Supplementary Information for

Cyano- and chloro-substituted coronene diimides as solution-processable electron-transporting semiconductors

Chenhao Zhang, Ke Shi, Kang Cai, Jiajun Xie, Ting Lei, Qifan Yan, Jie-Yu Wang, Jian Pei* and Dahui Zhao*

Beijing National Laboratory of Molecular Sciences, Centre for the Soft Matter Science and Engineering, the Key Laboratory of Polymer Chemistry and Physics of the Ministry of Education, College of Chemistry, Peking University, Beijing 100871, China. Email: dhzhao@pku.edu.cn, jianpei@pku.edu.cn

Table of Contents

I.	Synthetic procedures and characterizations	S2
II.	Absorption, emission and electrochemical characterizations	S7
III.	Fabrications and characterizations of OFET devices	S8
IV.	DFT calculations	S9
v.	XRD characterizations of thin film	S10
VI.	References	S11
VII.	Copies of NMR spectra	S12

I. Synthetic procedures and characterizations

General Methods. Chemicals and solvents were purchased and used as received unless otherwise indicated. All oxygen and moisture sensitive reactions were performed under nitrogen atmosphere. Dichloromethane (DCM) and triethylamine (TEA) were distilled over CaH₂. Toluene and tetrahydrofuran (THF) were distilled over sodium and benzophenone. ¹H and ¹³C NMR spectra were recorded on a Mercury plus 300 or on a Bruker-500 using CDCl₃ as the solvent unless otherwise noted. Chemical shifts are reported in parts per million(ppm), chemical shifts in ¹H NMR were referenced to TMS (0.0 ppm) and ¹³C NMR spectra were referenced to CDCl₃ (77.0 ppm). High-resolution ESI FT mass spectra were recorded on a Bruker APEX IV mass spectrometer. MALDI-TOF mass spectra were recorded on an ABI 4800 Plus MALDI TOF/TOF Analyzer. Elemental analyses were performed using a German Vario EL III elementa analyzer. The X-ray diffraction data were obtained on X'PertPro Panalytical Diffractometer at a wavelength of 1.5406 Å. Atomic force microscopy studies were performed with a Nanoscope IIIa microscope and carried out in tapping mode at ambient temperature.

Synthesis procedures

Compounds 4a and 5a were prepared using similar procedures as previously reported.^{1,2}



1. To a solution of compound **4a** (100 mg, 0.098 mmol) in dry DCM (40 mL) was added dropwise a solution of *tert*-butylhypochlorite (1.8 mmol) in dry DCM (4 mL). After stirring at 30 °C for 36 h, the reaction mixture was washed sequentially with Na₂SO₃ (aq.) and K₂CO₃ (aq.), and then dried over anhydrous Na₂SO₄. The solvent was evaporated and the residue was purified with silica gel column chromatography (PE/DCM, 5/1, v/v) to afford product **1** as an orange solid (69 mg, 75%).¹H NMR (CDCl₃, 300 MHz, ppm): δ 9.74 (s, 4H), 5.45-5.39 (m, 2H), 2.53-2.49 (m, 4H), 2.26-2.20 (m, 4H), 1.58-1.48 (m, 16H), 1.38-1.34 (m, 16H), 0.91-0.86 (m, 12H). ¹³C NMR (CDCl₃, 125 MHz, ppm): δ 163.5, 162.3, 131.0, 130.3, 128.2, 127.0, 125.8, 125.2, 124.5, 119.9, 118.1, 114.1, 56.5, 32.5, 31.8, 29.7, 29.2, 27.1, 22.6, 14.0. MALDI-TOFMS: Calcd. for C₅₄H₅₈Cl₄N₂O₄: 938.3. Found (M⁺): 938.1 (m/z). Elem. Anal.: Calcd. for C₅₄H₅₈Cl₄N₂O₄: C, 68.93; H, 6.21; N, 2.98. Found: C, 68.93; H, 6.24; N, 3.03.



3. A Schlenk tube containing **5a** (104 mg, 0.093 mmol) and CuCN (300 mg, 3.35 mmol) was evacuated and backfilled with nitrogen three times. After degassed and dried NMP (5 mL) was added, the tube was sealed under nitrogen atmosphere and heated at 120 °C for 24 h. After cooling to room temperature, the reaction mixture was diluted with DCM and the insoluble part was filtered out. The filtrate was washed with water five times to remove NMP and dried over anhydrous Na₂SO₄. Upon removal of solvents under reduced pressure, the residue was purified with silica gel column chromatography (petroleum ether/DCM=3/1, v/v) to afford a mixture of regioisomers of **3** as yellow crystals (39 mg, 46%). ¹H NMR (CDCl₃, 300 MHz, ppm): δ 10.49-10.46 (m, 2H), 10.33-10.29 (m, 2H), 5.49-5.43 (m, 2H), 2.49-2.41 (m, 4H), 2.08-2.01 (m, 4H), 1.42-1.36 (m, 16H), 1.27-1.22 (m, 16H), 0.84-0.79 (m, 12H). ¹³C NMR (CDCl₃, 125 MHz, ppm): δ 164.3, 163.1, 140.52, 129.5, 129.3, 127.5, 127.2, 126.7, 125.6, 125.5, 125.1, 122.2, 121.7, 120.2, 114.4, 112.8, 56.2, 32.6, 31.8, 29.7, 29.3, 27.1, 22.6, 14.0. HRESI FTMS: Calcd. for C₅₆H₅₈Cl₂N₄O₄: 920.38. Found (M + H⁺): 921.39 (m/z). Elem. Anal.: Calcd. for C₅₆H₅₈Cl₂N₄O₄: C, 72.95; H, 6.34; N, 6.08. Found: C, 72.97; H, 6.41; N, 5.97.



2a. A Schlenk tube containing compound **5a** (101 mg, 0.090 mmol), CuCN (246 mg, 2.75 mmol), 1,1'-bis(diphenylphosphino)ferrocene (dppf) (10 mg, 0.018 mmol) and Pd₂(dba)₃ (8 mg, 0.009 mmol) was evacuated and backfilled with nitrogen three times. After degassed and dried dioxane (5 mL) was added, the tube was sealed under nitrogen atmosphere and heated at 105 °C for 48 h. After cooling to room temperature, the reaction mixture was diluted with dichloromethane and insoluble part was filtered out. The filtrate was washed with water and then dried over anhydrous Na₂SO₄. Upon removal of solvents under reduced pressure, the residue was purified with silica gel column chromatography (PE/DCM=2/1, v/v) to afford product **2a** as yellow crystals (51 mg, 63%). ¹H NMR (CDCl₃, 300 MHz, ppm): δ 10.55 (s, 4H), 5.53-5.44 (m, 2H), 2.46-2.42 (m, 4H),

2.08-2.02 (m, 4H), 1.37-1.25 (m, 32H), 0.88-0.80 (m, 12H). ¹³C NMR (CDCl₃, 125MHz, ppm): δ 163.6, 132.4, 127.4, 127.0, 122.9, 122.4, 120.3, 118.2, 56.0, 32.6, 31.9, 29.4, 27.4, 22.7, 14.1. ESI FTMS: Calcd. for C₅₈H₅₈N₆O₄: 902.45. Found (M⁺): 902.45 (m/z). Elem. Anal.: Calcd. for C₅₈H₅₈N₆O₄: C, 77.13; H, 6.47; N, 9.31. Found: C, 77.07; H, 6.56; N, 9.15. CCDC No.: 1047207



6. A mixture of perylene-3,4,9,10-tetracarboxylic dianhydride (2.50 g, 6.3 mmol) and 4-octyltetradecan-1-amine (4.21 g, 12.9 mmol) in imidazole (8.0 g) were heated and stirred at 150 °C for 24 h. The reaction mixture was cooled to 100 °C, and then methanol (100 mL) was added with stirring. After cooling to room temperature, the dark red precipitate was filtered and rinsed thoroughly with methanol. The precipitate was dissolved in chloroform (300 mL) and filtered again. The solvent was evaporated to give product **6** as a red solid (5.12 g, 80%). ¹H NMR (CDCl₃, 300 MHz, ppm): δ 8.32-8.29 (d, 2H), 8.11-8.08 (d, 2H), 4.18-3.94 (m, 4H), 1.65-1.57 (m, 4H), 1.30-0.97 (m, 70H), 0.80-0.74 (m, 12H). ¹³C NMR (CDCl₃, 75 MHz, ppm): δ 162.8, 133.7, 130.8, 128.8, 125.6, 123.0, 122.6, 41.1, 37.3, 33.5, 31.9, 30.2, 29.7, 29.4, 26.7, 25.3, 22.7, 14.1. MALDI-TOF MS: Calcd. for C₆₈H₉₈N₂O₄: 1006.7. Found (M⁺): 1006.7 (m/z).



7. A mixture of compound **6** (3.42 g, 3.3 mmol), bromine (15.4 g, 97.4 mmol), and chloroform (50 ml) was stirred at 40 °C for 7 days. The reaction mixture was washed with Na₂SO₃ (aq.) and K₂CO₃ (aq.), and then dried over anhydrous Na₂SO₄. The solvent was evaporated and the residue was purified with silica gel column chromatography (PE/DCM=7/1, v/v) to give product **7** as an orange gel (2.63g, 67%).¹H NMR (CDCl₃, 300 MHz, ppm): δ 9.37-9.35 (d, 2H), 8.81 (s, 2H), 8.61-8.58 (m, 2H), 4.20-4.12 (m, 4H), 1.77-1.68 (m, 4H), 1.33-1.15 (m, 70H), 0.89-0.81 (m,

12H).¹³C NMR (CDCl₃, 75 MHz, ppm): δ 162.2, 161.6, 137.5, 131.9, 129.4, 128.4, 127.9, 126.3, 122.8, 122.3, 120.6, 41.1, 37.2, 33.5, 31.9, 30.9, 30.1, 29.7, 29.6, 29.3, 26.6, 25.2, 22.6, 14.1. MALDI-TOF MS: Calcd. for C₆₈H₉₆N₂O₄Br₂: 1162.6. Found (M + H⁺): 1163.6 (m/z).



8. A Schlenk tube containing compound **7** (1.24 g, 1.1 mmol), CuI (2 mg, 0.01 mmol) and Pd(PPh₃)₂Cl₂ (35 mg, 0.05 mmol) was evacuated and backfilled with nitrogen three times. After trimethylsilylacetylene (423 mg, 4.3 mmol), degassed and dried THF (15 mL) and triethylamine (15mL) were added, the tube was sealed under nitrogen atmosphere and heated at 40 °C for 6 h. After cooling to room temperature, the reaction mixture was washed with saturated NH₄Cl (aq.) and dried over anhydrous Na₂SO₄. The solvent was evaporated and the residue was purified with silica gel column chromatography (PE/DCM = 5/1, v/v) to afford product **9** as a red gel (1.03 g, 81%). ¹H NMR (CDCl₃, 300 MHz, ppm): δ 10.12-10.09 (d, 2H), 8.73 (s, 2H), 8.55-8.52 (d, 2H), 4.22-2.14 (m, 4H), 1.77-1.69 (m, 4H), 1.37-1.16 (m, 70H), 0.90-0.81 (m, 12H), 0.42 (s, 18H). ¹³C NMR (CDCl₃, 125 MHz, ppm): δ 162.6, 162.3, 137.8, 133.4, 133.3, 129.9, 127.2, 126.9, 122.9, 121.7, 119.4, 105.6, 41.1, 37.3, 33.5, 31.9, 31.0, 30.2, 29.7, 29.7, 29.7, 29.4, 29.4, 26.7, 25.2, 22.7, 14.1, 0.3.



4b. To a solution of **9** (1,6/1,7-isomer mixture, 840 mg, 0.70 mmol) in DCM (500 mL) was added ICl (500 mg, 3.0 mmol) in DCM (10 mL) dropwise at -78 °C. Then the solution was gradually warmed up to room temperature over 6 h and stirred at room temperature for additional 6 h. The reaction mixture was washed sequentially with Na₂SO₃ (aq.) and then exposed to sun light for 5 h. Upon completion of the reaction, the mixture was washed with Na₂SO₃ (aq.) and K₂CO₃ (aq.), and

then dried over anhydrous Na₂SO₄. The solvent was evaporated and the residue was purified with silica gel column chromatography (PE/DCM=8/1, v/v) to afford a mixture of regioisomers of **4b** as an orange gel (604 mg, 68%). ¹H NMR (CDCl₃, 300 MHz, ppm): δ 9.98 (m, 2H), 9.95 (m, 2H), 4.61-4.51 (m, 4H), 2.05-1.93 (m, 4H), 1.63-1.54 (m, 4H), 1.34-1.24 (m, 70H),1.08(s, 18H), 0.87-0.79 (m, 12H). ¹³C NMR (CDCl₃, 75 MHz, ppm): δ 163.5, 163.4, 141.8, 139.3, 133.2, 130.3, 127.1, 126.2, 122.7, 121.3, 121.2, 120.5, 120.4, 118.7, 43.6, 37.4, 33.6, 31.9, 30.2, 29.7, 29.4 26.7, 25.6, 22.6, 14.1, 4.1, 4.0. MALDI-TOF MS:Calcd. For C₇₂H₁₁₂Cl₂N₂O₄Si₂: 1266.8. Found (M + H⁺): 1267.7 (m/z). Elem. Anal.: Calcd. For C₇₂H₁₁₂Cl₂N₂O₄Si₂: C, 73.84; H, 8.90; N, 2.21. Found: C, 73.93; H, 8.78; N, 2.12.



5b. To compound **4b** (208 mg, 0.16 mmol) dissolved in DCM (50 mL) was added ICl (0.20 g, 1.23 mmol) under nitrogen atmosphere. After stirring at room temperature for 6 h, the reaction mixture was washed with Na₂SO₃ (aq.) and K₂CO₃ (aq.), and then dried over anhydrous Na₂SO₄. After removal of solvents under reduced pressure, the residue was purified by silica gel column chromatography (PE/DCM=6/1, v/v) to afford a mixture of regioisomers of **5b** as an orange gel (217 mg 91%). ¹H NMR (CDCl₃, 300 MHz, ppm): δ 8.76-8.53 (m, 4H), 4.30-4.14 (m, 4H), 1.91-1.79 (m, 4H), 1.54-1.45 (m, 4H), 1.41-1.24 (m, 70H), 0.88-0.94 (m, 12H). ¹³C NMR (CDCl₃, 125 MHz, ppm): δ 161.66, 161.64, 139.0, 135.4, 129.9, 127.8, 127.6, 124.8, 121.7, 121.3, 121.0, 119.4, 116.4, 107.3, 42.1, 37.5, 33.8, 32.1, 32.0, 30.4, 29.9, 29.8, 29.5, 26.9, 22.8, 14.5, 14.2. MALDI-TOF MS: Calcd. for C₅₄H₅₈Cl₂I₂N₂O₄: 1374.5. Found (M + H⁺): 1375.4 (m/z). Elem. Anal.: Calcd. for C₇₂H₉₄Cl₂I₂N₂O₄: C, 62.84; H, 6.88; N, 2.04. Found: C, 62.89; H, 6.92; N, 1.91.



2b. A Schlenk tube containing compound 5b (101 mg, 0.069 mmol), CuCN (350 mg, 3.9 mmol),

1,1'-bis(diphenylphosphino)ferrocene(dppf) (13 mg, 0.023 mmol) and Pd₂(dba)₃ (10 mg, 0.0011 mmol) was evacuated and backfilled with nitrogen three times. After degassed and dried dioxane (5 mL) was added, the tube was sealed under nitrogen atmosphere and heated at 105 °C for 48 h. After cooling to room temperature, the reaction mixture was diluted with dichloromethane and the solid residue was filtered out. The filtrate was washed with water and dried over anhydrous Na₂SO₄. Upon removal of solvents *in vacuo*, the residual was purified with silica gel column chromatography (PE/DCM=1/1, v/v) to afford product **2b** as a yellow solid (36.6 mg, 46%). ¹H NMR (CDCl₃, 300 MHz, ppm): δ 10.49 (s, 4H), 4.53-5.44 (m, 4H), 2.00-1.91 (m, 4H), 1.58-1.46 (m, 4H), 1.33-1.17 (m, 70H), 0.87-0.82 (m, 12H).¹³C NMR (CDCl₃, 75 MHz, ppm): δ 162.2, 130.4, 128.0, 126.7, 125.4, 124.5, 119.9, 118.1, 114.0, 42.3, 37.3, 33.6, 31.1, 30.2, 29.7, 29.4, 26.8, 25.5, 22.7, 22.7, 14.2. MALDI-TOF MS: Calcd. For C₇₆H₉₄N₆O₄:1154.7. Found (M + H⁺): 1155.6 (m/z). Elem. Anal.: Calcd. for C₇₆H₉₄N₆O₄: C, 78.99; H, 8.20; N, 7.27. Found: C, 78.77; H, 8.30; N, 7.15.

II. Absorption, emission and electrochemical characterizations

UV-Vis absorption spectra were recorded on a Hitachi U-4100 spectrophotometer using the absorption mode in a 1-cm quartz cell. Fluorescence emission spectra were recorded in 1-cm quartz cuvetteon a Horiba Jobin Yvon FluoroMax-4P spectrofluorometer. N,N'-bis(1-hexylheptyl)perylenediimides ($\Phi_f = 1.00$ in CH₂Cl₂) was used as the fluorescence quantum yield standard.

Cyclic voltammograms were recorded on a BASI Epsilon work-station with three-electrode configuration, using Pt plate as the counter electrode, a glassy carbon as the working electrode, and Ag/AgCl electrode as the reference electrode. Samples were dissolved in CH_2Cl_2 with tetrabutylammonium hexafluorophosphate (TBAPF₆, 0.1 M) as the supporting electrolyte. The scan speed was 100 mV s⁻¹. An energy level -4.8 eV below the vacuum level was used for reference Fc/Fc⁺. The LUMO levels of CDIs were estimated from the onset potentials of the first reduction waves.



Fig. S1 Emission spectra of **1** (excited at 506 nm), **2a/b** (excited at 417 nm), and **3** (excited at 420 nm) in CH₂Cl₂.

III. Fabrications and characterizations of OFET devices

Top-gate/bottom-contact FET devices were fabricated on n^{++} -Si/SiO₂ (300 nm) substrates. The gold source and drain bottom electrodes (with Ti as the adhesion layer) were patterned by photolithography on the SiO₂ surface. The substrates were subjected to cleaning using ultrasonication in acetone, cleaning agent, deionized water (twice), and isopropanol. The cleaned substrates were dried under vacuum at 80 °C for 2 h before transferring into a glove-box. A thin film of respective compound was deposited on the treated substrates by spin-coating, using a solution (10 mg/mL in trichloroethylene) at 2000 rpm for 60 s and annealed at 160 °C for 5 min. After thin film deposition, a CYTOP solution (CTL809M:CT-solv180 = 3:1) was spin-coated onto the semiconducting layer at 2000 rpm for 60 s to form a dielectric layer of 500 nm thick. The CYTOP layer was then baked at 100 °C for 1 h. Gate electrodes comprising a layer of Al (50 nm) were then evaporated through a shadow mask onto the dielectric layer by thermal evaporation. The OTFT devices had a channel length (*L*) of 5 µm and a channel width (*W*) of 200 µm.

The characterizations of the FETs were carried out in atmosphere (humidity 50-60%) on a probe stage using a Keithley 4200 SCS as parameter analyzer. The carrier mobility, μ , was calculated from the data in the saturated regime according to the equation $I_{SD} = (W/2L)Ci\mu(V_G-V_T)^2$, where I_{SD} is the drain current in the saturated regime. W and L are the semiconductor channel width and length, respectively. Ci (Ci= 3.7 nF) is the capacitance per unit area of the gate dielectric layer. V_G and V_T are the gate voltage and threshold voltage, respectively. V_G-V_T of the device was determined from the relationship between the square root of I_{SD} and V_G in the saturated regime.



Fig. S2 The transfer ($V_{DS} = 100$ V) and output characteristics of OFET devices fabricated with CDI 1 (top) and 3 (bottom)

CDI	$\mu \ [cm^2 \ V^{-1} \ s^{-1}]$	I_{on}/I_{off}	$V_{th}[V]$
1	2.3×10 ⁻³	10 ⁵	0-10
2a	0.026	10 ⁵	0-10
2b	0.16	10^{4}	0-10
3	0.015	10^{5}	40

 Table S1. Summaryof the transistor performance for CDI 1-3

IV. DFT calculations

The geometry was optimized with Density Functional Theory (DFT) using B3LYP hybrid functional with a basis set limited to $6-31g^{**}$. TD-DFT calculations were performed at optimized geometries using the same theory level. Quantum chemical calculations were performed with the Gaussian 03^3 package and the orbital pictures were prepared using Gaussview.⁴ All alkyl substituents were replaced with methyl groups in calculations.



Fig. S3 DFT calculated frontier molecular orbitals (FMOs) of CDI 1-3

		1	2	3 (anti)	3 (syn)	
LUMO+1 /eV		-2.68	-3.82	-3.24	-3.26	
LUMO /eV		-3.48	-4.08	-3.80	-3.79	
HOMO /eV		-6.58	-7.378	-6.96	-6.98	
HOMO-1 /eV		-6.73	-7.384	-7.09	-7.06	
S ₀ -S ₁	λ/nm	468.8	457.0	462.1	461.0	
	Transition dipole (Debye)	2.91	0.86	2.52	1.32	
	Assignments	H-0->L+0 (88%)	H-0->L+0 (67%)	H-0->L+0 (79%)	H-0->L+0 (81%)	
		H-1->L+1 (11%)	H-1->L+1 (32%)	H-1->L+1 (16%)	H-1->L+1 (18%)	
S ₀ -S ₂	λ/nm	422.4	424.6	422.2	424.0	
	Transition dipole (Debye)	4.60	2.82	1.52	2.36	
	Assignments	H-1->L+0 (86%)	H-1->L+0 (70%)	H-1->L+0 (76%)	H-1->L+0 (80%)	
		H-0->L+1 (14%)	H-0->L+1 (29%)	H-0->L+1 (19%)	H-0->L+1 (19%)	
H: HOMO; L: LUMO						

Table S2. DFT calculated FMO level and electronic transition of CDIs 1-3

V. XRD characterizations of thin films



Fig. S4 XRD patterns of thin films of 1-3 after thermal annealing at 160 °C on SiO₂/Si substrates.

VI. References

1. U. Rohr,; C. Kohl,; K. Mullen,; A. van de Craats; and J. Warman,; J. Mater. Chem., 2001, 11, 1789-1799.

2. I. Meager,; R. S. Ashraf,; S. Mollinger,; B. C. Schroeder,; H. Bronstein,; D. Beatrup,; M. S. Vezie,;
T. Kirchartz,; A. Salleo,; J, Nelson,; I. McCulloch, *J. Am. Chem. Soc.* 2013, 135, 11537–11540.

3. Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, J. A. Jr.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. Gaussian 03, Revision C.02; Gaussian Inc.: Wallingford CT, 2004.

S5. Dennington, R., II; Keith, T.; Millam, J.; Eppinnett, K.; Hovell, W. L.; Gilliland, R. GaussView, Version 3.09; Semichem, Inc.: Shawnee Mission, KS, 2003.



¹³C NMR spectrum of **1** (CDCl₃, 125 MHz)





¹³C NMR spectrum of **2a** (CDCl₃, 125 MHz)



