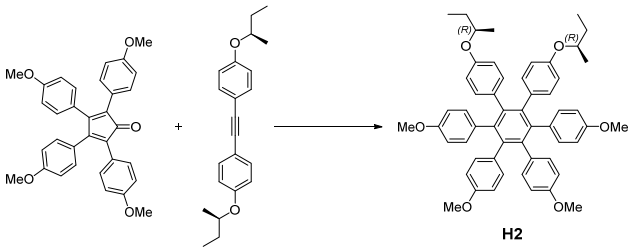
Supporting Information for

Solvent and Temperature Effects on Dynamics and Chiroptical Properties of Propeller Chirality and Toroidal Interaction of Hexaarylbenzenes

Tomoyo Kosaka, Satono Iwai, Yoshihisa Inoue, Toshiyuki Moriuchi, and Tadashi Mori*
Department of Applied Chemistry, Graduate School of Engineering, Osaka University, 2-1 Yamada-oka, Suita, Osaka, 565-0871, Japan

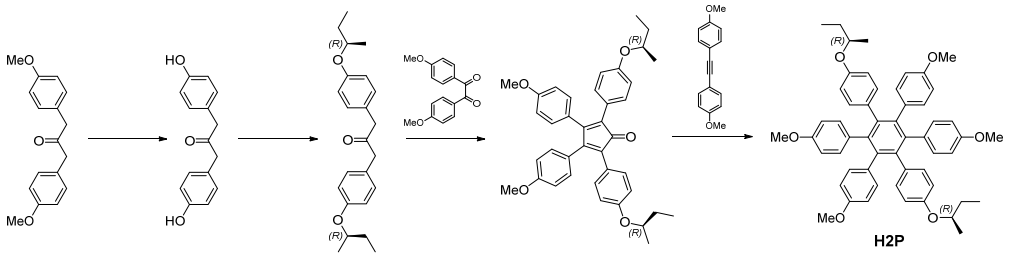
Contents

Preparation of 1,2-bis(4-((*R*)-1-methylpropyloxy)phenyl)-3,4,5,6-tetra-*p*-anisylbenzene (H2)



H2 was prepared by the procedure similar to that reported in the literature.[1] Thus, bis((*R*)-1-methylpropyloxyphenyl)acetylene[2] (322 mg, 1.0 mmol) and 2,3,4,5-tetra(*p*-anisyl)cyclopenta-2,4-dien-1-one[3] (505 mg, 1.0 mmol) were placed in pressure-resistant glass flask. Diphenyl ether (15 mL) was added and purged with argon. The mixture was heated to reflux for 14 h at 280 °C. The crude mixture was purified by silica-gel column chromatography with hexane-dichloromethane (1 : 1) as eluent to give yellow to brown material, which was further purified by recrystallization from ethanol to afford pale yellow solid in 0.44 g (53%). M.p. 223-224 °C. ^{1}H NMR: 0.87 (6H, t, J = 7.6 Hz), 1.12 (6H, d, J = 6.4 Hz), 1.47 (2H, sept d, J = 7.2, 1.6 Hz), 1.60 (2H, sept d, J = 7.2, 1.6 Hz), 3.62 (6H, s), 3.63 (6H, s), 4.07 (2H, sxt, J = 6.4 Hz), 6.40 (4H, d, J = 8.8 Hz), 6.41 (4H, d, J = 8.8 Hz), 6.42 (4H, d, J = 8.8 Hz), 6.63 (4H, d, J = 8.8 Hz), 6.67 (4H, d, J = 8.8 Hz), and 6.68 (2H, d, J = 8.8 Hz). ^{13}C NMR: 9.8, 19.2, 29.1, 55.1, 75.3, 112.3, 112.3, 115.0, 132.6, 133.8, 133.9, 140.29, 140.31, 140.6, 155.5, 156.9, and 157.0. EI-MS (direct): *m/z* = 800 (M^+ + 2, 18%), 799 (M^+ + 1, 58%), 798 (M^+, 100), 687 (25), and 686 (51). HRMS (EI): *m/z* = 798.3911. $C_{54}H_{54}O_6$ requires 798.3920. EA: Found: C, 81.09; H, 6.84%. Calcd for $C_{54}H_{54}O_6$: C, 81.17; H, 6.81. Specific rotation: $[\alpha]^{25}_D$ -71.7 ± 3.2° (*c* 0.10, chloroform).

Preparation of 1,4-bis(4-((*R*)-1-methylpropyloxy)phenyl)tetra-*p*-anisylbenzene (H2P)



This was prepared through the following 4 steps.

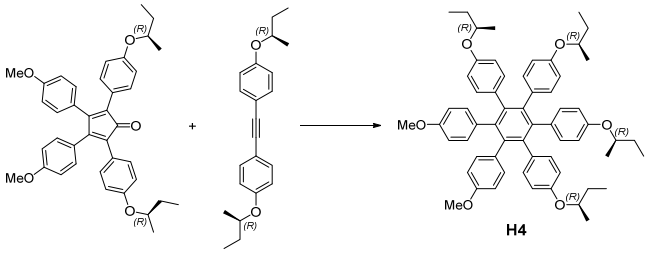
(1) Although bis(4-hydroxybenzyl)ketone has been reported,[4] the synthetic procedure was improved by applying the literature procedure for the synthesis of similar compounds.[5] Thus, bis(4-methoxybenzyl)ketone (7.20 g, 27 mmol) was mixed with pyridine hydrogen chloride (30.8 g, 0.27 mol, 10 eq) and heated up to 220 °C under an argon atmosphere and stirred for 3 h. The resulting mixture was cooled down to 100 °C and quenched with 0.1 M HCl (100 mL) and extracted with ethyl acetate (3 × 200 mL). The combined crude material was purified by silica-gel column chromatography with hexane-ethyl acetate (1 : 1) as eluent to give brown solid material in 5.43 g (84%).

(2) Bis(4-((*R*)-1-methylpropyloxy)benzyl)ketone was prepared by a slightly modified version of Mitsunobu reaction.[6] Thus, bis(4-hydroxybenzyl)ketone (5.42 g, 22 mmol), (*S*)-(+)-2-butanol (3.71 g, 50 mmol, 2.2 eq), and tetra-*n*-butylphosphine (12.5 g, 62 mmol, 2.8 eq) were dissolved in dry benzene (150 mL), to which was added 1,1'-azodicarbonyl dipiperidine (15.6 g, 62 mmol, 2.8 eq) as portions at an ambient temperature under an argon atmosphere. The solution was warmed to 60 °C and was stirred for 20 h. After cooling down, hexane (200 mL) was added and the resulting solid was filtrated off and washed with diethyl ether (100 mL). The oily residue was evaporated and purified by silica-gel column chromatography with hexane-ethyl acetate (50 : 1) as eluent to give the desired product as a pale yellow oil in 4.27 g (54%). ^{1}H NMR: 0.97 (6H, t, J = 7.5 Hz), 1.28 (6H, d, J = 6.1 Hz), 1.61 (2H, sept d, J = 6.6, 1.4 Hz), 1.74 (2H, sept d, J = 6.4, 1.4 Hz), 3.63 (4H, s), 4.26 (2H, sxt, J = 6.1 Hz), 6.83 (4H, AA'XX', J_{AX} = 8.8, $J_{AA'}$ = 2.4 Hz), and 7.02 (4H, AA'XX', J_{XA} = 8.8, $J_{XX'}$ = 2.4 Hz). ^{13}C NMR: 9.9, 19.4, 29.3, 48.2, 75.3, 116.3, 126.0, 130.7, 157.5, and 206.8. EI-MS (direct): *m/z* = 354 (M^+, 18%), 163 (32), and 107 (100). HRMS (EI): *m/z* = 354.2197. $C_{23}H_{30}O_3$ requires 354.2195. EA: Found: C, 77.67; H, 8.56%. Calcd for $C_{23}H_{30}O_3$: C, 77.93; H, 8.53; O, 13.54. Specific rotation: $[\alpha]^{25}_D$ -63.1 ± 6.8° (*c* 0.10, chloroform).

(3) 2,5-Bis(4-((*R*)-1'-methylpropyloxy)phenyl)-3,4-di(*p*-anisyl)cyclopenta-2,4-dien-1-one was prepared according to the literature procedure for the preparation of related molecules.[3] Thus, to a boiling solution of bis(4-((*R*)-1-methylpropyloxy)benzyl)ketone, (4.28 g, 12 mmol) and *p*-anisil (3.26 g, 12 mmol) in dry ethanol (25 mL) was added an ethanol solution of KOH (1.9 M, 5.0 mL, prepared from 0.54 g of KOH dissolved in 5.0 mL of ethanol). The solution was refluxed for 5 days under an argon atmosphere and then cooled to 0 °C and kept at this temperature overnight with an ice-bath. The greenish crystalline precipitate was filtrated and washed with cold ethanol (2 × 20 mL). The crude material (3.44 g) contain the desired product as well as *p*-anisil, which was separated by silica-gel column chromatography with hexane-chloroform (1 : 1) as eluent to give the desired product as a greenish dark brown powder in 1.08 g (15%). The yield would be improved by prolonged reflux, although not verified. M.p. 172-173 °C. ^{1}H NMR: 0.96 (6H, t, J = 7.6 Hz), 1.28 (6H, d, J = 6.0 Hz), 1.60 (2H, sept d, J = 7.6, 1.2 Hz), 1.73 (2H, sept d, J = 7.6, 1.2 Hz), 3.79 (6H, s), 4.27 (2H, sxt, J = 6.1 Hz), 6.71 (4H, AA'XX', J_{AX} = 9.2, $J_{AA'}$ = 2.6 Hz), and 6.75 (4H, AA'XX', J_{AX} = 9.2, $J_{AA'}$ = 2.6 Hz), 6.86 (4H, AA'XX', J_{XA} = 9.2, $J_{XX'}$ = 2.4 Hz), and 7.16 (4H, AA'XX', J_{XA} = 9.2, $J_{XX'}$ = 2.4 Hz). ^{13}C NMR: 10.0, 19.5, 29.4, 55.3, 75.0, 113.5, 115.5, 123.5, 124.1, 126.0, 131.3, 131.5, 152.7, 157.7, 159.7, and 201.6. EI-MS (direct): *m/z* = 590 (M^+ +2, 12%), 589 (M^+ +1, 43), 588 (M^+, 100), 477 (14), 476 (43), 475 (14), 238 (19), 224 (28), 223 (16), and 209 (11). HRMS (EI): *m/z* = 588.2878. $C_{39}H_{40}O_5$ requires 588.2876. EA: Found: C, 79.32; H, 6.57%. Calcd for $C_{39}H_{40}O_5$: C, 79.56; H, 6.85. Specific rotation: $[\alpha]^{25}_D$ -2110 ± 460° (*c* 0.10, chloroform). The value was gradually increased during the measurement under the exposure to Na-D line.

(4) **H2P** was prepared according to the literature procedure of the synthesis of similar compounds.[1] Thus, 1-methoxy-4-(4'-methoxyphenylethynyl)benzene (0.14 g, 0.6 mmol) and 2,5-bis(4-((*R*)-1-methylpropyloxy)phenyl)-3,4-di(4-anisyl)cyclopenta-2,4-dien-1-one (0.35 g, 0.6 mmol) were placed in a pressure-resistant glass flask. Diphenyl ether (10 mL) was added and purged with argon. The mixture was heated to reflux for 12 h at 280 °C. The resulting mixture was purified by silica-gel column chromatography with hexane-dichloromethane (1 : 1) as eluent to give yellowish powder, which was further purified by recrystallization from hexane-dichloromethane to afford colorless solid in 0.20 g (43%). M.p. 250-251 °C. ^{1}H NMR: 0.88 (6H, t, J = 7.2 Hz), 1.12 (6H, d, J = 6.2 Hz), 1.48 (2H, pseudo sept d, J = 7.2, 1.6 Hz), 1.60 (2H, pseudo sept d, J = 7.2, 1.6 Hz), 3.62 (12H, s), 4.09 (2H, sxt, J = 6.2 Hz), 6.41 (12H, d, J = 8.8 Hz), 6.63 (4H, d, J = 8.8 Hz), and 6.68 (8H, d, J = 8.8 Hz). ^{13}C NMR: 9.8, 19.1, 29.1, 55.1, 75.3, 112.25, 112.30, 115.2, 132.6, 132.7, 133.7, 133.9, 140.3, 140.6, 155.4, and 157.0. EI-MS (direct): *m/z* = 800 (M^+ +2, 19%), 799 (M^+ +1, 59), 798 (M^+, 100), 687 (22), and 686 (45). HRMS (EI): *m/z* = 798.3912. $C_{54}H_{54}O_6$ requires 798.3920. EA: Found: C, 80.88; H, 6.73%. Calcd for $C_{54}H_{54}O_6$: C, 81.17; H, 6.81. Specific rotation: $[\alpha]^{25}_D$ -33.8 ± 8.0° (*c* 0.10, chloroform).

Preparation of 1,2,3,4-tetrakis(4-((*R*)-1-methylpropyloxy)phenyl)-5,6-di-*p*-anisylbenzene (H4)



H2P was prepared according to the literature procedure for the synthesis of similar compounds.[1] Thus, bis((*R*)-1-methylpropyloxyphenyl)acetylene (0.20 g, 0.6 mmol) and 2,5-bis(4-((*R*)-1-methylpropyloxy)phenyl)-3,4-bis(4-anisyl)cyclopenta-2,4-dien-1-one (0.35 g, 0.6 mmol) were placed in a pressure-resistant glass flask. Diphenyl ether (10 mL) was added and purged with argon. The mixture was heated to reflux for 20 h at 290 °C. The crude mixture was purified by silica-gel column chromatography with hexane-dichloromethane (1 : 1) as eluent to give yellow material (0.30 g), which was further purified by recrystallization from hexane-dichloromethane to afford colorless solid in 0.14 g (27%). M.p. 142-143 °C. ^{1}H NMR: 0.87 (6H, td, J = 7.0, 1.4 Hz), 1.11 (12H, dd, J = 6.2, 2.0 Hz), 1.47 (4H, pseudo sept d, J = 7.0, 1.4 Hz), 1.60 (4H, pseudo sept d, J = 7.0, 1.4 Hz), 3.62 (6H, s), 4.07 (4H, sept, J = 6.2 Hz), 6.397 (4H, d, J = 8.8 Hz), 6.406 (4H, d, J = 8.8 Hz), 6.412 (4H, d, J = 8.8 Hz), 6.64 (8H, d, J = 8.8 Hz), and 6.68 (4H, d, J = 8.8 Hz). ^{13}C NMR: 9.8, 19.15, 19.17, 29.13, 29.15, 55.1, 75.20, 75.24, 112.25, 112.32, 114.9, 115.02, 115.05, 132.7, 133.77, 133.82, 133.86, 140.2, 140.45, 140.47, 155.46, 155.51, and 157.0. EI-MS (direct): *m/z* = 884 (M^+ +2, 22%), 883 (M^+ +1, 64), 882 (M^+, 100), 659 (15), and 658 (32). HRMS (EI): *m/z* = 882.4854. $C_{60}H_{66}O_6$ requires 882.4859. EA: Found: C, 81.40; H, 7.51%. Calcd for $C_{60}H_{66}O_6$: C, 81.60; H, 7.53. Specific rotation: $[\alpha]^{25}_D$ -118.6 ± 10.0° (*c* 0.10, chloroform).

X-ray crystal structure of H2P

The crystals of **H2P** suitable for X-ray analysis were obtained by slow evaporation of aqueous dichloromethane solution, which were directly deposited on Rigaku R-AXIS RAPID diffractometer that uses graphite monochromated Cu-Kα radiation. Crystallographic data for **H2P** (CCDC #1852769): $C_{54}H_{54}O_6$, M = 799.02, monoclinic, $P2_1$ (#4), a = 11.5859(3) Å, b = 20.1144(4) Å, c = 18.9328(4) Å, β = 95.8180(10) °, V = 4389.44(17) Å^3, Z = 4. Crystal size: 0.15 × 0.10 × 0.05 mm^3, T = 123 K, ρ_{calcd} = 1.209 g·cm^{-3}, R_1 = 0.0479 ($I > 4\sigma(I)$), wR_2 = 0.1418 (all data), GOF = 1.010, reflections collected/unique: 2735/2214 (R_{int} = 0.0590), Data: 2735, restraints: 1740, parameters: 1095.

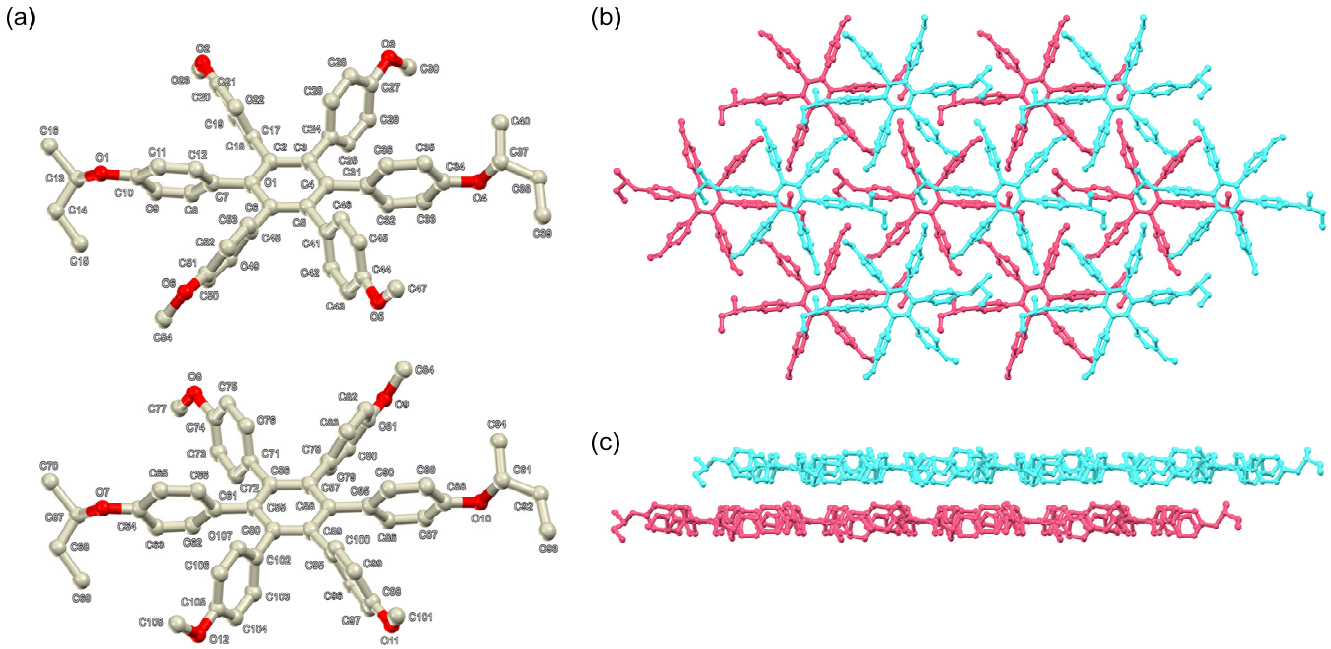


Figure S1. (a) Two independent molecules in the asymmetric unit of **H2P**, (b) top view, and (c) side view of the crystal packing in the asymmetric unit of **H2P**.

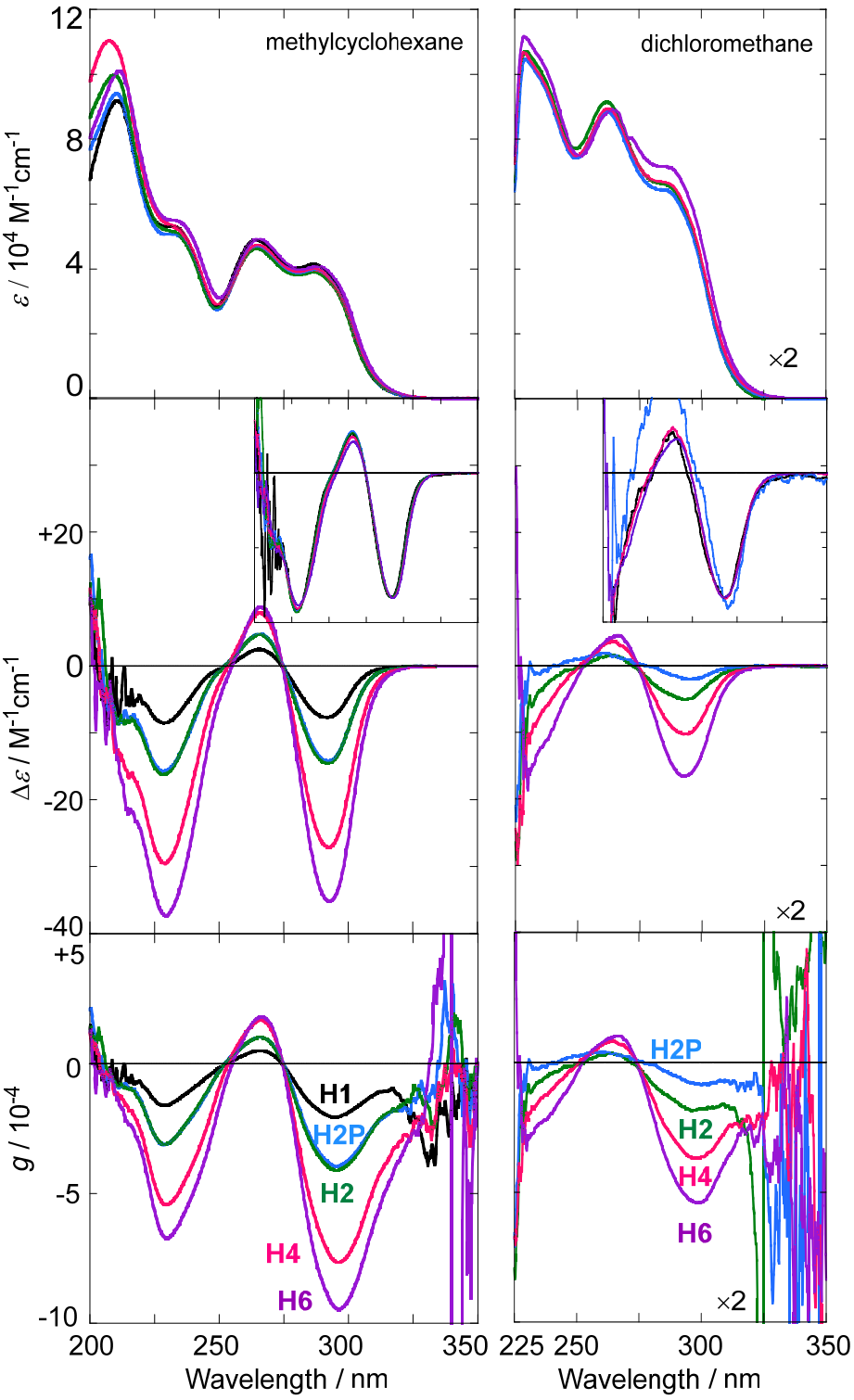


Figure S2. Experimental UV-vis (top), CD (middle), and absorption anisotropy (*g*) factor spectra (bottom) of **H1**-**H6** in methylcyclohexane (left) and dichloromethane (right) at 25 °C. Inset: normalized CD spectra.

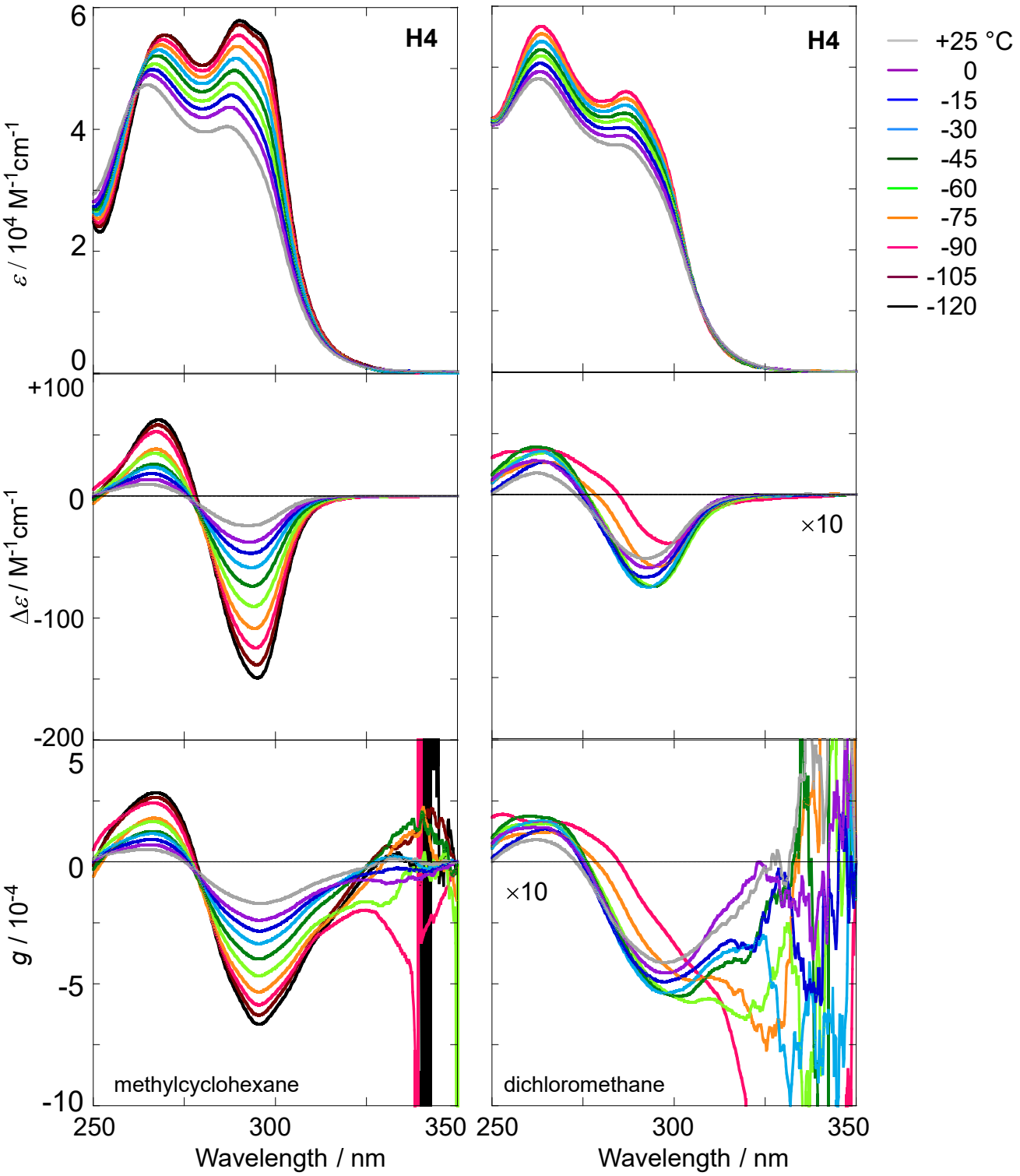


Figure S3. Experimental UV-vis (top), CD (middle), and absorption anisotropy (*g*) factor spectra (bottom) of **H4** in methylcyclohexane (left) and dichloromethane (right) at various temperatures.

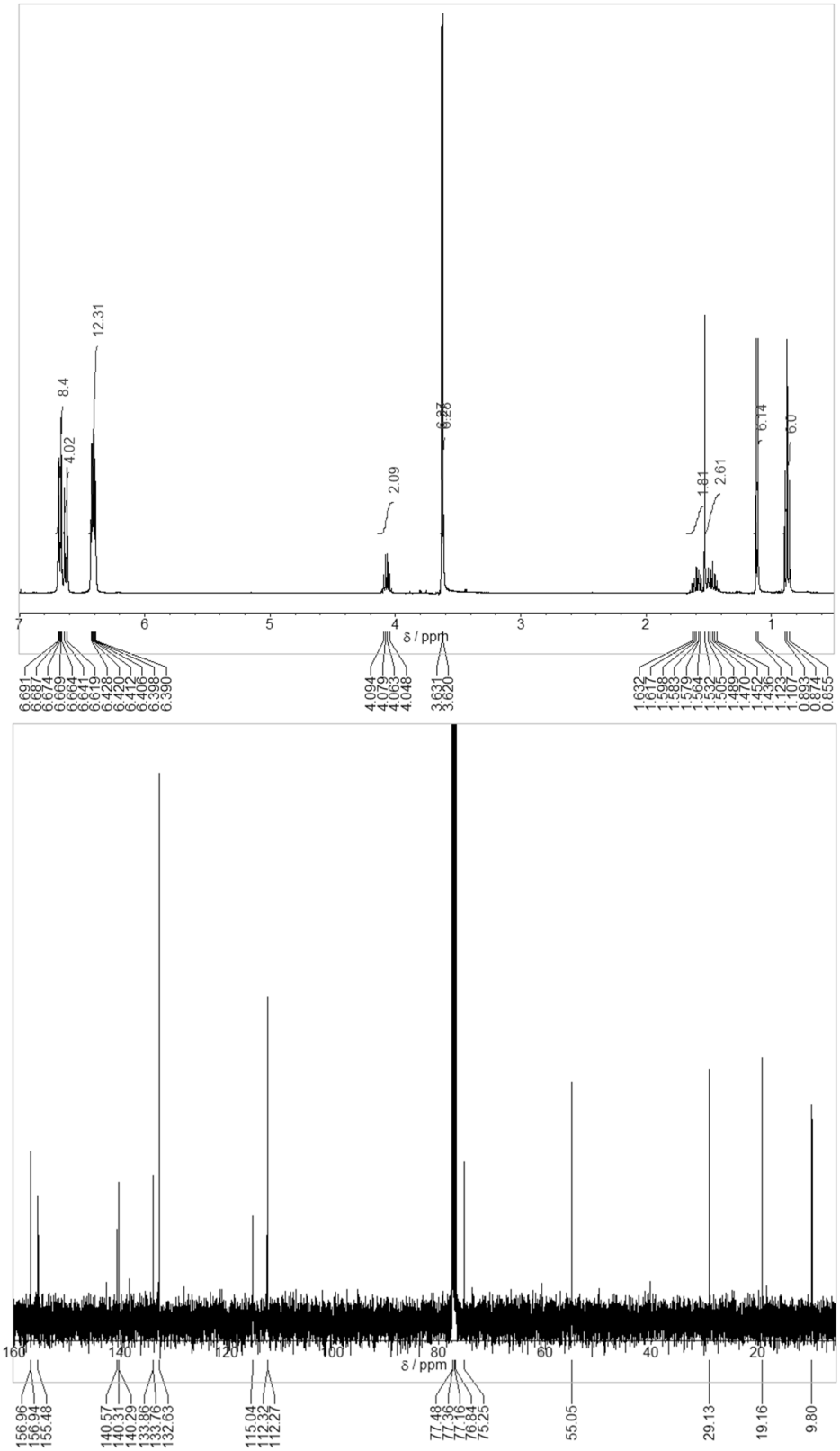


Figure S4. ^{1}H- and ^{13}C-NMR spectra of **H2**.

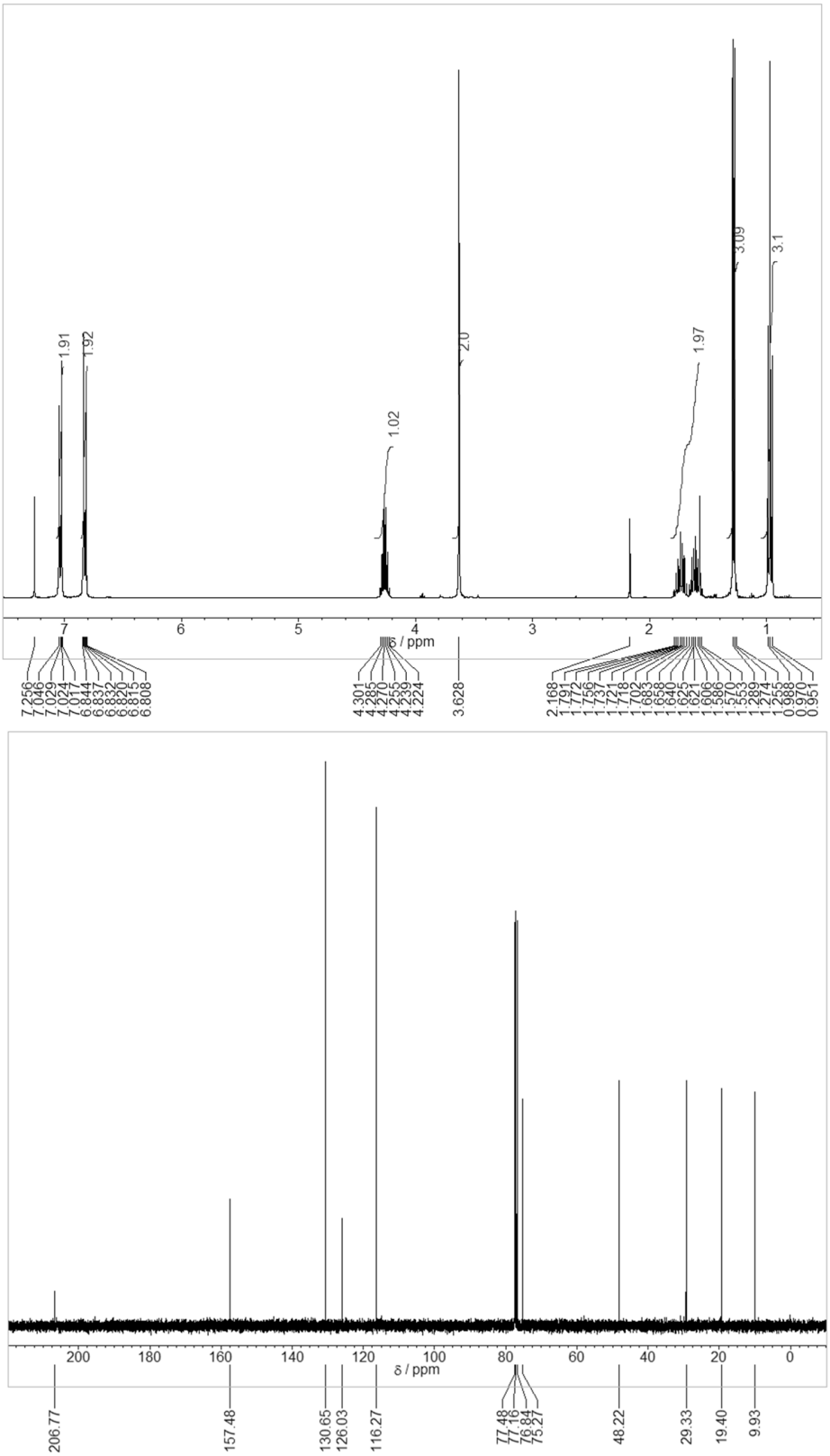


Figure S5. ^{1}H- and ^{13}C-NMR spectra of bis(4-(*R*)-1'-methylpropyloxybenzyl)ketone.

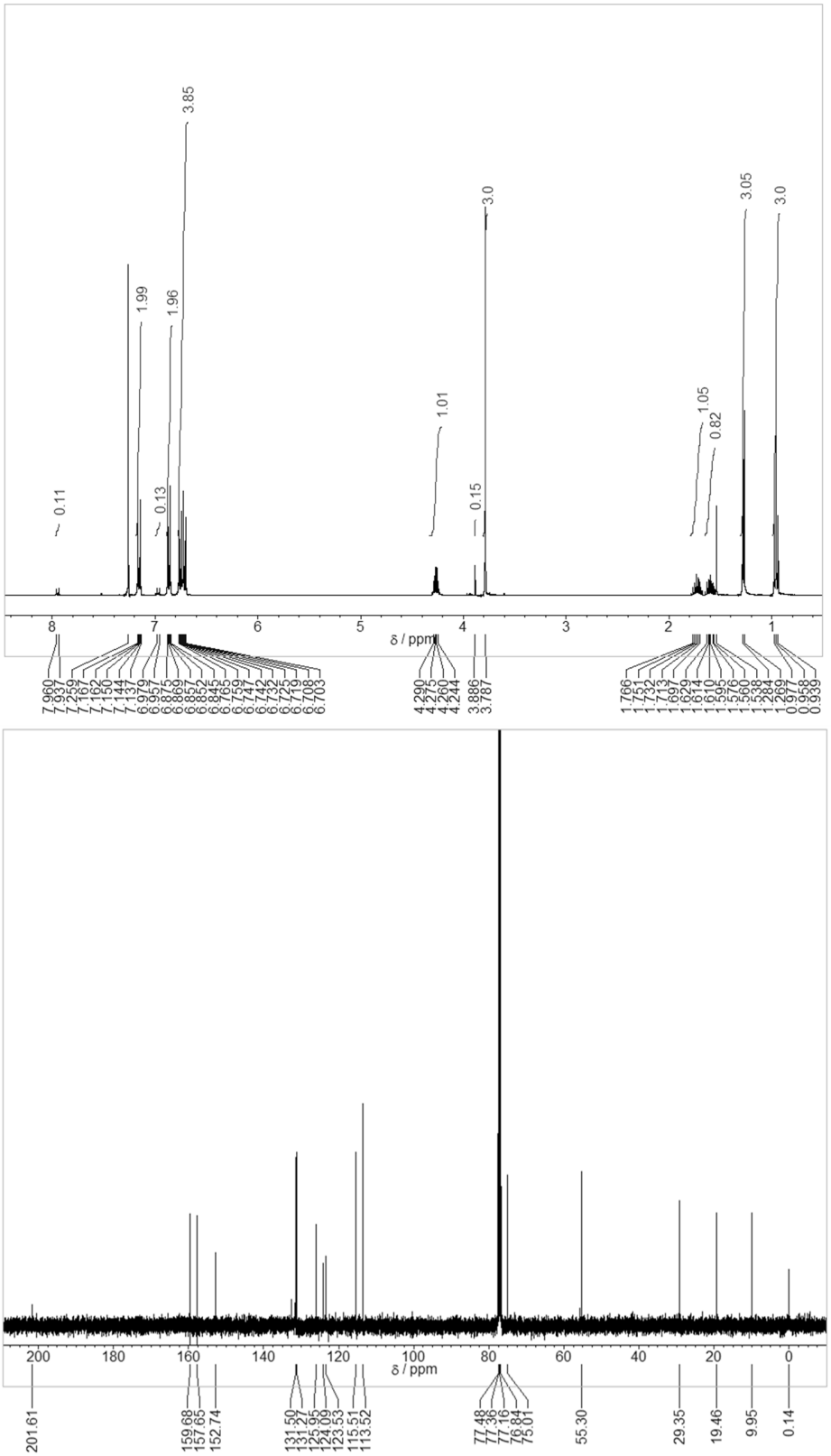


Figure S6. ^{1}H- and ^{13}C-NMR spectra of 2,5-bis(4-(*R*)-1'-methylpropyloxybenzyl)-3,4-bis(p-anisyl)cyclopenta-2,4-dien-1-one.

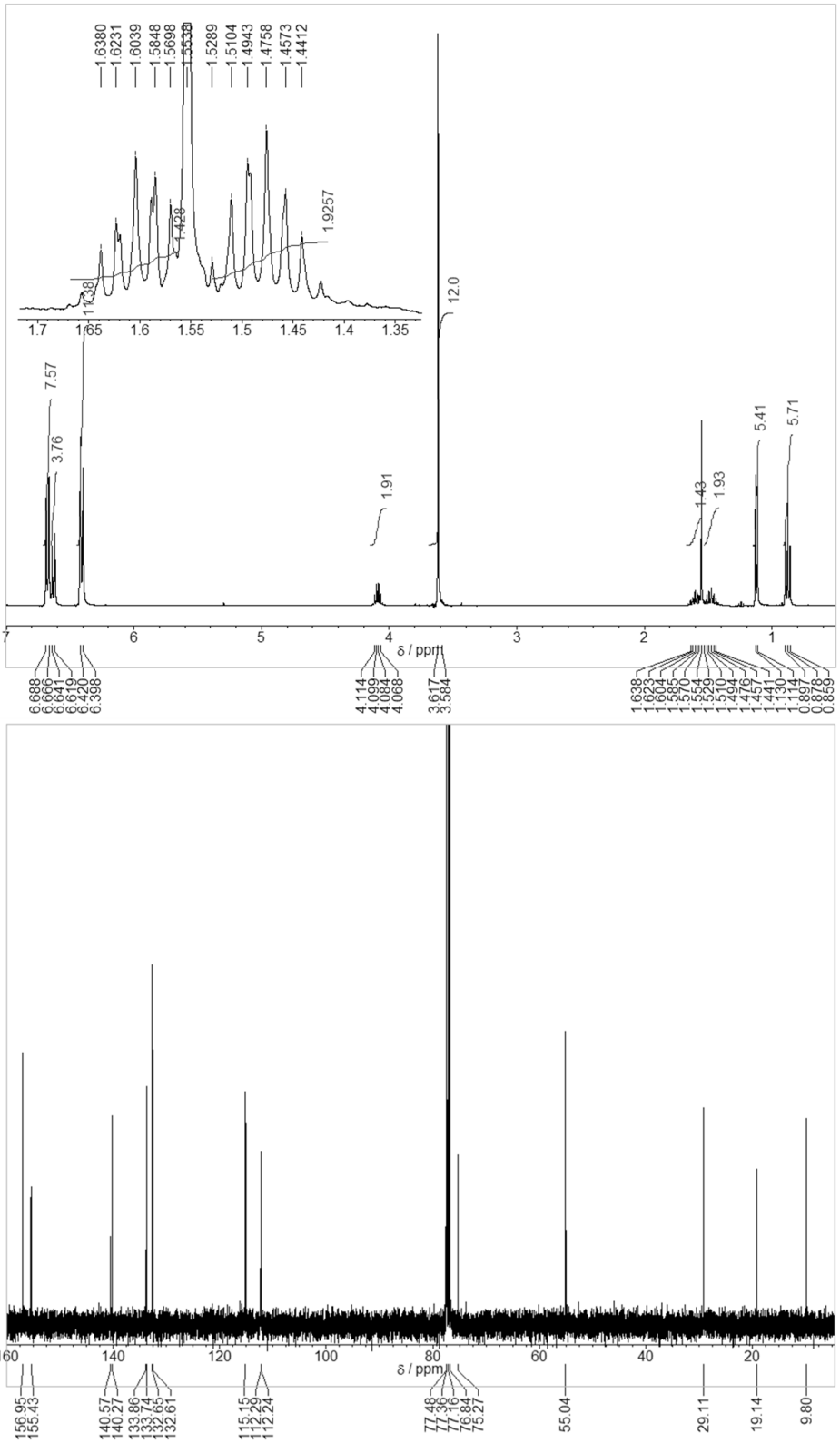


Figure S7. ^{1}H- and ^{13}C-NMR spectra of **H2P**.

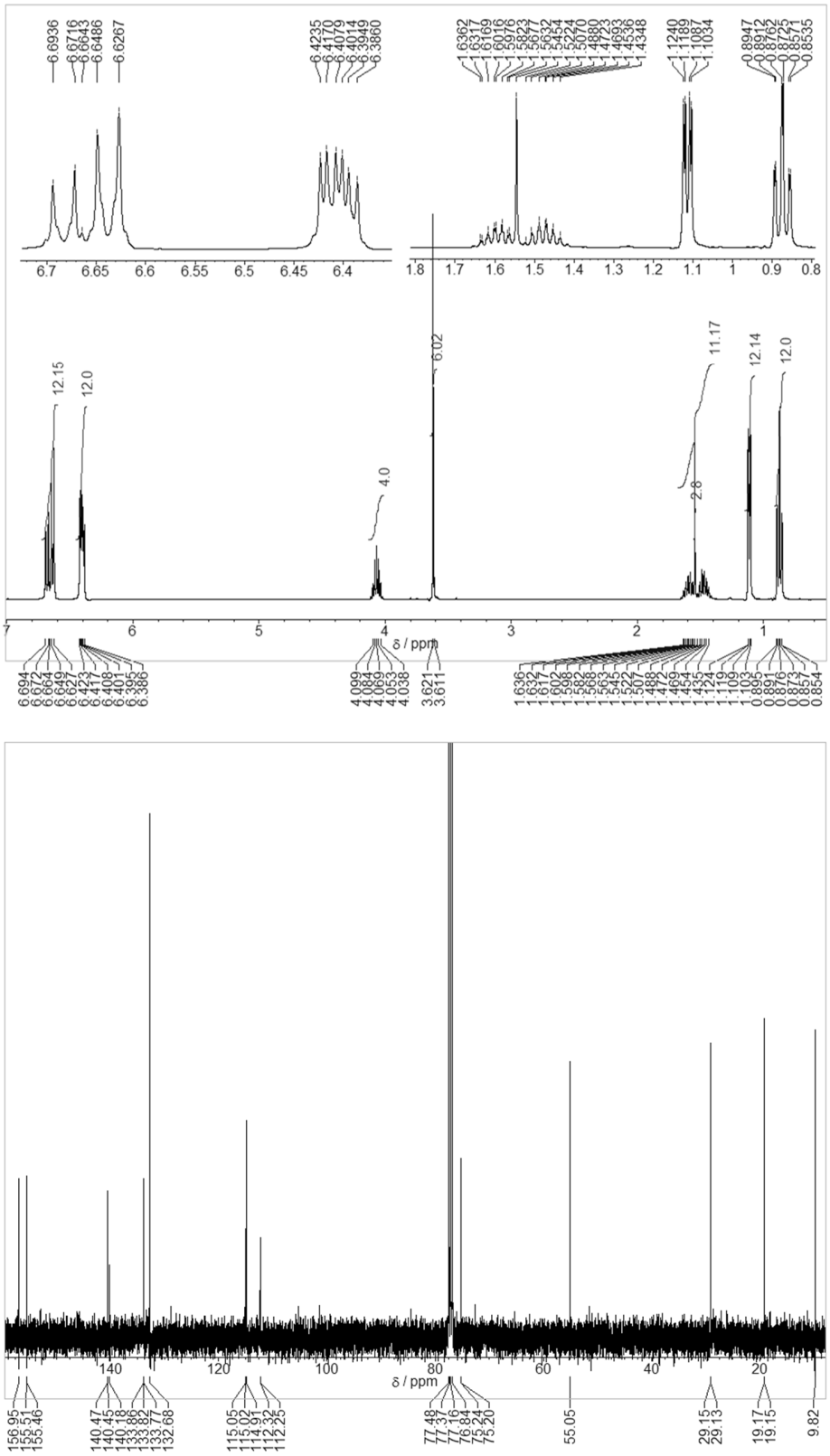


Figure S8. ^{1}H- and ^{13}C-NMR spectra of **H4**.

TABLE S1. Optimized Geometries of the Hexaarylbenzenes at the DFT-D3(BJ)-TPSS/def2-TZVP level.

H2 (clockwise)
Energy = -2543.156287696 au

C	2.4462406	-0.5172952	0.2330932	H	-1.7830937	1.1687497	1.8348103
C	3.9215057	-0.4752591	0.4345206	H	-3.0065203	3.3113479	2.1002013
C	1.6873587	0.6672490	0.3377433	H	0.5690690	2.9157085	-1.2944662
C	1.8070914	-1.7410757	-0.0631752	H	-0.6472188	5.0246672	-1.0630717
C	0.4100785	-1.7784319	-0.2549261	H	-1.8475748	0.7655813	-1.9791857
C	0.2887274	0.6298644	0.1438262	H	-4.2866379	0.5668560	-2.3911972
C	-0.3499880	-0.5926774	-0.1468874	H	-2.1741764	-2.0575166	1.2301930
C	2.6062002	-2.9933779	-0.1719336	H	-4.5834018	-2.2423303	0.8535054
C	-0.2726047	-3.0661599	-0.5654733	H	-1.1048518	-2.3861592	-2.4262539
C	2.3551803	1.9630657	0.6468916	H	-2.2972449	-4.4703082	-2.9239903
C	-0.5055627	1.8844380	0.2546852	H	0.3857289	-4.0691855	1.2240735
C	-1.8246452	-0.6410381	-0.3476464	H	-0.8394967	-6.1744432	0.7475977
C	-0.2219302	2.9884380	-0.5541330	H	2.0098040	-3.4213990	-2.1975025
C	-1.5326492	2.0146891	1.2017145	H	3.3668023	-5.4911346	-2.3834886
C	-2.2227802	3.2088495	1.3558111	H	3.4014657	-2.8790764	1.8210722
C	-0.9100547	4.1929020	-0.4198095	H	4.7233792	-4.9394347	1.6617731
C	-1.9103516	4.3131903	0.5517567	H	4.3967217	-1.2645998	-1.5068157
C	-2.6299504	-1.4682170	0.4402602	H	6.8289980	-1.2018203	-1.1935287
C	-2.4469478	0.1047502	-1.3601638	H	3.8147311	0.3259952	2.4315984
C	-3.8105534	0.0005711	-1.5965056	H	6.2725620	0.3657371	2.7740807
C	-4.0020833	-1.5792544	0.2233593	H	1.2130597	2.3362935	2.4284099
C	-4.5995381	-0.8514734	-0.8121845	H	2.2501254	4.5032325	2.9206096
C	-0.2050161	-4.1558383	0.3171528	H	3.6638928	1.9167948	-1.0639761
C	-1.0315816	-3.2154249	-1.7292254	H	4.7016352	4.1219758	-0.5943216
C	-1.7165703	-4.3973263	-2.0113978	H	8.8483611	-0.1605790	-0.8172257
C	-0.8854585	-5.3369143	0.0582864	H	9.9526817	-0.6496406	0.5036654
C	-1.6517901	-5.4625927	-1.1076522	H	6.4005903	-6.2451254	0.7878102
C	3.3811494	-3.4496339	0.8974144	H	5.0094808	-7.2074083	1.3803241
C	2.6092726	-3.7507372	-1.3542317	H	6.1135217	-7.8929447	0.1496163
C	3.3624560	-4.9102543	-1.4663053	H	2.6982204	6.7076137	2.4144679
C	4.1376400	-4.6185080	0.8078181	H	3.9707226	5.9367269	3.4140273
C	4.1322521	-5.3524743	-0.3826511	H	-2.0791253	6.4663670	-0.9336197
C	4.4750737	-0.0146536	1.6398647	H	-3.6862082	7.7481993	1.3145590
C	4.7990235	-0.8978120	-0.5672759	H	-3.1808341	8.5843606	-0.1540847
C	6.1825784	-0.8676185	-0.3899173	H	-1.2101232	7.5056168	1.8267146
C	5.8475609	0.0137650	1.8391229	H	-0.1798451	6.5362790	0.7520578
C	6.7115191	-0.4127240	0.8222138	H	-0.6898744	8.1637263	0.2576554
C	3.3515354	2.4852247	-0.1931528	H	-4.5100730	6.9597022	-1.5518299
C	1.9851107	2.7146204	1.7652919	H	-4.9997444	6.1003921	-0.0819693
C	2.5684250	3.9507331	2.0437998	H	-5.5513804	7.7627874	-0.3647083
C	3.9381231	3.7163074	0.0623374	H	-6.5676516	-1.8773691	0.5838148
C	3.5450571	4.4604250	1.1822770	H	-8.3827814	-1.3405525	-1.8030332
C	8.9535937	-0.7764978	0.0851013	H	-8.8837565	-2.1841150	-0.3371061
C	5.6353405	-6.9804935	0.5077281	H	-6.7614337	-3.2641623	-2.1536256
C	3.7660126	6.4586332	2.4704801	H	-5.4524000	-3.5364341	-0.9838101
C	-2.2603487	6.6793497	0.1294342	H	-7.1136100	-4.0167305	-0.5802771
C	-1.0046297	7.2543476	0.7810017	H	-8.3769652	-0.1289767	1.0339920
C	-3.4684507	7.6049100	0.2486242	H	-7.8484910	0.7147176	-0.4314622
C	-4.7065987	7.0759281	-0.4795115	H	-9.5481793	0.2423811	-0.2422918
C	-6.7768641	-1.8799814	-0.4953042	H	-3.9103023	-6.0514088	-2.4629530
C	-6.5057956	-3.2606013	-1.0889645	H	-2.5038323	-6.7134133	-3.3553375
C	-8.2106434	-1.4072335	-0.7213219	H	-3.5400129	-7.8014362	-2.3831253
C	-8.5147545	-0.0647592	-0.0517681	H	4.3614548	7.3708219	2.4173185
C	-3.1088696	-6.8014937	-2.4438781				
O	8.0521540	-0.3488520	1.1069769				
O	4.8438594	-6.5082713	-0.5832561				
O	4.1686941	5.6713544	1.3490287				
O	-2.6435916	5.4467952	0.7875845				
O	-5.9319277	-0.8894294	-1.1310796				
O	-2.3013811	-6.6598159	-1.2744456				

H2 (counterclockwise)

Energy = -2543.155644812 au

C	2.4254427	-0.5188425	0.2473749
C	3.8989953	-0.4838805	0.4635703
C	1.6671312	0.6653093	0.3651536
C	1.7879120	-1.7359401	-0.0768781
C	0.3919808	-1.7689155	-0.2802662
C	0.2707628	0.6323006	0.1608416
C	-0.3664439	-0.5841446	-0.1624680
C	2.5885144	-2.9858841	-0.2032868
C	-0.2836231	-3.0519589	-0.6222270
C	2.3370655	1.9510666	0.7079628
C	-0.5293535	1.8825833	0.2837323
C	-1.8398726	-0.6186777	-0.3773009
C	-0.5453790	2.6158603	1.4730457
C	-1.2852706	2.3692342	-0.7938878
C	-2.0141469	3.5450455	-0.6902518
C	-1.2813129	3.7935637	1.6001536
C	-2.0161783	4.2711160	0.5086330
C	-2.3829068	-1.0529033	-1.5893131
C	-2.7301480	-0.2241580	0.6332766
C	-4.1035007	-0.2742957	0.4438851
C	-3.7602606	-1.0991422	-1.8025954
C	-4.6321948	-0.7160190	-0.7767223
C	0.0730716	-3.7761669	-1.7709721
C	-1.3034383	-3.5660529	0.1827398
C	-1.9561739	-4.7578577	-0.1331774
C	-0.5701463	-4.9584358	-2.1070399
C	-1.5915659	-5.4570329	-1.2881738
C	3.6335681	-3.0828913	-1.1255101
C	2.3216538	-4.1022552	0.6053465
C	3.0733741	-5.2635644	0.5028422
C	4.3947899	-4.2454365	-1.2506661
C	4.1163752	-5.3423728	-0.4290226
C	4.7271530	0.3334933	-0.3222642
C	4.5025189	-1.2681741	1.4498143
C	5.8818205	-1.2489079	1.6590637
C	6.1015132	0.3593338	-0.1361430
C	6.6881775	-0.4330550	0.8590282
C	3.0637549	2.0946657	1.9006941
C	2.2499596	3.0578635	-0.1403570
C	2.8583922	4.2729213	0.1753843
C	3.6682594	3.2971688	2.2367930
C	3.5682008	4.3962763	1.3740391
C	8.6740434	-1.1397831	1.9812321
C	5.8718020	-6.6342721	-1.4046289
C	4.0993319	6.6814637	0.9293870
C	-2.8429467	6.2161269	1.7096877
C	-3.8718312	5.6025362	2.6553112
C	-3.2146826	7.6273081	1.2606926
C	-2.1391465	8.2831714	0.3911336
C	-6.6295313	-1.1485945	-2.0930312
C	-6.6271929	0.0145467	-3.0811374
C	-8.0365712	-1.6064924	-1.7164585
C	-8.0434173	-2.8340546	-0.8020776
C	-3.2225057	-7.1539307	-0.8848755
O	8.0526400	-0.3428685	0.9720659
O	4.8048169	-6.5288311	-0.4612222
O	4.1944272	5.5446487	1.7885920
O	-2.7498040	5.4282277	0.4976312
O	-5.9998553	-0.7473973	-0.8516317
O	-2.1728198	-6.6300359	-1.6993272
H	-1.2980527	1.8149404	-1.7275429
H	-2.5911038	3.9230175	-1.5287767
H	0.0330109	2.2641200	2.3221854
H	-1.2682900	4.3231701	2.5456675
H	-2.3357016	0.1256774	1.5825612
H	-4.7894288	0.0239541	1.2309151
H	-1.7173312	-1.3671464	-2.3877915
H	-4.1333686	-1.4360786	-2.7627529
H	-1.6031492	-3.0221032	1.0734072
H	-2.7419357	-5.1226156	0.5186171
H	0.8676100	-3.4020041	-2.4094587
H	-0.2962052	-5.5132745	-2.9991117
H	1.5100487	-4.0549197	1.3250884
H	2.8678318	-6.1235152	1.1328560
H	3.8651234	-2.2314879	-1.7584481
H	5.1955012	-4.2805373	-1.9807271
H	3.8855581	-1.9143219	2.0670347
H	6.3102691	-1.8709584	2.4367691
H	4.2819075	0.9579941	-1.0908179
H	6.7398305	0.9888144	-0.7484965
H	1.6882644	2.9756277	-1.0659406
H	2.7671604	5.1072493	-0.5108396
H	3.1528585	1.2473485	2.5737994
H	4.2246575	3.4069797	3.1625599
H	8.3102227	-0.8662695	2.9799678
H	8.4945997	-2.2085014	1.8067050
H	9.7412175	-0.9274774	1.9066771
H	5.5034134	-6.5179512	-2.4319529
H	6.6486846	-5.8842884	-1.2076418
H	6.2829184	-7.6356483	-1.2715366
H	4.5556084	6.4774338	-0.0477652
H	3.0533930	6.9833841	0.7886357
H	-1.8515187	6.2430999	2.1833091
H	-4.1652353	7.5745996	0.7150907
H	-3.3946629	8.2293155	2.1603518
H	-4.8623098	5.6171609	2.1893201
H	-3.6187774	4.5659189	2.8948130
H	-3.9158331	6.1729983	3.5894967
H	-1.1931895	8.3700555	0.9388079
H	-1.9560790	7.6881252	-0.5079474
H	-2.4433032	9.2886289	0.0827065
H	-6.0747739	-2.0042227	-2.5030518
H	-8.5520756	-0.7679523	-1.2315669
H	-8.5793128	-1.8220954	-2.6455142
H	-7.2154649	0.8460885	-2.6800086
H	-5.6103890	0.3705717	-3.2690225
H	-7.0667210	-0.2973171	-4.0348763
H	-7.5586227	-3.6877791	-1.2903945
H	-7.5047760	-2.6247946	0.1263743
H	-9.0668635	-3.1281145	-0.5477643
H	-2.8607251	-7.3856754	0.1251078
H	-4.0611537	-6.4486441	-0.8199850
H	-3.5475600	-8.0701915	-1.3791348
H	4.6489965	7.4770059	1.4338484

H2P (clockwise)

Energy = -2543.156282974 au

C	1.3916703	0.1873655	0.1974696
C	2.8690935	0.2179540	0.3825542
C	0.6305322	1.3681750	0.3231254
C	0.7533367	-1.0379557	-0.0971145
C	-0.6447500	-1.0791595	-0.2737272
C	-0.7701408	1.3262620	0.1498479
C	-1.4072246	0.1032326	-0.1465257
C	1.5631549	-2.2822627	-0.2247181
C	-1.3235413	-2.3674778	-0.5896856
C	1.3067014	2.6564832	0.6415664
C	-1.5771570	2.5716295	0.2766804
C	-2.8832309	0.0478673	-0.3370239
C	-1.3257532	3.6801913	-0.5357904
C	-2.6129283	2.6708083	1.2195017
C	-3.3602182	3.8320650	1.3508560
C	-2.0726227	4.8535372	-0.4258043
C	-3.0943560	4.9326183	0.5259152
C	-3.6778271	-0.7889244	0.4515343
C	-3.5166809	0.7924405	-1.3434952
C	-4.8805992	0.6783040	-1.5731846
C	-5.0501023	-0.9102193	0.2412300
C	-5.6586703	-0.1834286	-0.7884917
C	-1.2388738	-3.4652694	0.2813105
C	-2.0929242	-2.5110397	-1.7473531
C	-2.7723633	-3.6950475	-2.0340051
C	-1.9136772	-4.6486579	0.0179443
C	-2.6909298	-4.7685097	-1.1413237
C	2.3631789	-2.7315826	0.8292340
C	1.5744313	-3.0222459	-1.4176911
C	2.3701188	-4.1500703	-1.5593408
C	3.1639793	-3.8673754	0.7093759
C	3.1761562	-4.5765486	-0.4959301
C	3.4440025	0.6346131	1.5927019
C	3.7280387	-0.2179441	-0.6301773
C	5.1090528	-0.2682146	-0.4504683
C	4.8163761	0.5837101	1.7929101
C	5.6613334	0.1209099	0.7752689
C	2.3110363	3.1733010	-0.1925747
C	0.9597248	3.3916589	1.7779799
C	1.5834067	4.6008966	2.0868870
C	2.9359589	4.3785719	0.0921290
C	2.5755400	5.1006114	1.2371997
C	7.9144321	-0.5379505	0.1520968
C	7.7807572	-2.0563870	0.2445380
C	9.3047836	-0.0393163	0.5374896
C	9.4730200	1.4718024	0.3607850
C	4.7901981	-6.1296675	0.3311184
C	2.8986294	7.0333666	2.6019132
C	-3.6330348	7.1718889	-0.1050446
C	-7.8251789	-1.2328151	-0.4664408
C	-7.5440341	-2.6081137	-1.0677230
C	-9.2642300	-0.7722354	-0.6838029
C	-9.5775541	0.5643128	-0.0067005
C	-4.1519941	-6.1048590	-2.4758129
O	6.9983432	0.1001571	1.0756983
O	3.9407626	-5.6917162	-0.7301822
O	3.2466153	6.2801475	1.4395230
O	-3.8835151	6.0372104	0.7252393
O	-6.9921237	-0.2316027	-1.1013364
O	-3.3338312	-5.9686191	-1.3131635
H	-2.8326526	1.8209825	1.8585424
H	-4.1574514	3.9073660	2.0839466
H	-0.5259682	3.6321253	-1.2686869
H	-1.8474367	5.6901300	-1.0775177
H	-2.9257863	1.4604904	-1.9629794
H	-5.3653554	1.2439437	-2.3630846
H	-3.2131493	-1.3779108	1.2365313
H	-5.6227624	-1.5805886	0.8715829
H	-2.1788651	-1.6758238	-2.4357392
H	-3.3616647	-3.7634414	-2.9414070
H	-0.6394986	-3.3830771	1.1829719
H	-1.8550611	-5.4923284	0.6987571
H	0.9539917	-2.7001956	-2.2485693
H	2.3851396	-4.7141664	-2.4868516
H	2.3762417	-2.1752461	1.7615224
H	3.7729623	-4.1795746	1.5502255
H	3.3096830	-0.5472197	-1.5765623
H	5.7335222	-0.6247928	-1.2613767
H	2.8013840	0.9906326	2.3923885
H	5.2570979	0.8915543	2.7362351
H	0.1815661	3.0175205	2.4364552
H	1.2868745	5.1390271	2.9800965
H	2.6037635	2.6178346	-1.0783697
H	3.7088927	4.7779820	-0.5572725
H	7.6823565	-0.1925648	-0.8653053
H	9.4938269	-0.3238432	1.5803121
H	10.0360857	-0.5773013	-0.0789579
H	8.0586304	-2.3935819	1.2485367
H	6.7542187	-2.3760526	0.0425545
H	8.4426363	-2.5390556	-0.4826934
H	9.3179059	1.7631454	-0.6847062
H	8.7481952	2.0143927	0.9738743
H	10.4787590	1.7904402	0.6532587
H	5.5165822	-5.3520471	0.6012810
H	4.2050356	-6.4071562	1.2172028
H	5.3130324	-7.0057653	-0.0543149
H	1.8428581	7.3326154	2.5771535
H	3.0948176	6.4601742	3.5171154
H	3.5342862	7.9193004	2.5782919
H	-2.6121113	7.5486183	0.0385078
H	-3.7872440	6.9280119	-1.1640071
H	-4.3533719	7.9287212	0.2077152
H	-7.6111665	-1.2332455	0.6117266
H	-9.4419466	-0.7022677	-1.7644072
H	-9.9284117	-1.5570112	-0.3000864
H	-7.8042678	-2.6090361	-2.1312814
H	-6.4877004	-2.8747510	-0.9684220
H	-8.1426736	-3.3721650	-0.5600030
H	-9.4342189	0.4964098	1.0781120
H	-8.9202015	1.3516120	-0.3857779
H	-10.6146094	0.8628219	-0.1911019
H	-4.9588359	-5.3603628	-2.4796832
H	-3.5567581	-6.0037766	-3.3923592
H	-4.5754748	-7.1083798	-2.4203655

H2P (counterclockwise)

Energy = -2543.155640598 au

C	1.3871637	0.1704938	0.2433850
C	2.8588881	0.2017456	0.4705970
C	0.6300235	1.3564515	0.3490593
C	0.7507502	-1.0472907	-0.0809018
C	-0.6432420	-1.0790918	-0.2959365
C	-0.7643291	1.3249829	0.1321255
C	-1.4006085	0.1076822	-0.1907978
C	1.5529493	-2.2976478	-0.1929619
C	-1.3176762	-2.3629866	-0.6367361
C	1.3033602	2.6406798	0.6904899
C	-1.5654849	2.5760751	0.2428110
C	-2.8721217	0.0727303	-0.4186723
C	-1.5893889	3.3158971	1.4276910
C	-2.3173923	3.0525106	-0.8430879
C	-3.0561851	4.2228978	-0.7510626
C	-2.3338865	4.4902957	1.5432994
C	-3.0699830	4.9495927	0.4464899
C	-3.4039353	-0.3668439	-1.6337869
C	-3.7717076	0.4699500	0.5825066
C	-5.1433089	0.4171075	0.3812578
C	-4.7792285	-0.4159674	-1.8589293
C	-5.6606677	-0.0302050	-0.8421448
C	-0.9508000	-3.0945415	-1.7775940
C	-2.3458883	-2.8709894	0.1614068
C	-2.9975051	-4.0635108	-0.1540185
C	-1.5927725	-4.2776451	-2.1131770
C	-2.6230271	-4.7697960	-1.3015205
C	2.6105882	-2.3962822	-1.1006737
C	1.2804030	-3.4096946	0.6196412
C	2.0408233	-4.5670609	0.5372108
C	3.3810878	-3.5545576	-1.2051655
C	3.0988926	-4.6459614	-0.3774882
C	3.6985128	1.0055105	-0.3157929
C	3.4517110	-0.5781066	1.4670886
C	4.8291968	-0.5705828	1.6837532
C	5.0722712	1.0176377	-0.1227414
C	5.6516770	0.2254798	0.8778910
C	2.0240834	2.7845211	1.8868977
C	1.2337863	3.7423308	-0.1659113
C	1.8572858	4.9515501	0.1436583
C	2.6427015	3.9813323	2.2171155
C	2.5637529	5.0742403	1.3443326
C	7.6934916	-0.4619264	2.0037523
C	7.5940349	0.2719407	3.3382207
C	9.1328991	-0.6286632	1.5225970
C	9.2440923	-1.4489477	0.2350332
C	4.8866919	-5.9276659	-1.3063469
C	3.1422822	7.3436427	0.8778623
C	-3.8620625	6.8490455	1.6576852
C	-7.6457698	-0.4710802	-2.1741417
C	-7.6366952	0.6883898	-3.1664861
C	-9.0552887	-0.9296351	-1.8078556
C	-9.0681054	-2.1546848	-0.8901796
C	-4.2613540	-6.4611104	-0.9048121
O	7.0169253	0.2936063	0.9692947
O	3.7980012	-5.8266328	-0.3875546
O	3.2067953	6.2159093	1.7516858
O	-3.8294949	6.0924130	0.4469192
O	-7.0274835	-0.0641460	-0.9288434
O	-3.2026120	-5.9439267	-1.7117983
H	-2.3207890	2.4921955	-1.7731008
H	-3.6332096	4.5910801	-1.5937932
H	-1.0108798	2.9733912	2.2804061
H	-2.3278189	5.0333616	2.4815896
H	-3.3861867	0.8236520	1.5340445
H	-5.8364635	0.7172639	1.1611758
H	-2.7308612	-0.6835371	-2.4249946
H	-5.1434909	-0.7576671	-2.8207936
H	-2.6533864	-2.3215126	1.0459953
H	-3.7900313	-4.4233181	0.4923144
H	-0.1493743	-2.7254183	-2.4103765
H	-1.3110301	-4.8380539	-2.9993151
H	0.4587016	-3.3615912	1.3277914
H	1.8315737	-5.4232333	1.1711521
H	2.8464879	-1.5483829	-1.7365966
H	4.1926471	-3.5901238	-1.9231069
H	2.8260750	-1.2118169	2.0886094
H	5.2414131	-1.1876620	2.4736411
H	3.2641440	1.6283387	-1.0920275
H	5.7196490	1.6343188	-0.7387263
H	0.6766992	3.6599657	-1.0943308
H	1.7814907	5.7815386	-0.5496952
H	2.0989050	1.9409976	2.5664381
H	3.1956247	4.0909563	3.1449979
H	7.2241862	-1.4533780	2.0726488
H	9.5635544	0.3698485	1.3759433
H	9.7027617	-1.1080789	2.3285794
H	8.0988753	1.2408773	3.2697851
H	6.5507501	0.4456144	3.6163105
H	8.0703139	-0.3159348	4.1304540
H	8.8452872	-2.4600162	0.3800441
H	8.6791974	-0.9751163	-0.5726323
H	10.2877818	-1.5409137	-0.0825283
H	4.5399944	-5.8244896	-2.3425851
H	5.6502300	-5.1668010	-1.0988172
H	5.3062470	-6.9230092	-1.1554791
H	3.6012139	7.1175048	-0.0931663
H	2.1042544	7.6662500	0.7254256
H	3.7050708	8.1335792	1.3766355
H	-4.2791261	6.2567552	2.4822568
H	-2.8587419	7.2004764	1.9309086
H	-4.5092541	7.7026453	1.4526922
H	-7.0862221	-1.3274293	-2.5760797
H	-9.5757814	-0.0904300	-1.3294909
H	-9.5901098	-1.1484286	-2.7407455
H	-8.2294123	1.5206117	-2.7734187
H	-6.6188194	1.0450805	-3.3471779
H	-8.0677625	0.3723544	-4.1227073
H	-8.5780948	-3.0091061	-1.3720442
H	-8.5375337	-1.9421109	0.0421594
H	-10.0932494	-2.4494260	-0.6436146
H	-3.9100251	-6.6878718	0.1099788
H	-5.0991535	-5.7537909	-0.8521590
H	-4.5834391	-7.3794709	-1.3971140

H4 (clockwise)

Energy = -2779.196238337 au

C	2.2119104	0.5420624	0.4115647
C	3.6852437	0.5727730	0.6317360
C	1.4549246	1.7280975	0.5053285
C	1.5727349	-0.6816033	0.1119895
C	0.1789761	-0.7163297	-0.0995771
C	0.0584117	1.6926719	0.2953466
C	-0.5794474	0.4709088	-0.0030031
C	2.3792793	-1.9297359	0.0157033
C	-0.4949438	-2.0031431	-0.4278047
C	2.1234897	3.0215675	0.8217433
C	-0.7342717	2.9491830	0.3975804
C	-2.0530598	0.4295749	-0.2138723
C	-0.4414267	4.0512128	-0.4105304
C	-1.7698540	3.0829902	1.3348777
C	-2.4607721	4.2778739	1.4789899
C	-1.1301110	5.2565454	-0.2861622
C	-2.1404816	5.3796628	0.6744988
H	-2.0273924	2.2387328	1.9673618
H	-3.2518116	4.3827350	2.2153018
H	0.3567961	3.9759995	-1.1428541
H	-0.8602393	6.0864743	-0.9288882
C	-2.8698411	-0.3822411	0.5779565
C	-2.6667124	1.1866621	-1.2235096
C	-4.0351630	1.1201038	-1.4430578
C	-4.2479680	-0.4543742	0.3791578
C	-4.8394431	0.2969312	-0.6431414
H	-2.0578175	1.8336715	-1.8477937
H	-4.5055359	1.7014911	-2.2301984
H	-2.4205031	-0.9836633	1.3625111
H	-4.8391038	-1.1013900	1.0168219
C	-0.4335691	-3.1015435	0.4433450
C	-1.2273447	-2.1498612	-1.6090127
C	-1.8862993	-3.3380176	-1.9221428
C	-1.0912974	-4.2884852	0.1537313
C	-1.8254355	-4.4175653	-1.0331770
H	-1.2970237	-1.3136416	-2.2982480
H	-2.4448858	-3.4022719	-2.8487007
H	0.1363379	-3.0191702	1.3639525
H	-1.0478592	-5.1337617	0.8337905
C	3.1535606	-2.3690036	1.0931186
C	2.4228459	-2.6800988	-1.1691499
C	3.2309624	-3.8027398	-1.2811964
C	3.9646506	-3.4987769	1.0021219
C	4.0170755	-4.2173943	-0.1977480
H	1.8213902	-2.3693930	-2.0181672
H	3.2735390	-4.3729371	-2.2042043
H	3.1403303	-1.8058590	2.0214276
H	4.5549407	-3.7943705	1.8616909
C	4.2285482	1.0182044	1.8472307
C	4.5701178	0.1281543	-0.3541863
C	5.9493864	0.1085463	-0.1467648
C	5.5969360	0.9991954	2.0757558
C	6.4669469	0.5378304	1.0794737
H	4.1759726	-0.2260515	-1.3018516
H	6.6007512	-0.2474343	-0.9369377
H	3.5632451	1.3776165	2.6264618
H	6.0135091	1.3348179	3.0204950
O	7.8019254	0.5418288	1.3974821
C	3.1350374	3.5368633	-0.0042682
C	1.7418787	3.7765742	1.9339857
C	2.3283591	5.0096165	2.2194457
C	3.7251290	4.7648546	0.2582579
C	3.3204040	5.5124994	1.3716224
H	0.9584676	3.4034026	2.5865808
H	2.0007186	5.5650066	3.0909838
H	3.4564414	2.9655540	-0.8698982
H	4.5002634	5.1653592	-0.3878803
C	8.7054692	0.0506819	0.4065956
H	8.4867774	-0.9960000	0.1576555
H	8.6620640	0.6600760	-0.5051968
H	9.6981037	0.1248526	0.8523091
O	4.7838107	-5.3329989	-0.4123467
C	5.7489613	-5.7249950	0.5944310
C	6.9581916	-4.7932594	0.5538093
H	5.2632240	-5.6822406	1.5795798
C	6.1061528	-7.1760938	0.2826925
C	4.9155426	-8.1297401	0.4095216
H	6.5194256	-7.2165600	-0.7330560
H	6.9088587	-7.4778668	0.9674066
H	7.4607270	-4.8783532	-0.4152761
H	6.6593837	-3.7510441	0.6995108
H	7.6696498	-5.0624822	1.3420329
H	4.5143997	-8.1212607	1.4298232
H	4.1123825	-7.8357503	-0.2717800
H	5.2099615	-9.1571611	0.1721728
O	3.9489710	6.7198606	1.5462973
C	3.5343132	7.5109523	2.6606073
H	2.4688827	7.7659237	2.5885189
H	3.7220393	6.9892548	3.6078084
O	-2.8769614	6.5135975	0.8989723
C	-2.4928220	7.7423378	0.2345078
C	-1.2451244	8.3274649	0.8924209
H	-2.3013993	7.5215715	-0.8251638
C	-3.7055550	8.6640296	0.3355642
C	-4.9349121	8.1243371	-0.3995897
H	-3.9335797	8.8147247	1.3983318
H	-3.4181989	9.6414835	-0.0721634
H	-1.4607698	8.5862042	1.9342625
H	-0.4174154	7.6123865	0.8765096
H	-0.9292237	9.2339056	0.3646690
H	-4.7281998	8.0006150	-1.4691514
H	-5.2276087	7.1506724	0.0028635
H	-5.7835237	8.8085255	-0.2977662
O	-6.1778441	0.3116329	-0.9362629
C	-7.0689617	-0.5678252	-0.2074939
C	-6.9485501	-1.9945720	-0.7366958
H	-6.8011658	-0.5285953	0.8579492
C	-8.4676884	0.0168105	-0.3885531
C	-8.6207388	1.4116523	0.2229742
H	-8.6903063	0.0457823	-1.4627118
H	-9.1832511	-0.6786865	0.0680833
H	-7.2496410	-2.0292434	-1.7887426
H	-5.9209023	-2.3592709	-0.6589062
H	-7.5972665	-2.6669389	-0.1647826
H	-8.4330598	1.3881443	1.3028872
H	-7.9105142	2.1100218	-0.2282299
H	-9.6324121	1.7993576	0.0655095
O	-2.4272287	-5.6330414	-1.2279672
C	-3.2652451	-5.8262263	-2.3937428
C	-4.6253688	-5.1674555	-2.1786845
H	-2.7573500	-5.3857223	-3.2634570
C	-3.3615046	-7.3373820	-2.5892252
C	-2.0124411	-7.9915973	-2.8974012
H	-3.7970544	-7.7730964	-1.6811268
H	-4.0700039	-7.5250851	-3.4059718
H	-1.5833077	-7.5868710	-3.8215445
H	-1.3017185	-7.8090339	-2.0866827
H	-2.1215885	-9.0737265	-3.0226691
H	-5.2484764	-5.2841234	-3.0720515
H	-5.1373172	-5.6356946	-1.3317374
H	-4.5185991	-4.0995288	-1.9707177
H	4.1356845	8.4196707	2.6150748

H4P (counterclockwise)

Energy = -2779.195076170 au

C	2.2716036	0.5721572	0.4154096
C	3.7471577	0.6065316	0.6172527
C	1.5134280	1.7567315	0.5316733
C	1.6322781	-0.6484314	0.1058308
C	0.2362289	-0.6821396	-0.0864935
C	0.1158357	1.7235402	0.3317160
C	-0.5207486	0.5060414	0.0161792
C	2.4303244	-1.8991348	-0.0217730
C	-0.4560418	-1.9626052	-0.4034389
C	2.1847815	3.0436498	0.8666050
C	-0.6876989	2.9709385	0.4570521
C	-1.9926195	0.4548772	-0.2080814
C	-0.6961391	3.7071759	1.6447971
C	-1.4568836	3.4507373	-0.6142263
C	-2.1898826	4.6238156	-0.5067286
C	-1.4360185	4.8819433	1.7757725
C	-2.1831929	5.3534145	0.6899192
H	-1.4759551	2.8942109	-1.5464058
H	-2.7764599	4.9968732	-1.3407628
H	-0.1080324	3.3603295	2.4892465
H	-1.4164519	5.4140503	2.7197695
C	-2.5135026	-0.0082143	-1.4193590
C	-2.9013049	0.8170304	0.7975484
C	-4.2702962	0.6819688	0.6129720
C	-3.8852853	-0.1393315	-1.6279874
C	-4.7744821	0.1853386	-0.5969305
H	-2.5254720	1.1950052	1.7437198
H	-4.9704450	0.9433806	1.4006453
H	-1.8325219	-0.2911999	-2.2164031
H	-4.2396019	-0.5035764	-2.5851910
C	-0.1501879	-2.6957572	-1.5597925
C	-1.4745932	-2.4456994	0.4225374
C	-2.1917567	-3.5987440	0.1084316
C	-0.8611651	-3.8395332	-1.8956353
C	-1.9014924	-4.2919995	-1.0723762
H	-1.7288331	-1.8999979	1.3262214
H	-2.9731743	-3.9321672	0.7812359
H	0.6470465	-2.3525309	-2.2124702
H	-0.6360594	-4.3932938	-2.8020817
C	3.4674662	-2.0006720	-0.9528441
C	2.1723426	-3.0126001	0.7925241
C	2.9294343	-4.1708330	0.6906967
C	4.2314666	-3.1605048	-1.0781097
C	3.9703627	-4.2541065	-0.2441403
H	1.3665827	-2.9649928	1.5188577
H	2.7330721	-5.0269252	1.3289951
H	3.6903536	-1.1534257	-1.5945447
H	5.0207680	-3.1934622	-1.8201243
C	4.5692919	1.4199825	-0.1788757
C	4.3596687	-0.1814344	1.5951784
C	5.7418454	-0.1721573	1.7842063
C	5.9464278	1.4364420	-0.0124049
C	6.5421865	0.6377955	0.9722724
H	3.7475177	-0.8245971	2.2201623
H	6.1772011	-0.7983021	2.5547428
H	4.1174149	2.0473756	-0.9411835
H	6.5800818	2.0620240	-0.6335560
O	7.9091760	0.7156733	1.0635186
C	2.9221661	3.1897029	2.0525066
C	2.0886759	4.1493798	0.0177605
C	2.6984699	5.3655637	0.3264706
C	3.5281969	4.3933727	2.3816524
C	3.4190047	5.4912478	1.5184622
H	1.5187636	4.0652460	-0.9026197
H	2.6000719	6.1989229	-0.3599485
H	3.0183138	2.3433219	2.7258121
H	4.0927127	4.5050563	3.3022702
C	8.5400040	-0.0956521	2.0551487
H	8.1984852	0.1746829	3.0625972
H	8.3444850	-1.1609400	1.8764787
H	9.6080374	0.1047078	1.9619556
O	4.6702136	-5.4321097	-0.2465689
C	5.7372890	-5.6165978	-1.2087136
C	5.1565249	-5.9926276	-2.5690995
H	6.3076671	-4.6796870	-1.2784369
C	6.6393770	-6.7021709	-0.6263986
C	7.3015797	-6.2893679	0.6904855
H	6.0370258	-7.6078836	-0.4819052
H	7.4034110	-6.9418484	-1.3767326
H	4.6246693	-6.9467421	-2.4969057
H	4.4542438	-5.2322699	-2.9221081
H	5.9582343	-6.0936707	-3.3087923
H	7.9318982	-5.4032017	0.5499774
H	6.5448443	-6.0503505	1.4429371
H	7.9334761	-7.0936640	1.0808860
O	4.0476678	6.6409462	1.9258532
C	3.9432646	7.7765080	1.0661547
H	4.3909172	7.5718761	0.0851401
H	2.8956951	8.0769059	0.9344709
O	-2.9215503	6.5076244	0.6827699
C	-3.0018315	7.3013071	1.8919025
C	-4.0185950	6.6908057	2.8525474
H	-2.0049684	7.3322042	2.3537281
C	-3.3813336	8.7096406	1.4404181
C	-2.3171192	9.3631640	0.5553200
H	-4.3380053	8.6525682	0.9060588
H	-3.5520601	9.3157049	2.3391640
H	-5.0144436	6.7014164	2.3980259
H	-3.7610036	5.6558667	3.0944070
H	-4.0527304	7.2660258	3.7842360
H	-1.3650524	9.4544156	1.0915809
H	-2.1433442	8.7640304	-0.3428875
H	-2.6266672	10.3665550	0.2455092
O	-6.1359752	0.0425951	-0.6585025
C	-6.7306641	-0.5157655	-1.8560216
C	-6.9103820	0.5763493	-2.9064177
H	-6.0695434	-1.3081328	-2.2334489
C	-8.0497589	-1.1450451	-1.4139142
C	-7.8566467	-2.3171533	-0.4483004
H	-8.6646857	-0.3648427	-0.9480182
H	-8.5821786	-1.4784432	-2.3137002
H	-7.5977100	1.3431093	-2.5348020
H	-5.9559419	1.0549592	-3.1433542
H	-7.3237990	0.1525881	-3.8282027
H	-7.2726856	-3.1175228	-0.9184513
H	-7.3229110	-1.9918191	0.4491469
H	-8.8199779	-2.7381071	-0.1428267
O	-2.5736274	-5.3992255	-1.5197569
C	-3.6951550	-5.8990434	-0.7504762
C	-3.1945416	-6.7927277	0.3805167
H	-4.2479617	-5.0396429	-0.3464180
C	-4.5895135	-6.6357215	-1.7449096
C	-5.1827662	-5.7115023	-2.8114164
H	-3.9985694	-7.4311787	-2.2160235
H	-5.3917185	-7.1249672	-1.1780478
H	-5.8045658	-4.9340235	-2.3515051
H	-4.3878250	-5.2176855	-3.3774012
H	-5.8087112	-6.2717873	-3.5134164
H	-4.0356585	-7.1421134	0.9893043
H	-2.6761218	-7.6638089	-0.0328589
H	-2.4985032	-6.2534506	1.0292662
H	4.4963713	8.5734577	1.5646168

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