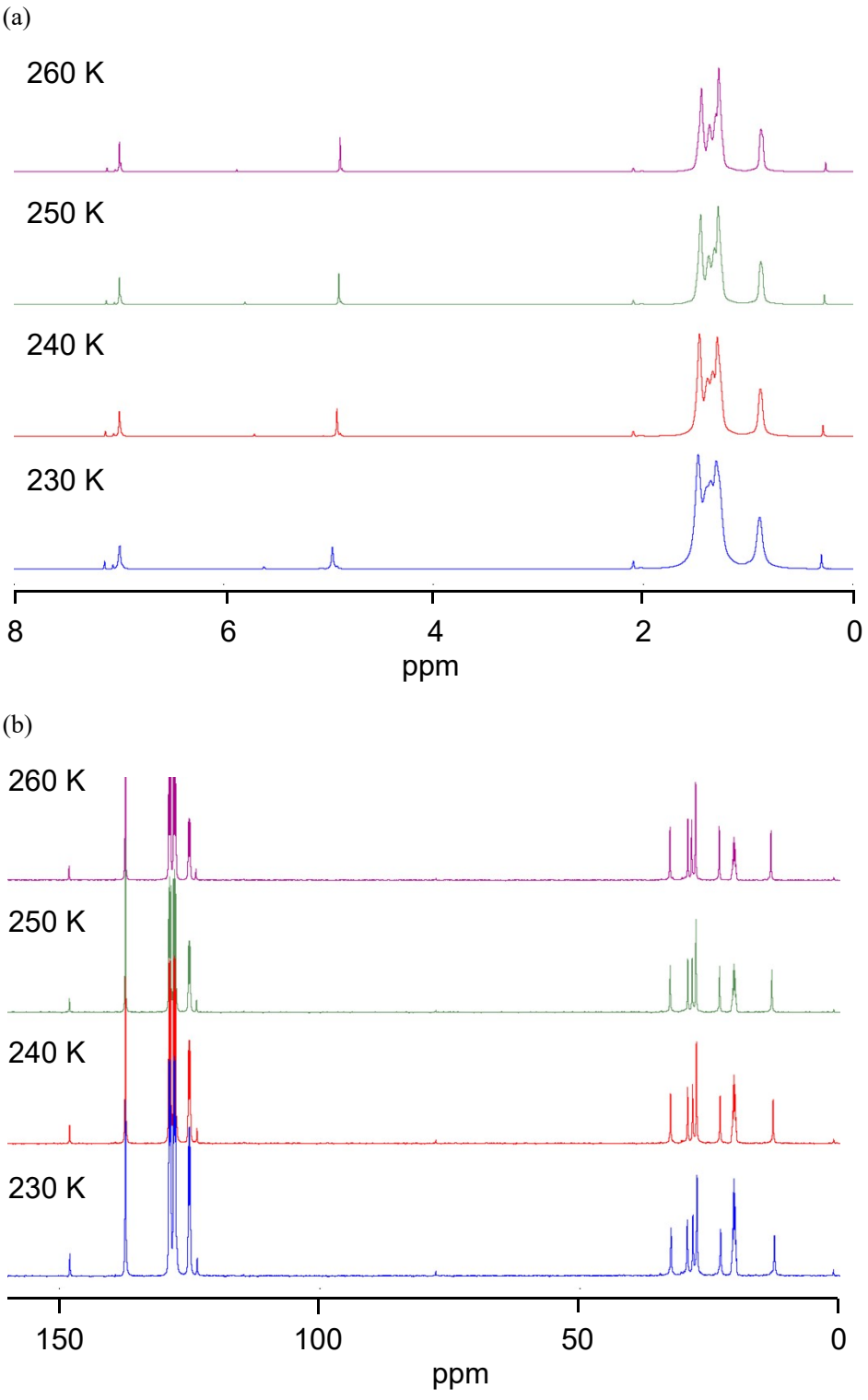
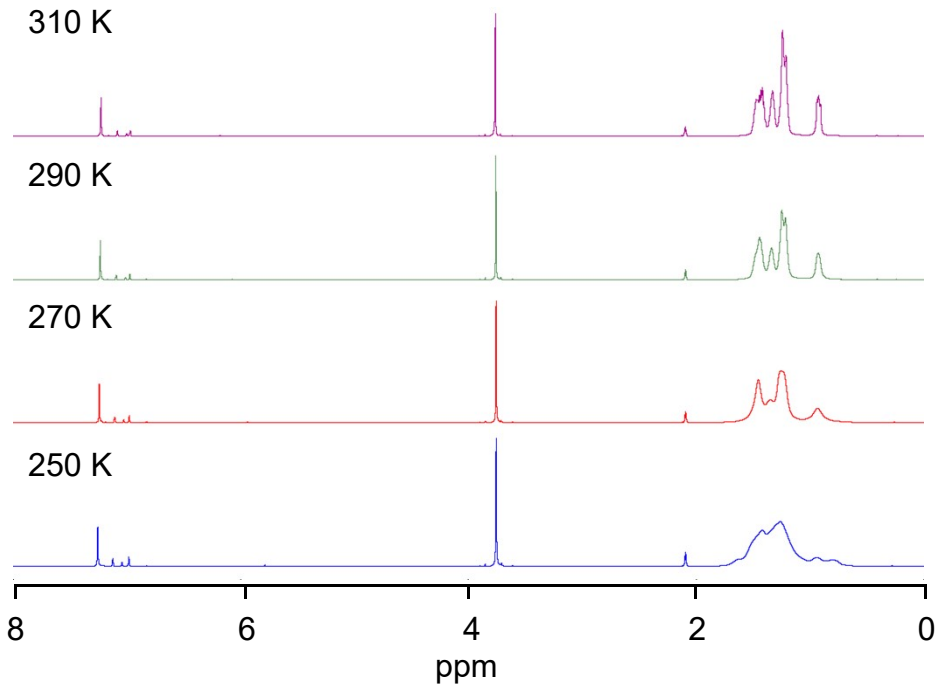


Fig. S25. Temperature-dependent NMR spectra of **1a** in toluene-d_8: (a) ^{1}H NMR; (b) ^{13}C NMR.

(a)



(b)

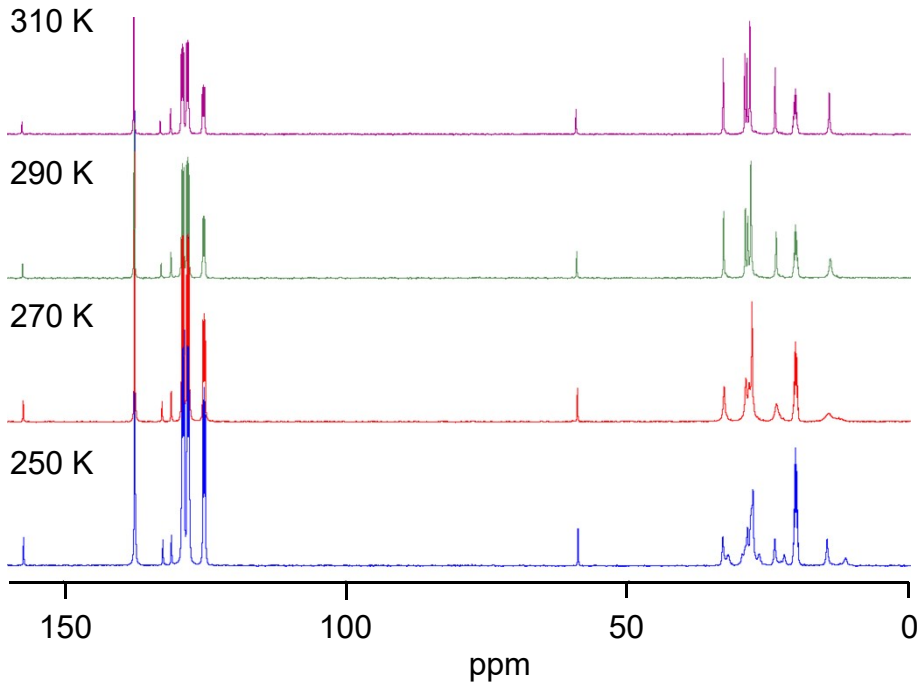
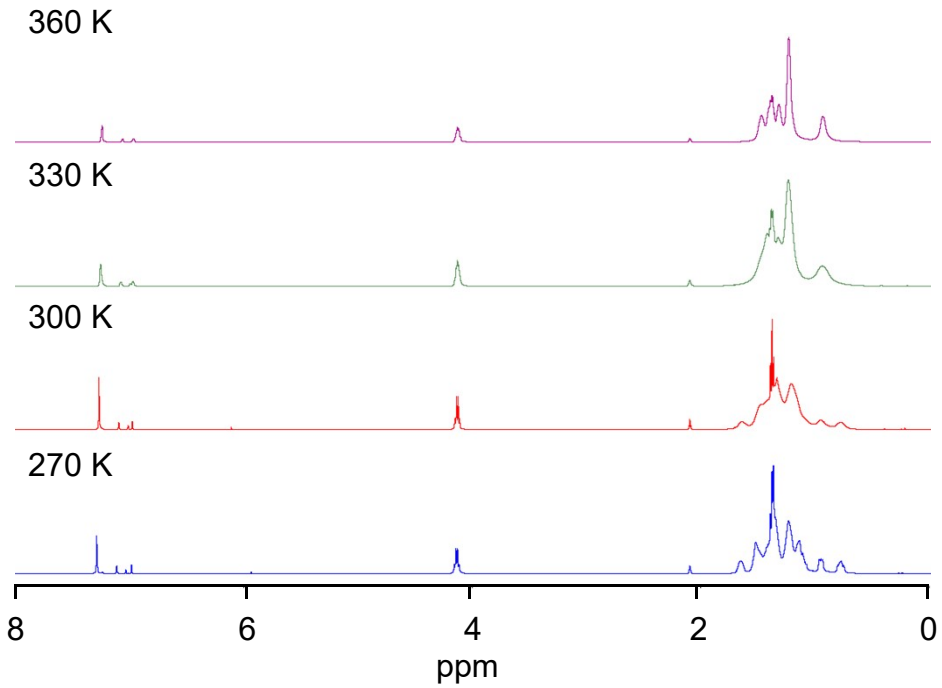


Fig. S26. Temperature-dependent NMR spectra of **1b** in toluene-d_8: (a) ^{1}H NMR; (b) ^{13}C NMR.

(a)



(b)

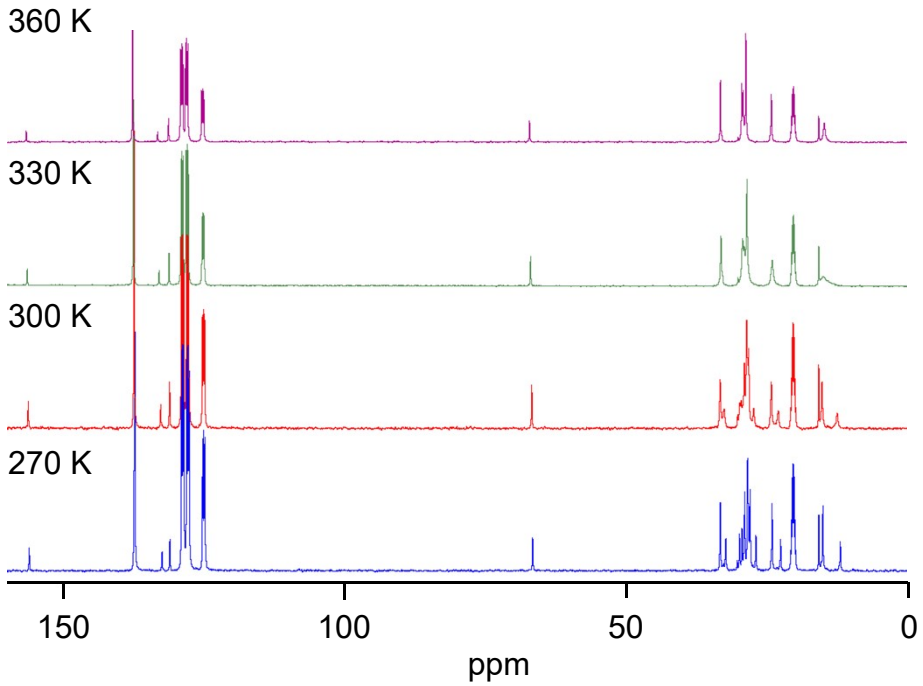


Fig. S27. Temperature-dependent NMR spectra of **1c** in toluene-d_8: (a) ^{1}H NMR; (b) ^{13}C NMR.

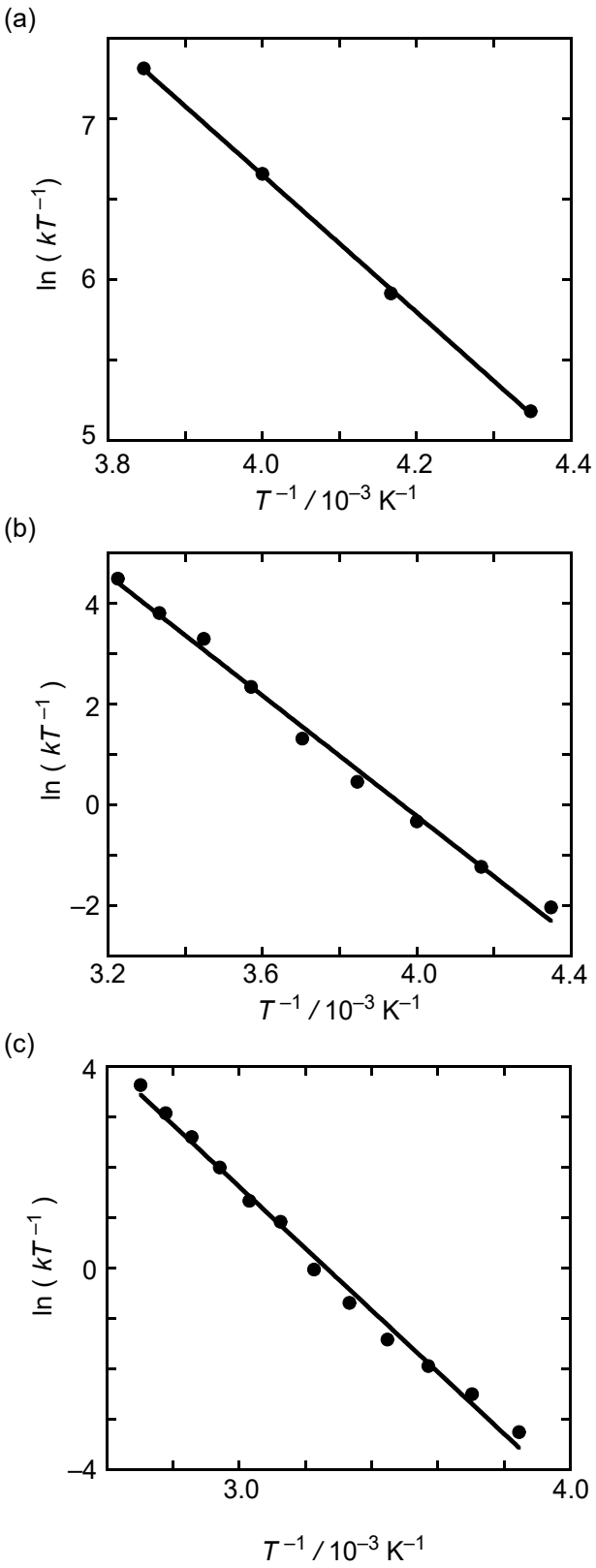


Fig. S28. Eyring plots for phenylene rotation: (a) **1a**, (b) **1b**, and (c) **1c**.