Supporting Information

A Novel Symmetrically Multifunctionalized Dodecamethoxy-

Cycloparaphenylene: Synthesis, Photophysical, and Supramolecular

Properties

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General. All glassware was oven-dried. Air-sensitive reactions were carried out using the standard Schlenk technique under nitrogen. Work-up and purification procedures were carried out with reagent-grade solvents under air. Mass spectrometry (MS) analyses were carried out using APCI-LTQ Orbitrap MS and MALDI-TOF-MS techniques. NMR spectra were recorded on a Bruker BioSpin (¹H 400 MHz, ¹³C 100 MHz) spectrometer. Chemical shifts for ¹H NMR are expressed in parts per million (ppm) relative to residual peak of CHCl₃ (δ 7.26 ppm). Chemical shifts for ¹³C NMR are expressed in ppm relative to CDCl₃ (δ 77.0 ppm). Coupling constants (*J*) are given in Hz. The apparent resonance multiplicity is described as s (singlet), br s (broad singlet), d (doublet), t (triplet), q (quartet), and m (multiplet). Flash chromatography was performed on silica gel (300~400 mesh). Preparative thin-layer chromatography (PTLC) were performed using silica gel GF 254 precoated plates. UV-vis absorption measurements were carried out on a UNIC-3802 spectrophotometer.

Materials. Tetrahydrofuran (THF) were distilled after reflux with sodium under nitrogen prior to use. Other chemicals including the solvents were obtained from commercial suppliers and used without further purification unless otherwise stated. Sodium naphthalenide (1.0 M in THF) was prepared according to the literature reports.^{S1}

Synthesis of 1,4-dibromo-2,5-dimethoxybenzene 1. The starting material 1,4-dibromo-2,5-dimethoxybenzene **1** was synthesized according to the literature reports.^{S2}

$$MeO \xrightarrow{OMe} \frac{Br_2}{AcOH, rt, 5 h} \xrightarrow{Br}_{MeO} \frac{OMe}{1}$$

Synthesis of 1,4-bis(2',5'-dimethoxy-4'-bromophenyl)-1,4-dimethoxycyclohexa-2,5-dienes (*cis*-isomer) 3.



1,4-dibromo-2,5-dimethoxybenzene (2.96 g, 10.0 mmol, 2.35 equiv.) was dissolved in 50 mL of anhydrous THF in a dry 100mL round bottom flask and cooled to -78 °C. To this solution was added *n*-butyllithium in hexane (4.2 mL, 2.5 M, 10.5 mmol) dropwise over 10 min. The reaction mixture was allowed to stir at -78 °C for 2 h, then benzoquinone (460 mg, 4.26 mmol, 1 equiv.) dissolved in 12 mL of anhydrous THF was added dropwise over 15 min. The color of the solution changed from pale yellow to green, then blue, and finally dark purple while benzoquinone was added. The reaction mixture was allowed to stir at -78 °C for another 2 h before it was moved to

room temperature. Water (20 mL) was added with stirring to quenching the reaction, which was further diluted by the addition of diethyl ether (30 mL). After stirring for an additional 20 min, the biphasic mixture was separated. The aqueous layer was extracted by diethyl ether (3 x 20 mL) and the organic phase combined was dried over anhydrous Na₂SO₄. Concentrated in *vacuo* delivered the diol **2**, which was carried forward without further purification.

To a dry 50mL round bottom flask was added 511 mg of sodium hydride (60% in mineral, 12.8 mmol) and 12 mL of anhydrous THF. The suspension was cooled to 0 °C and the crude diol 2 dissolved in 8 mL of anhydrous THF was added by syringe dropwise. The mixture was allowed to stir at 0 °C for 30 min before iodomethane (1.50 mL, 24 mmol) was added. Then, the mixture was warmed to room temperature and stirred for an additional 16 h. The excess sodium hydride was guenched by the addition of water (15 mL) slowly! The reaction mixture was further diluted with 20 mL of diethyl ether. The aqueous layer was extracted by diethyl ether (3 x 15 mL) and the organic phase combined was dried and concentrated in vacuo. The crude product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (v/v, 5:1) as the eluent to delivere a yellow solid, that was recrystallized from methol to afford the white dibromide 3 (510 mg, 21% over two steps). ¹H NMR (400 MHz, CDCl₃) § 7.04 (s, 2H), 7.02 (s, 2H), 6.28 (s, 4H), 3.71 (s, 6H), 3.50 (s, 6H), 3.35 (s, 6H). ¹³C NMR (101 MHz, CDCl₃) δ 152.39, 149.79, 131.59, 130.65, 117.89, 113.16, 110.97, 73.68, 56.92, 56.55, 51.41. FT-IR: 3120.08, 3039.59, 3022.68, 3003.69, 2962.18, 2928.33, 2848.81, 2841.83, 2830.59, 1652.84, 1638.53, 1566.01, 1487.97, 1464.40, 1442.11, 1395.11, 1374.61, 1290.08, 1261.01, 1212.34, 1182.50, 1147.41, 1079.91, 1055.19, 1021.65, 956.43, 875.01, 865.71, 803.71, 775.26, 763.58, 663.76. Melting point: 144-146 °C. HR-MS (APCI-LTQ Orbitrap MS) m/z calcd. for C₂₄H₂₆Br₂O₆ [M]⁺: 570.0076, Found 570.0075.

Synthesis of dodecamethoxy-[9]CPP 5b.



An oven dried 100-mL Schlenk flask containing Ni(cod)₂ (363 mg, 1.3 mmol), 2,2'-bipyridyl (bpy) (206 mg, 1.3 mmol), and a magnetic stirring bar (oven dried) was evacuated and backfilled with nitrogen for 3 cycles. Then, freshly-distilled THF (degassed) (20 mL) and cod (160 μ L, 1.3 mmol) was added sequentially by syringe under nitrogen. The suspension was allowed to stir at 65 °C for 1 h in the absence of light for activation. Then, **3** (262 mg, 0.46 mmol) dissolved in anhydrous THF (degassed) (40 ml) was added by syringe, and the reaction mixture was stirred at reflux for 48 h. After cooling to room temperature, the reaction mixture was passed through a short pad of silica with DCM as the eluent. The filtrate was concentrated, then wash by methanol to afford the crude product containing cyclic precursors **4** as white powder, which was used for next step without further purification.

The above crude product containing cyclic precursors 4 was dissolved in anhydrous THF (15 mL) in a 50-mL oven dried flask with a magnetic stirring bar and cooled to -78 °C. Then, sodium naphthalenide (1.7 mL, 1.7 mmol, 1.0 M in THF) was added into the reaction mixture dropwise. It was stirred at -78 °C for 2 h before quenching the reaction by the addition of I_2 (1.3 mL, 1.3 mmol, 1.0 M in THF). The resulting mixture was warmed up to room temperature and sodium thiosulfate (aqueous saturated solution) was carefully added to remove excess I₂. Then, water (10 mL) was added and the mixture was extracted with DCM (3×15 mL). The organic phase was combined and dried over anhydrous Na₂SO₄. After removing the solvent under reduced pressure, the crude solid was purified initially by silica gel column chromatography with petroleum ether/DCM (ν/ν , 1:1~1:5) as the eluent, then by preparative thin-layer chromatography with petroleum ether/diethyl ether (v/v, 1:2) as the eluent to afford **5b** as a yellow solid (8.0 mg, 5 % over two steps). ¹H NMR (400 MHz, CDCl₃) δ 7.59 (s, 12H), 7.02 (s, 6H), 6.85 (s, 6H), 3.68 (s, 36H), 3.67 (s, 36H). ¹³C NMR (101 MHz, CDCl₃) & 152.44, 151.38, 136.89, 129.75, 128.58, 126.69, 116.94, 115.38, 57.10, 56.83. FT-IR: 2918.52, 2849.91, 1653.76, 1637.91, 1459.79, 1438.07, 1384.02, 1209.14, 1161.11, 1113.26, 1043.65, 844.34, 699.94. Melting point: 137-139 °C. MALDI-TOF-MS m/z calcd. for C₆₆H₆₀O₁₂ [M]⁺: 1044.41, Found 1044.39. HR-MS (APCI-LTQ Orbitrap MS) m/z calcd. for C₆₆H₆₁O₁₂ [M+H]⁺: 1045.4163, Found 1045.4209.



Figure S1. HR-MS (APCI-LTQ Orbitrap MS) for compound 3.



Figure S2. (a) The observed peaks by MALDI-TOF-MS from the crude product. The measured and simulated data for (b) the partially aromatized product **5a** (c) hexadecamethoxy-[12]CPP **5c** (d) icosamethoxy-[15]CPP **5d**.



Figure S3. HR-MS (APCI-LTQ Orbitrap MS) for compound 5b.

Computational details.

To identify the potential-minimal structure, the initial configurations were relaxed using molecular dynamic program GULP. ^{S3} In flexible simulations, UFF^{S4} force filed was used for bond stretching, angle bending, and dihedral torsions.

Base on the previous relaxed structure, density functional theory (DFT) calculations were carried out using quantum chemical program of ORCA 4.0.1. ^{S5} The basic sets, consisting of C, O for def2-TZVP and H for def2/SVP, were used to describe wave function. Hybrid functional B3LYP, together with CAM corrections, was used in geometrical optimizations and frequency validation of ground state. For the calculation of absorption spectra, time-dependent DFT (TD-DFT) calculation, including 54 excited states, were performed. Specifically, solvent effect with CPCM model was corrected in SCF calculation. Furthermore, geometrical configuration of the 1st existed state was identified by TD optimization. Hybrid functional B3LYP was used in all the TD-DFT calculations.



Figure S4. The computational method for strain energy of 5b.

5b Bimethoxyl-triphenyl	-3453.08447	
Bimethoxyl-triphenyl	000 0000	
· · ·	-923.22009	
Triphenyl	-694.18619	
Biphenyl	-463.18683	

 Table S1. The strain energy calculation of 5b

λ(nm)	fosc	Main electronic transfers
291.7	0.1509	HOMO-7→ LUMO
294	0.114	HOMO-7→ LUMO
296.4	0.034	HOMO→ LUMO+5
300.7	0.0282	HOMO→ LUMO+4
304.6	0.0124	HOMO-5→ LUMO+1
312.9	0.0946	HOMO-6→ LUMO
320	0.0365	HOMO-3→ LUMO+2
349	0.0953	HOMO-4→ LUMO
349.4	0.0187	HOMO-1→ LUMO+2
353.7	0.0332	HOMO-1→ LUMO+1
359.5	0.7417	HOMO→ LUMO+1
360.9	0.4383	HOMO→ LUMO+2
364.3	0.0514	HOMO-5→ LUMO
380.7	0.2262	HOMO-2→ LUMO
426.4	0.1448	HOMO → LUMO
427.9	0.2822	HOMO-1→ LUMO

 Table S2. Theoretical data for the main electronic transfers of 5b in absorption spectra.



Figure S5. The optimized structures of ground state and 1st excited state of **5b**: (a) ground state of **5b**, (b) 1st excited state of **5b**

	Ground state	1 st excited state
	39.07	22.40
A-A ^a	26.13	25.96
	39.59	18.78
	52.80	29.79
	49.06	29.63
A-B ^a	43.31	29.04
	49.64	22.43
	49.96	30.61
	16.95	6.15

Table S3. The torsion angles (unit: deg.) between adjacent phenyl rings of $\mathbf{5b}$ in

ground and 1st excited state.

^a: **A-A**: torsion angle between two adjacent methoxyl-substituted phenyl rings; **A-B**: torsion angle between two adjacent methoxyl-substituted and unsubstituted phenyl rings. (**A**: methoxyl-substituted phenyl ring; **B**: unsubstituted phenyl rings)

Ground	state						
С	5.0613	-0.5822	-3.6302	С	1.5126	-4.1075	-2.958
С	6.2932	0.3733	0.6097	0	-3.0543	-1.6499	7.281
С	5.2864	1.5514	4.4265	С	-2.0493	-2.3567	7.9739
С	1.2003	0.5921	5.5129	0	-5.3446	-3.9703	3.7226
С	-2.7207	-0.4947	6.637	С	-5.1849	-4.8215	4.8345
С	-5.4342	-2.6254	3.9301	0	5.6213	-1.3357	-0.94
С	-5.1067	-3.2553	-0.3208	С	5.4085	-2.2145	0.1361
С	-3.303	-3.048	-4.0296	0	7.2423	0.5144	3.4765
С	0.9841	-2.0959	-4.1314	С	7.5073	-0.0965	4.7219
С	3.9294	-1.0101	-4.3033	Н	5.9435	-1.2064	-3.6358
С	6.0163	-0.0624	-0.6738	Н	6.1647	-0.3025	1.4384
С	6.2309	1.4268	3.4207	Н	5.3217	0.8905	5.2789
С	2.4833	0.8813	5.1009	Н	0.8302	-0.4186	5.4063
С	-1.4571	0.0666	6.7418	Н	-4.3255	-3.9199	-0.6639
С	-4.7611	-2.006	4.9679	Н	3.9552	-1.9587	-4.8191
С	-5.39	-3.2183	1.0263	Н	3.0877	0.0948	4.6694
С	-4.3705	-3.2122	-3.1605	Н	-0.6939	-0.4415	7.3099
С	-0.356	-2.4276	-4.1554	Н	-4.0712	-2.5887	5.5548
С	5.9582	0.8626	-1.7213	Н	-4.8389	-3.8656	1.6848
С	6.0995	2.1783	2.2419	Н	-4.7311	-4.204	-2.932
С	2.9669	2.1871	5.1035	Н	-0.6829	-3.3456	-3.6994
С	-1.0962	1.2391	6.0886	Н	3.8453	2.2719	-2.3324
С	-4.834	-0.629	5.193	Н	0.2145	3.689	6.3843
С	-6.2576	-2.2593	1.5549	Н	-4.0727	1.8121	4.6147
С	-4.9552	-2.14	-2.4888	Н	-7.2173	-0.8687	-1.3857
С	-1.3365	-1.5632	-4.6442	Н	-3.0115	0.2868	-3.8032
С	2.7355	-0.295	-4.2369	Н	0.7307	0.8995	-5.6504
С	5.0384	0.5733	-2.8546	Н	1.8608	1.5266	-3.524
С	6.5433	1.708	0.9009	Н	6.4654	2.8508	-2.2816
С	4.2069	2.432	4.3273	Н	5.0413	3.8214	1.3823
С	0.3345	1.5973	5.9347	Н	2.4977	4.1967	5.6826
С	-3.6781	0.0931	5.7986	Н	-7.7266	-0.7922	0.9794
С	-5.6768	-2.3499	-1.2118	Н	-7.0282	0.0832	2.7574
С	-2.7373	-1.7796	-4.1944	Н	6.5895	4.9734	-1.5232
С	1.4066	-0.8442	-4.6098	Н	7.9132	5.5858	-0.505
С	3.8953	1.3672	-2.9238	Н	8.2092	4.2483	-1.6408
С	6.7641	2.5643	-0.1816	Н	1.541	4.738	2.0914
С	4.2158	3.3273	3.2634	Н	1.5151	3.1287	2.8439
С	0.85	2.8875	6.037	Н	2.4842	3.406	1.3767
С	-3.3474	1.3366	5.2521	Н	-3.5781	4.0746	4.6201
С	-6.6998	-1.5407	-0.7185	Н	-2.222	4.6397	3.6116

Table S4. Relaxed configuration of ground and 1st excited state of **5b**.

С	-3.4268	-0.6969	-3.6566	Н	-3.0853	3.1481	3.1849
С	0.4471	-0.0556	-5.2287	Н	-5.8905	1.431	6.82
С	2.7674	0.941	-3.5965	Н	-7.0943	2.5454	6.1374
С	6.4434	2.1426	-1.466	Н	-7.4906	0.822	6.3309
С	5.1518	3.1926	2.2539	Н	-5.4834	2.1649	-2.077
С	2.1455	3.1761	5.6401	Н	-4.891	1.6917	-3.685
С	-2.1009	1.9183	5.3955	Н	-3.7781	1.7277	-2.2914
С	-5.8503	0.0343	4.4912	Н	-3.3706	-0.6752	-6.4433
С	-6.9862	-1.5013	0.6351	Н	-3.0926	0.8398	-7.325
С	-4.5424	-0.8529	-2.8527	Н	-2.0208	-0.5569	-7.598
С	-0.897	-0.4005	-5.2701	Н	-2.5317	-6.0309	-5.0909
С	-6.1252	-1.8583	2.9786	Н	-4.1898	-5.5318	-4.7013
С	-6.416	-0.5561	3.3774	Н	-2.9716	-5.6837	-3.4063
0	7.1831	3.8258	0.1075	Н	2.412	-4.5641	-2.551
C	7.4831	4.6953	-0.9566	Н	1.0561	-4.784	-3.6858
0	3.2297	4.2734	3.11	Н	0.8071	-3.9322	-2.1419
C	2.1343	3.8532	2.3108	Н	-2.5357	-3.2315	8.3975
0	-1 7619	3 0892	4 7919	Н	-1 6146	-1 765	8 7833
Č	-2.7242	3.7628	4.0133	Н	-1.2512	-2.6744	7.2976
0	-6 2297	1 328	4 7651	Н	-5 8229	-4 5041	5 6617
Č	-6 6969	1 5339	6 0923	Н	-5 4872	-5 811	4 4969
0	-5 1852	0 1969	-2 2744	Н	-4 1486	-4 864	5 1809
Č	-4 8006	1 5094	-2.6104	Н	6 3 3 6 3	-2.425	0.6759
Õ	-1 7612	0 5038	-5 8378	Н	4 6722	-1 8182	0.8405
Č	-2.6074	-0.0129	-6 8542	Н	5 0258	-3 134	-0.3
Õ	-2 7068	-4 0769	-4 696	Н	8 4263	-0.6628	4 5961
C	-3 1347	-5 3945	-4 4491	Н	6 709	-0 7799	5 0232
0	1 9226	-2 9018	-3 5616	Н	7 6458	0.6547	5 50292
	10220		0.0010		110.00		
1 st Excit	ed state						
С	4.9146	-0.9818	-3.5751	С	1.6147	-4.7542	-4.373
С	6.0009	0.257	0.5781	Ο	-3.1574	-1.6018	7.6439
С	4.9816	1.3629	4.5506	С	-2.2985	-2.2722	8.5468
С	1.2173	0.7032	6.5314	Ο	-4.885	-3.7454	3.7365
С	-2.757	-0.4058	7.1123	С	-4.2438	-4.562	4.6983
С	-5.0399	-2.4104	3.989	Ο	5.8391	-1.5345	-1.014
С	-4.8421	-3.1158	-0.3481	С	5.9415	-2.4841	0.0307
С	-3.1631	-3.1876	-4.1742	Ο	6.7564	0.2567	3.3522
С	1.0778	-2.5017	-5.0084	С	7.0387	-0.5395	4.4895
С	3.9365	-1.4357	-4.435	Н	5.7272	-1.6446	-3.3212
С	5.8511	-0.2061	-0.7175	Н	6.0511	-0.4544	1.3832
С	5.7725	1.2012	3.4307	Н	5.1038	0.6871	5.3834
С	2.4607	0.9307	5.9885	Н	0.9065	-0.3232	6.677
-							

С	-1.5249	0.1546	7.3757	Н	-4.2045	-3.9174	-0.699
С	-4.5213	-1.8252	5.1258	Н	4.0176	-2.4369	-4.8252
С	-5.0986	-3.052	1.0016	Н	3.0683	0.0723	5.7317
С	-4.1119	-3.21	-3.1726	Н	-0.8078	-0.4025	7.9601
С	-0.275	-2.7831	-4.9565	Н	-3.8926	-2.4108	5.7727
С	5.5584	0.7021	-1.7728	Н	-4.6745	-3.8089	1.6385
С	5.579	2.0211	2.2767	Н	-4.4644	-4.1605	-2.8023
С	2.8811	2.2247	5.6024	Н	-0.5922	-3.7476	-4.6019
С	-1.1258	1.4198	6.8793	Н	3.7694	2.1698	-3.1225
С	-4.6661	-0.4464	5.4204	Н	0.189	3.9069	6.8295
С	-5.7926	-1.9598	1.5807	Н	-4.0705	2.1525	5.3534
С	-4.6279	-2.0412	-2.5645	Н	-6.568	-0.3938	-1.3528
С	-1.2733	-1.8118	-5.1982	Н	-2.9172	0.1587	-4.5082
С	2.8031	-0.6508	-4.7568	Н	0.8295	0.6753	-6.1346
С	4.8486	0.2986	-2.9813	Н	2.0647	1.3805	-4.5983
С	5.9407	1.6215	0.9189	Н	5.6771	2.7786	-2.2777
С	3.9766	2.3557	4.647	Н	4.6209	3.8402	1.6701
С	0.2856	1.751	6.7312	Н	2.3731	4.3055	5.8775
С	-3.6712	0.2467	6.2279	Н	-7.0367	-0.2786	0.9896
С	-5.2505	-2.1056	-1.2497	Н	-6.7309	0.2829	2.8455
С	-2.5994	-1.9494	-4.6037	Н	5.2682	4.8509	-1.454
С	1.5332	-1.1707	-5.2494	Н	6.46	5.7439	-0.4748
С	3.8537	1.1602	-3.5028	Н	7.0148	4.5507	-1.6771
С	5.9762	2.5274	-0.1852	Н	1.4938	5.3503	2.981
С	3.9777	3.3195	3.6095	Н	1.4905	3.5865	2.7168
С	0.8014	3.059	6.5671	Н	2.5085	4.6462	1.7017
С	-3.3713	1.6013	5.9596	Н	-3.7704	4.3585	5.8793
С	-6.1229	-1.1324	-0.7047	Н	-2.4036	5.2449	5.1553
С	-3.2814	-0.7934	-4.1617	Н	-3.1	3.839	4.31
С	0.5456	-0.3022	-5.7674	Н	-6.1244	1.4393	7.0009
С	2.8728	0.7055	-4.3515	Н	-7.1232	2.6733	6.1915
С	5.7501	2.0686	-1.4674	Н	-7.6443	0.9678	6.1899
С	4.7458	3.1376	2.478	Н	-5.0744	2.3156	-2.7529
С	2.0487	3.2869	6.0244	Н	-4.6375	1.6395	-4.3433
С	-2.1684	2.1934	6.2968	Н	-3.407	1.7677	-3.0547
С	-5.6433	0.219	4.6244	Н	-3.1396	-0.8457	-7.1325
С	-6.3888	-1.0734	0.6446	Н	-3.004	0.8321	-7.7169
С	-4.2813	-0.8191	-3.2077	Н	-1.8075	-0.3863	-8.2308
С	-0.7961	-0.6036	-5.7847	Н	-2.7733	-6.3113	-5.0552
С	-5.7068	-1.6255	2.9956	Н	-4.3392	-5.5948	-4.5966
С	-6.1011	-0.3468	3.4579	Н	-3.0613	-5.8159	-3.3687
0	6.2102	3.8383	0.107	Н	2.5344	-5.3166	-4.2195
С	6.2363	4.7873	-0.9444	Н	1.0357	-5.2182	-5.179
0	3.1408	4.4099	3.6845	Н	1.0257	-4.7643	-3.4501

C	2.1069	4.4912	2.7079	Н	-2.8416	-3.1575	8.8745
0	-1.8816	3.4852	5.9668	Н	-2.0661	-1.6471	9.4157
С	-2.8531	4.2618	5.2892	Н	-1.363	-2.5801	8.0663
0	-6.0933	1.4963	4.9065	Н	-4.7611	-4.5222	5.663
С	-6.7806	1.6393	6.1487	Н	-4.2906	-5.5764	4.3035
0	-4.8755	0.3185	-2.7489	Н	-3.1954	-4.2773	4.8403
С	-4.4642	1.5727	-3.2639	Н	6.8884	-2.3856	0.5723
0	-1.6418	0.3595	-6.296	Н	5.1075	-2.3951	0.7354
С	-2.4426	-0.0487	-7.4052	Н	5.903	-3.4592	-0.4526
0	-2.7014	-4.3226	-4.7825	Н	7.8886	-1.1619	4.2129
С	-3.2589	-5.5732	-4.4187	Н	6.1916	-1.1815	4.7564
0	2.0205	-3.4417	-4.7175	Н	7.3075	0.0793	5.352
C O C O	-1.0418 -2.4426 -2.7014 -3.2589 2.0205	-0.0487 -4.3226 -5.5732 -3.4417	-6.296 -7.4052 -4.7825 -4.4187 -4.7175	H H H H H	5.903 7.8886 6.1916 7.3075	-2.3931 -3.4592 -1.1619 -1.1815 0.0793	0.7334 -0.4526 4.2129 4.7564 5.352

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¹³C NMR spectrum of **3** in CDCl₃.



¹³C NMR spectrum of **5b** in CDCl₃.