Supporting Information

REVERSIBILITY OF 3-PHENYL 2-OXINDOLE DIMER FORMATION: APPLICATION TO CONSTRUCT COMPOUNDS WITH TWO DISTINCT VICINAL ALL-CARBON QUATERNARY CENTERS

Yoshihiro Sohtome,[1,2]* Masumi Sugawara,[1] Daisuke Hashizume,[3] Daiki Hojo,[2] Miki Sawamura,[1] Atsuya Muranaka,[2,4] Masanobu Uchiyama,[2,4] and Mikiko Sodeoka[1,2]*

[1] Synthetic Organic Chemistry Laboratory, RIKEN, 351-0198, Japan. [2] RIKEN Center for Sustainable Resource Science, 351-0198, Japan. [3] RIKEN Center for Emergent Matter Science, 351-0198, Japan. [4] Elements Chemistry Laboratory, RIKEN, 351-0198, Japan; E-mail: sohtome@riken.jp, sodeoka@riken.jp

Dedicated to Professor Dr. Masakatsu Shibasaki on the occasion of his 70th birthday

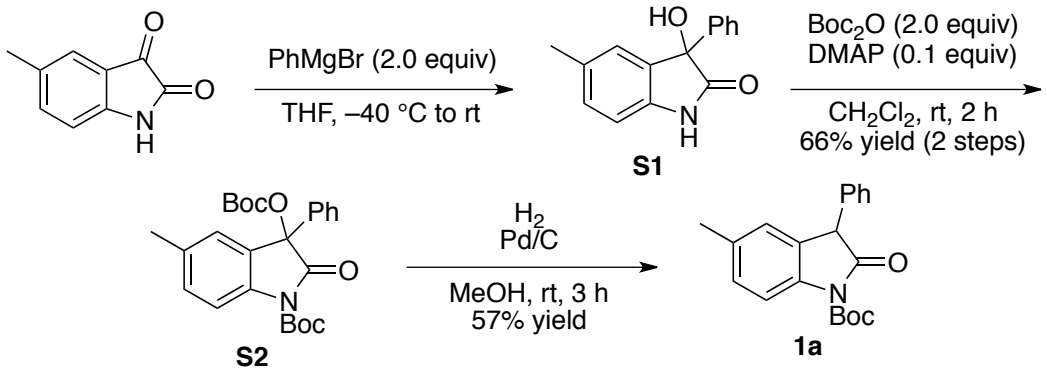
Contents

1. General

^{1}H and ^{13}C NMR spectra were recorded at room temperature on a JEOL JNM-ECS-400 NMR spectrometer at 400 and 100 MHz, respectively. The proton chemical shift values are reported in parts per million (ppm) downfield from tetramethylsilane and referenced to the proton resonance of $CHCl_3$ (δ 7.26), CD_3OD (δ 3.31) or C_6D_6 (δ 7.16). The carbon chemical shift values are reported in parts per million (ppm) downfield from tetramethylsilane and referenced to the carbon resonance of $CDCl_3$ (δ 77.0), CD_3OD (δ 49.0) or C_6D_6 (δ 128.1). Chemical shifts are reported in ppm and *J* values in Hz. The data are presented in the following order: chemical shift, signal area integration in natural numbers, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, quint = quintet, m = multiplet and/or multiple resonances, and br = broad) and coupling constant. ESI-MS spectra were measured on a Bruker micrOTOF-QII-RSL. UV-Vis spectra were recorded by JASCO V-660 spectrophotometer.

All reactions were performed under an argon atmosphere in flame-dried glassware with magnetic stirring. Anhydrous methanol (MeOH), dichloromethane (CH_2Cl_2) and tetrahydrofuran (THF) were purchased from Kanto. Other solvents used were purchased from Wako Pure Chemical Industries, Ltd. (Wako) or Tokyo Chemical Industry Co. Ltd. (TCI), and were used as received. Reactions conducted below room temperature were cooled using a PSL-1400 (Tokyo Rikakikai Co., Ltd.) or a PSL-1810 (EYELA). Analytical thin-layer chromatography (TLC) was performed on Silica gel 60 F254-coated glass plates (Merck); visualization of the developed chromatogram was performed by ultraviolet illumination (254 nm) and/or staining with cerium molybdate stain (Hanessian's stain). Flash column chromatography was performed using silica gel 60N (40-50 μm, Kanto Chemical Co., Inc.) and CHROMATOREX® NH (NH–DM1020, 100–200 mesh, Fuji Silysia Chemical, Ltd.). Gel permeation chromatography (GPC) was performed using a Recycling Preparative HPLC LC-918 (Japan Analytical Industry Co., Ltd.) equipped with two polystyrene columns (YMC-GPC T2000 and YMC-GPC T4000).

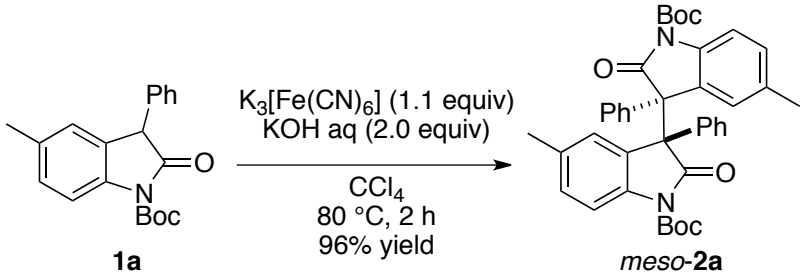
2. Preparation of 1a and *meso*-2a[11]



To a stirred, cold (–40 °C) suspension of 5-methylisatin (1.61 g, 10.0 mmol) in THF (25 mL, 0.4 M) under an atmosphere of N_2, a solution of PhMgBr in THF (20 mL, 2.0 equiv, 1.0 M solution) was added dropwise. The mixture was allowed to warm to room temperature and stirred until the isatin was consumed. The reaction mixture was quenched with 1 M HCl. The aqueous layer was extracted with EtOAc, and the combined organic layers were washed with brine and then dried over Na_2SO_4. After removal of the solvent, the crude **S1** was used for the next reaction without further purification.

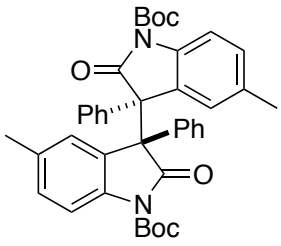
To a solution of the crude **S1** in CH_2Cl_2 (25 mL, 0.4 M) were added DMAP (122 mg, 1.0 mmol) and $(Boc)_2O$ (4.40 g, 20 mmol). The reaction mixture was stirred at room temperature for 2 h, and then the reaction was quenched with saturated aqueous NH_4Cl. The aqueous layer was extracted with CH_2Cl_2, and the combined organic layer was washed with brine and dried over Na_2SO_4. After removal of the solvent, the resulting solid was washed with hexane and filtered to give **S2** in 66% yield in 2 steps (2.90 g, 6.6 mmol).

S2 (1.54 g, 3.5 mmol) was dissolved in MeOH (70 mL, 0.05 M). 10% Pd/C (374.5 mg) was added to this solution, and the resulting mixture was stirred under a hydrogen atmosphere (balloon) for 3 h at room temperature. The reaction mixture was passed through Celite to remove Pd/C, and the residue was washed with MeOH. After removal of the solvent, the crude product was dissolved in EtOAc and passed through a short pad of silica gel. After evaporation of EtOAc under reduced pressure, the residue was triturated with hexane at room temperature. The resulting solid was collected by filtration, washed with hexane, and dried under reduced pressure to give **2** in 57% yield (644.0 mg, 2.0 mmol) as a white solid. The NMR spectra for **1a** were identical with reported data.[S1]



A flame-dried test tube was charged with *N*-Boc oxindole **1a** (64.7 mg, 0.20 mmol) and CCl_4 (670 μL, 0.3 M) and heated at 80 °C. A solution of $K_3[Fe(CN)_6]$ (72.4 mg, 0.22 mmol, 1.1 equiv) and KOH (22.4 mg, 0.40 mmol, 2 equiv) in H_2O (800 μL) was added dropwise to it. The mixture was stirred for 2 h at 80 °C, then cooled to room temperature. The organic layer was separated and the aqueous layer was extracted with CCl_4. The combined organic layer was washed with brine and dried over Na_2SO_4. After evaporation of the solvent, the crude product was purified by silica gel column chromatography (hexane/EtOAc = 10/1 to 7/1) to afford *meso*-**2a** in 96% yield (62.2 mg, 96 μmol).

di-*tert*-Butyl 5,5'-dimethyl-2,2'-dioxo-3,3'-diphenyl-(3,3'-biindoline)-1,1'-dicarboxylate

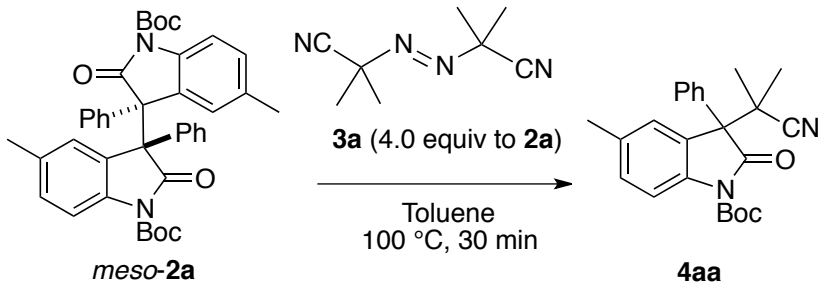


meso-**2a**

10/1 mixture

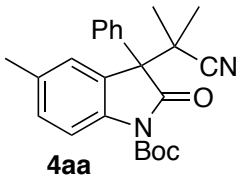
Yellow solid; mp. 195-196 °C; IR (neat) 2975, 2357, 1790, 1760, 1733, 1489, 1339, 1281, 1153, 752 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$, only signals of the major product are shown) δ 7.68 (d, J = 8.2 Hz, 2H), 7.52-7.19 (m, 10H), 7.13 (d, J = 8.2 Hz, 2H), 2.16 (s, 6H), 1.73-1.46 (m, 18H); ^{13}C NMR (100 MHz, $CDCl_3$, only signals of the major product are shown) δ 172.7, 148.8, 138.2, 132.3, 131.4, 131.2, 129.4, 128.1, 127.8, 127.1, 126.9, 126.5, 114.8, 83.9, 60.8, 28.0, 21.1; HRMS (ESI) Calcd for $C_{40}H_{40}N_2NaO_4$ $[M+Na]^+$ 667.2779, Found: 667.2756.

3. A typical procedure for reaction of *meso*-2a with azo compounds



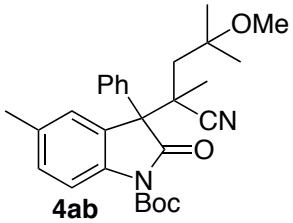
A flame-dried test tube was charged with oxindole dimer *meso*-**2a** (16.1 mg, 25 μmol), AIBN (16.4 mg, 0.1 mmol, 4 equiv), and toluene (0.5 mL, 0.05 M). The mixture was stirred at 100 °C under an argon atmosphere. After 30 min, the solvent was evaporated and the resultant product was purified by silica gel column chromatography (hexane/EtOAc = 10/1) to afford the product **4aa** in 86% yield (16.8 mg, 43 μmol).

***tert*-Butyl 3-(2-cyanopropan-2-yl)-5-methyl-2-oxo-3-phenylindoline-1-carboxylate**



Colorless oil; IR (neat) 2980, 2378, 1786, 1757, 1735, 1490, 1337, 1307, 1248, 1152, 1113, 754 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.85 (br s, 1H), 7.84 (dd, J = 8.3, 2.3 Hz, 2H), 7.71 (d, J = 8.3 Hz, 1H), 7.40-7.30 (m, 3H), 7.17 (d, J = 8.3 Hz, 1H), 2.43 (s, 3H), 1.64 (s, 9H), 1.62 (s, 3H), 1.33 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.3, 148.7, 136.9, 134.8, 134.3, 129.7, 128.6, 128.2, 128.1, 127.7, 126.6, 123.9, 114.7, 84.9, 58.8, 40.2, 28.1, 24.2, 22.9, 21.4; HRMS (ESI) Calcd for $C_{24}H_{26}N_2NaO_3$ $[M+Na]^+$ 413.1836, Found: 413.1845.

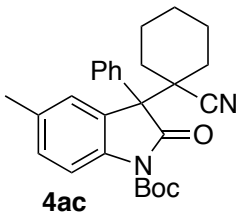
***tert*-Butyl 3-(2-cyano-3-methoxy-3-methylpentan-2-yl)-5-methyl-2-oxo-3-phenylindoline-1-carboxylate**



The crude mixture was purified by silica gel column chromatography (hexane/EtOAc = 10/1) followed by GPC ($CHCl_3$) to afford **4ab** as a diastereo mixture (1:1) in 86% yield (19.8 mg, 42.8 μmol). Colorless oil; IR (neat) 2978, 2938, 2828, 1788, 1756, 1737, 1489, 1370, 1337, 1307, 1281, 1246, 1152, 1114, 754 cm^{-1}; ^1H NMR (400 MHz, CD_3OD, signals of both diastereomers are shown) δ 8.03 (brs, 1H), 7.86-7.79 (m, 4H), 7.78 (s, 1H), 7.73 (d, J = 8.0 Hz, 1H), 7.72 (d, J = 8.4 Hz, 1H), 7.43-7.31 (m, 6H), 7.30-7.21 (m, 2H), 3.11 (s, 3H), 3.05 (s, 3H), 2.45 (s, 3H), 2.39 (s, 3H), 2.31 (d, J = 15.4 Hz, 1H), 1.87 (d, J = 15.4 Hz, 1H), 1.76 (d, J = 14.8 Hz, 1H),1.72-1.59 (m, 22H), 1.45 (s, 3H), 1.28 (s, 3H), 1.21 (s, 3H), 1.19 (s, 3H), 1.17 (s, 3H).; ^{13}C NMR (100 MHz, CD_3OD, signals of both diastereomers are shown) δ 175.5, 174.8, 150.1, 138.5, 138.3, 136.9, 135.6, 135.1, 131.0, 130.9, 130.1, 129.8, 129.5, 129.3, 129.1, 128.3. 128.2, 124.6, 124.1, 115.8, 115.6, 86.28, 86.26, 75.9, 75.7, 62.1, 61.6, 45.5, 43.7, 43.0, 42.6, 28.2, 27.00, 26.97, 26.0, 25.4, 23.1, 23.0, 21.4, 21.3; HRMS (ESI) Calcd for $C_{28}H_{34}N_2NaO_3$ $[M+Na]^+$ 485.2416, Found:

485.2449.

***tert*-Butyl 3-(1-cyanocyclohexyl)-5-methyl-2-oxo-3-phenylindoline-1-carboxylate**



4ac

The crude mixture was purified by silica gel column chromatography (Hex/Et_2O = 20/1) followed by GPC ($CHCl_3$) to afford **4ac** in 81% yield (17.4 mg, 40.4 μmol). Colorless oil; IR (neat) 2936, 2862, 1786, 1754, 1735, 1488, 1337, 1307, 1247, 1153, 755 cm^{-1}; ^1H NMR (400 MHz, C_6D_6) δ 8.35 (s, 1H), 8.20-8.12 (m, 3H), 7.08 (m, 2H), 6.98-6.94 (m, 1H), 6.92 (ddd, J = 8.4, 1.84, 0.9 Hz, 1H), 2.56 (td, J = 13.2, 3.6 Hz, 1H), 2.10 (s, 3H), 1.84 (dd, J = 13.2, 2.3 Hz, 1H), 1.63-1.42 (m, 12H), 1.38-1.20 (m, 3H), 1.13 (d, J = 12.8 Hz, 1H), 0.66 (m, 1H); ^{13}C NMR (100 MHz, C_6D_6) δ 173.4, 149.7, 137.9, 135.0, 134.6, 130.0, 129.0, 128.9, 128.7, 127.3, 121.6, 115.1, 84.3, 59.9, 48.1, 31.9, 29.5, 27.9, 24.7, 23.2, 23.0, 21.2; HRMS (ESI) Calcd for $C_{27}H_{30}N_2NaO_3$ $[M+Na]^+$ 453.2154, Found: 453.2171.

4. X-Ray analysis of *meso*-2a

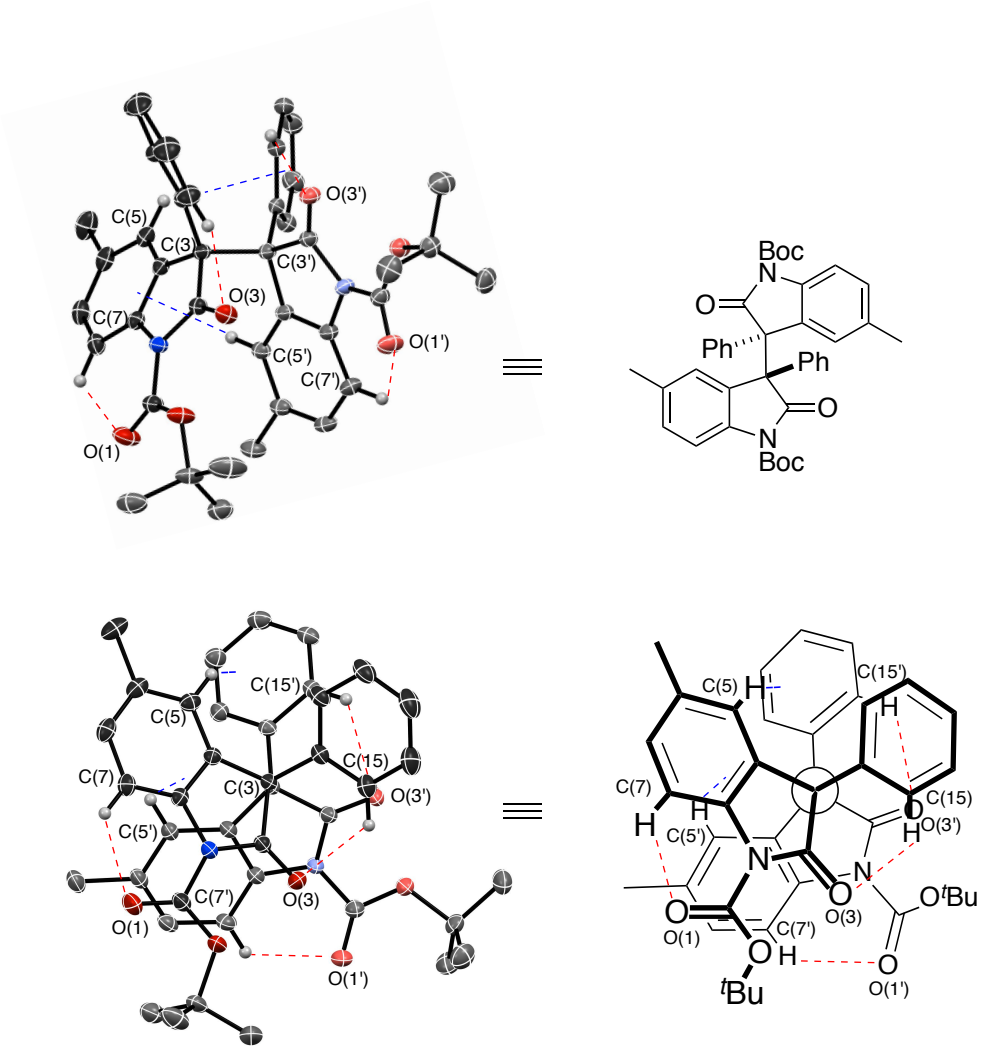


Figure S1. ORTEP drawings (50% probability ellipsoids) and chemical structures of *meso*-**2a**. CH/O interactions are represented by red broken lines, while CH/π interactions are represented by blue broken lines. Only hydrogen atoms associated with CH/O and CH/π interactions are shown for the sake of clarity.

Table S1. Crystal data of *meso*-**2a** (CCDC 1499431).

Molecular formula	$C_{40}H_{40}N_2O_6$
Formula weight	644.74
T (K)	90
Wavelength (Å)	0.71073
Color	colorless
Crystal system	triclinic
Space group	*P*-1
a (Å)	11.0727(2)
b (Å)	11.9236(2)
c (Å)	14.6792(3)
V (Å)	1703.06(5)
Z	2
Density (Mg/m^3)	1.257
Absorption coefficient (mm^{-1})	0.084
F (000)	684
Crystal size (mm^3)	0.21 x 0.17 x 0.08
Theta range for data collection (°)	1.48 to 31.07
Reflections collected	57180
Independent reflections	8401
Software for refinements	SHELXL-97
Goodness of fit on F_2	1.071
R_1, wR_2 [I>2σ (I)]	0.0450, 0.1142
R_1, wR_2 (all data)	0.0602, 0.1234

5. Temperature-Dependent UV-Vis Measurements

A 1 cm quartz cell containing 6.4 mg (10 μmol) of *meso*-**2a** in 2.5 mL of $CHCl_3$ (4 mM) was capped. Absorbance measurements were taken at 5 degree intervals with at least 5 minutes between measurements to allow the temperature and the solution to equilibrate.

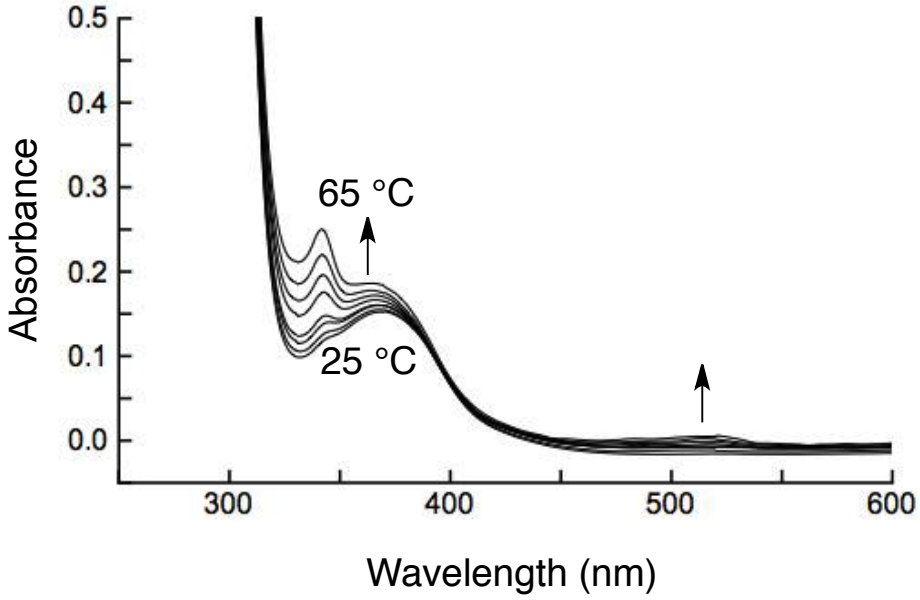


Figure S2. Absorption spectra of *meso*-**2a** at different temperatures in $CHCl_3$ (4 mM).

6. Computational Details

For dimer **2**, density functional theory (DFT) calculations were performed for singlet configurations using the Gaussian 09 program package.[14] For monomeric radical **1**, DFT calculations were conducted for doublet configurations. All geometry optimizations, vibrational analyses, NMR analyses and time-dependent density functional theory (TD-DFT) calculations were carried out using the M06-2X functional for **2** or UM06-2X functional[15] for **1** with the 6-311G(d,p) basis set.

To identify plausible rotamers and their rotation barriers for *meso*-**2a**, *dl*-**2a**, *meso*-**2c** and *dl*-**2c**, we first examined the energy profile through partial geometry optimization varying the dihedral angles (ω) of C(14)–C(3)–C(3')–C(14') by 20° jumps (Figure S3). For example, the energy profile plots for *meso*-**2a** gave the three local minima at ω = –63.35 (*meso*-**2aI**), 56.65 and 156.65°. The structure obtained at ω = 56.65° using the ModRedundant option involves only one CH/π interaction of C(5')–H and the electron-rich oxindole core, likely due to the constrained optimization. Unconstrained optimization starting from the coordinates involving four CH/O and two CH/π interactions gave roughly the same structure **DFT-*meso*-2aI** with ω = 63.35, as a (±)-*sc* conformation. On the other hand, the local minimum at ω = 156.65° gave **DFT-*meso*-2aII**, which has *ap* (antiperiplanar) conformation. The energy value of **DFT-*meso*-2aII** (ΔG_{II-I} = 2.8 kcal/mol) is higher than that of **DFT-*meso*-2aI**, suggesting that the population of **2aI** should be larger than that of **2aII**, considering the rotation barrier (13.9 kcal/mol from **DFT-*meso*-2aII**). The ΔG values plotted in Figure 4 (main text) were obtained from the energetics of a series of simulated structures in the ground and transition states (Table S2).

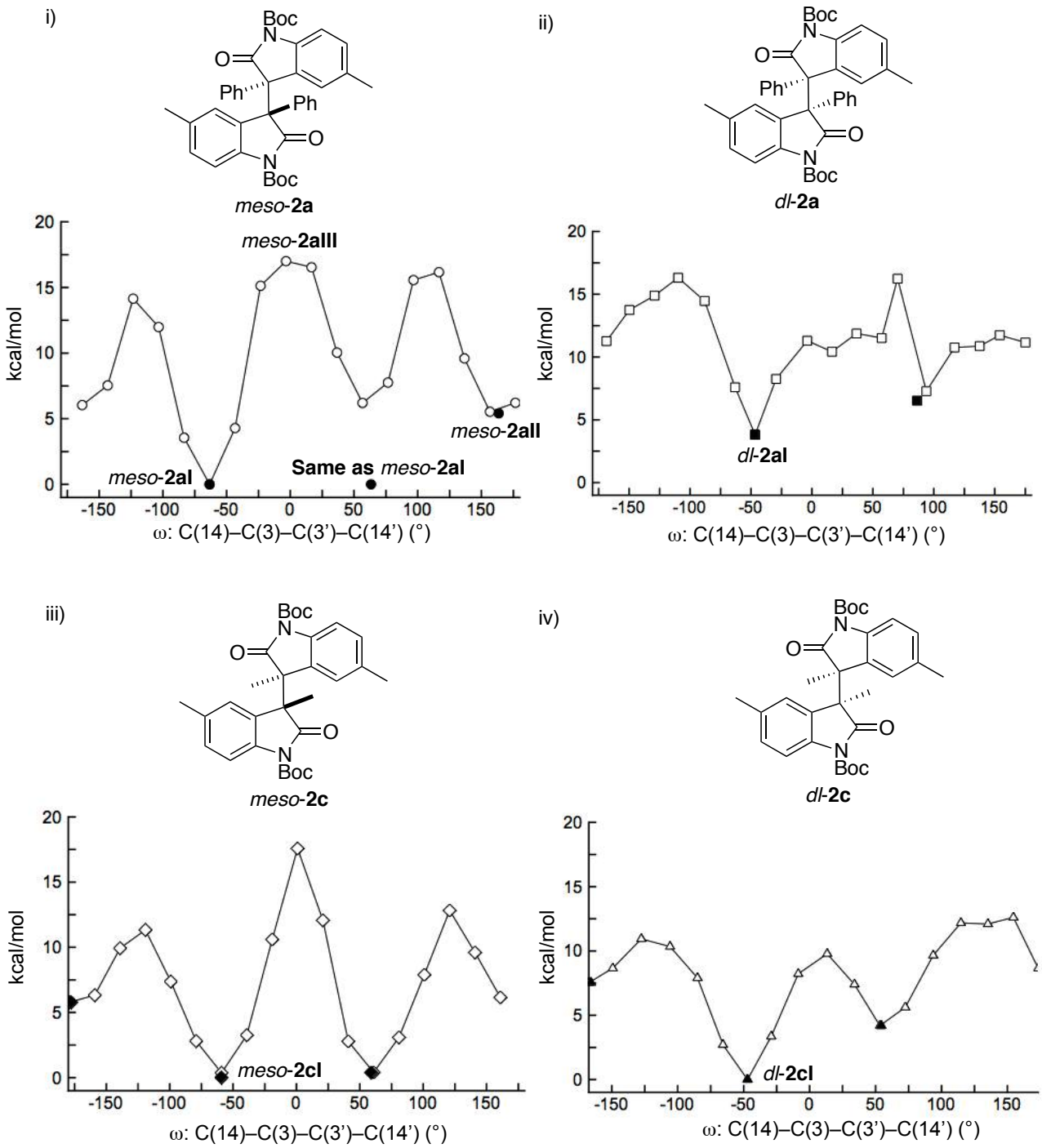


Figure S3. Rotational energy profile of *meso*-**2a**, *dl*-**2a**, *meso*-**2c** and *dl*-**2c** (open symbols: optimized with the ModRedundant option, closed symbols: optimized without the ModRedundant option); the total energies were plotted.

Table S2.

Entry		Imaginary number	Sum of electronic and thermal free energies (Hartree)	Sum of electronic and thermal free energies (kcal/mol)
1	**DFT-*meso*-2aI**	0	–2108.346635	–1323008.597
2	**DFT-*meso*-2aII**	0	–2108.342237	–1323005.837
3	**DFT-*meso*-2aIII**	1	–2108.320147	–1322991.975
4	**DFT-*dl*-2aI**	0	–2108.342354	–1323005.911
5	**DFT-radical-1a**	0	–2108.309404	–1322985.234
6	**DFT-*meso*-2cI**	0	–1725.044936	–1082482.948
7	**DFT-*dl*-2cI**	0	–1725.047331	–1082484.451
8	**DFT-radical-2a**	0	–1724.99026	–1082448.638

Cartesian coordinates (in Å) and energy of DFT-*meso*-2aI

E(RM062X) =: –2108.99501534 au

Center number	Atomic number	Atomic type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.322398	-0.419994	1.121602
2	8	0	-0.956487	3.707605	1.504102
3	8	0	-2.317892	1.969508	1.034102
4	8	0	0.106895	-2.891598	-1.166698
5	8	0	-3.439699	-0.780089	-1.774498
6	8	0	-2.504204	-2.575791	-0.775098
7	7	0	-0.136893	1.574803	1.346002
8	7	0	-1.167700	-1.009895	-1.656398
9	6	0	-0.297297	0.197203	1.086002
10	6	0	1.093402	-0.387601	0.731202
11	6	0	1.999805	0.794897	0.975802
12	6	0	1.241208	1.916799	1.314102
13	6	0	1.831511	3.159998	1.492802
14	1	0	1.239213	4.022399	1.754202
15	6	0	3.206811	3.258994	1.292602
16	1	0	3.681014	4.226693	1.419002
17	6	0	3.988109	2.163292	0.928802
18	6	0	3.365505	0.921794	0.772302
19	1	0	3.956203	0.065292	0.465002
20	6	0	-1.166190	2.538305	1.312402
21	6	0	-3.569990	2.727712	1.033202
22	6	0	-4.591693	1.639614	0.735502
23	1	0	-5.586192	2.079017	0.635002
24	1	0	-4.604395	0.906114	1.543902
25	1	0	-4.326494	1.123714	-0.190398
26	6	0	-3.549387	3.772712	-0.074598

27	1	0	-4.515586	4.282214	-0.098398
28	1	0	-3.390888	3.287311	-1.038498
29	1	0	-2.766485	4.511710	0.092002
30	6	0	-3.798488	3.345212	2.407702
31	1	0	-4.810787	3.752815	2.450002
32	1	0	-3.086686	4.145210	2.606302
33	1	0	-3.704690	2.578912	3.180502
34	6	0	1.365699	-1.614601	1.605402
35	6	0	2.551898	-1.726504	2.334502
36	1	0	3.280800	-0.930006	2.317402
37	6	0	2.818895	-2.853205	3.103902
38	1	0	3.750195	-2.912707	3.654402
39	6	0	1.898493	-3.890003	3.170002
40	1	0	2.107690	-4.771803	3.764002
41	6	0	0.699193	-3.776099	2.476602
42	1	0	-0.037309	-4.569298	2.529602
43	6	0	0.428596	-2.651199	1.707902
44	1	0	-0.516204	-2.590396	1.188602
45	6	0	5.475009	2.294888	0.722402
46	1	0	6.020708	2.009387	1.625902
47	1	0	5.749512	3.322187	0.478502
48	1	0	5.813207	1.645787	-0.087698
49	6	0	-0.011802	-1.706698	-1.218398
50	6	0	1.071701	-0.655200	-0.883498
51	6	0	0.486504	0.587501	-1.532298
52	6	0	-0.837796	0.345305	-1.903398
53	6	0	-1.641594	1.352307	-2.418398
54	1	0	-2.658694	1.148309	-2.715498
55	6	0	-1.095190	2.629505	-2.517798
56	1	0	-1.712488	3.432507	-2.907398
57	6	0	0.212511	2.912702	-2.127698
58	6	0	1.008208	1.869200	-1.651098
59	1	0	2.026208	2.081197	-1.342098
60	6	0	-2.487801	-1.429491	-1.426198
61	6	0	-3.764305	-3.160388	-0.319798
62	6	0	-3.286709	-4.376389	0.462202
63	1	0	-4.144310	-4.962587	0.798102
64	1	0	-2.711708	-4.060391	1.335302
65	1	0	-2.650210	-4.999791	-0.167998
66	6	0	-4.599806	-3.577386	-1.523898
67	1	0	-5.491808	-4.103483	-1.176698
68	1	0	-4.025708	-4.252687	-2.161798
69	1	0	-4.909304	-2.709185	-2.103998
70	6	0	-4.496403	-2.182186	0.593102
71	1	0	-5.281904	-2.718984	1.130402
72	1	0	-4.946401	-1.368785	0.026402
73	1	0	-3.796502	-1.762088	1.319602
74	6	0	2.432200	-1.125204	-1.378098
75	6	0	3.172302	-0.382606	-2.299498
76	1	0	2.761904	0.521895	-2.725498
77	6	0	4.440401	-0.796209	-2.695798
78	1	0	4.995902	-0.201211	-3.410998
79	6	0	4.987798	-1.965411	-2.183898
80	1	0	5.977397	-2.285313	-2.487698
81	6	0	4.241496	-2.734709	-1.298098
82	1	0	4.641693	-3.665410	-0.913398
83	6	0	2.972797	-2.327405	-0.904398
84	1	0	2.398995	-2.954904	-0.238298

85	6	0	0.744114	4.321700	-2.149798
86	1	0	1.823514	4.334698	-2.308898
87	1	0	0.544015	4.809401	-1.190498
88	1	0	0.270716	4.913902	-2.934498

Cartesian coordinates (in Å) and energy of DFT-*meso*-2aII

E(RM062X) = –2108.98893808 au

Center number	Atomic number	Atomic type	Coordinates (Angstroms) X	Y	Z
1	8	0	2.596035	1.291029	0.122791
2	7	0	2.192305	-0.670136	-1.053181
3	6	0	1.028027	-1.329227	-1.522210
4	6	0	0.921363	-2.601998	-2.064925
5	1	0	1.783518	-3.245161	-2.149579
6	6	0	-0.340217	-3.030963	-2.460305
7	6	0	-1.470829	-2.226183	-2.324831
8	6	0	-1.326785	-0.947908	-1.784823
9	1	0	-2.211113	-0.330681	-1.670168
10	6	0	-0.075884	-0.492050	-1.383496
11	6	0	0.339421	0.798606	-0.695707
12	6	0	1.854485	0.574470	-0.486530
13	8	0	-2.554642	1.482167	0.004571
14	7	0	-2.252825	-0.525023	1.129862
15	6	0	-1.146775	-1.207081	1.696119
16	6	0	-1.125829	-2.460676	2.286129
17	1	0	-2.038550	-3.013261	2.447356
18	6	0	0.110503	-2.978121	2.660755
19	1	0	0.149561	-3.963924	3.111350
20	6	0	1.295183	-2.273566	2.466140
21	6	0	1.232645	-0.997699	1.900613
22	1	0	2.155462	-0.443792	1.766775
23	6	0	0.014603	-0.458491	1.507263
24	6	0	-0.318258	0.835928	0.778855
25	6	0	-1.844305	0.697035	0.564443
26	6	0	-0.034959	2.116650	1.572951
27	6	0	0.889710	2.130802	2.618375
28	6	0	-0.702803	3.308310	1.265516
29	6	0	1.156078	3.298843	3.322592
30	1	0	1.409838	1.227178	2.898677
31	6	0	-0.439050	4.473728	1.974691
32	1	0	-1.426945	3.329624	0.463390
33	6	0	0.494934	4.477550	3.002719
34	1	0	1.881100	3.280717	4.127475
35	1	0	-0.968216	5.382434	1.713439
36	1	0	0.702004	5.387970	3.552756
37	6	0	0.135216	2.076538	-1.516495
38	6	0	-0.787540	2.131429	-2.561981
39	6	0	0.880483	3.226673	-1.229115
40	6	0	-0.975538	3.301841	-3.287619
41	1	0	-1.365636	1.258504	-2.826564
42	6	0	0.694591	4.393565	-1.959238
43	1	0	1.603025	3.213776	-0.424817
44	6	0	-0.237056	4.439531	-2.988738

45	1	0	-1.700502	3.318214	-4.092596
46	1	0	1.281857	5.270477	-1.713534
47	1	0	-0.382984	5.351516	-3.555459
48	6	0	3.434035	-1.313932	-0.889510
49	8	0	3.543074	-2.511493	-0.854534
50	8	0	4.401773	-0.424096	-0.808778
51	6	0	5.754031	-0.815563	-0.409575
52	6	0	6.457928	0.529004	-0.297697
53	6	0	5.711320	-1.516846	0.943551
54	6	0	6.382734	-1.680758	-1.494486
55	1	0	7.495833	0.381377	0.006420
56	1	0	6.439653	1.044511	-1.259163
57	1	0	5.950318	1.154595	0.438142
58	1	0	6.729393	-1.620091	1.324550
59	1	0	5.138593	-0.914419	1.653387
60	1	0	5.264509	-2.506993	0.868279
61	1	0	7.431442	-1.860044	-1.246775
62	1	0	5.871317	-2.638152	-1.579527
63	1	0	6.340466	-1.163198	-2.455110
64	6	0	-3.546566	-1.073418	1.072441
65	8	0	-3.935745	-1.891022	1.861537
66	8	0	-4.210229	-0.591763	0.036265
67	6	0	-5.662809	-0.754974	-0.064759
68	6	0	-5.994742	0.072768	-1.298247
69	6	0	-6.018882	-2.221989	-0.272144
70	6	0	-6.325155	-0.167221	1.175893
71	1	0	-7.073829	0.080001	-1.462145
72	1	0	-5.641511	1.096344	-1.164739
73	1	0	-5.510689	-0.348811	-2.181739
74	1	0	-7.086808	-2.299709	-0.489149
75	1	0	-5.467055	-2.627717	-1.122736
76	1	0	-5.793362	-2.812033	0.614197
77	1	0	-7.407853	-0.164100	1.034759
78	1	0	-6.092048	-0.751529	2.065326
79	1	0	-5.991689	0.862599	1.321715
80	6	0	2.631807	-2.881613	2.802982
81	1	0	3.099073	-3.279099	1.897078
82	1	0	2.527190	-3.698033	3.518541
83	1	0	3.309762	-2.138638	3.228242
84	1	0	-0.447271	-4.026951	-2.877595
85	6	0	-2.830224	-2.731720	-2.735366
86	1	0	-3.118298	-3.601510	-2.138788
87	1	0	-3.587549	-1.959346	-2.592923
88	1	0	-2.839821	-3.032738	-3.785718

Cartesian coordinates (in Å) and energy of DFT-*meso*-2aIII

E(RM062X) =: –2108.96791484 au

Center number	Atomic number	Atomic type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.148260	0.227733	-2.724264
2	8	0	-1.549086	-3.331429	-1.213532
3	8	0	-2.203437	-1.228520	-1.735387
4	8	0	-1.096090	1.864600	-0.653139

5	8	0	-3.342371	-0.237880	2.150449
6	8	0	-3.348959	1.381252	0.584844
7	7	0	-0.064612	-1.591028	-1.269744
8	7	0	-1.423556	0.292846	1.032643
9	6	0	0.362125	-0.339370	-1.811943
10	6	0	1.572297	0.072999	-0.952009
11	6	0	2.098046	-1.309869	-0.587679
12	6	0	1.053417	-2.234307	-0.685708
13	6	0	1.201612	-3.548220	-0.283185
14	1	0	0.379824	-4.244388	-0.350725
15	6	0	2.458282	-3.936431	0.187705
16	1	0	2.597912	-4.962563	0.510965
17	6	0	3.540407	-3.063416	0.217883
18	6	0	3.348277	-1.735757	-0.187200
19	1	0	4.185376	-1.047629	-0.164958
20	6	0	-1.331681	-2.165916	-1.413416
21	6	0	-3.578053	-1.557309	-2.106211
22	6	0	-4.115587	-0.195079	-2.521919
23	1	0	-5.182936	-0.261858	-2.744672
24	1	0	-3.583752	0.160501	-3.406121
25	1	0	-3.947614	0.523534	-1.717847
26	6	0	-4.314853	-2.113209	-0.893757
27	1	0	-5.377546	-2.208563	-1.130475
28	1	0	-4.213950	-1.439974	-0.040131
29	1	0	-3.926217	-3.092267	-0.617050
30	6	0	-3.584211	-2.530119	-3.279445
31	1	0	-4.604924	-2.622558	-3.657095
32	1	0	-3.228785	-3.515596	-2.981938
33	1	0	-2.953540	-2.145689	-4.084064
34	6	0	2.631507	0.918695	-1.632672
35	6	0	3.744035	1.330347	-0.887264
36	1	0	3.795678	1.103506	0.171283
37	6	0	4.761718	2.074111	-1.463189
38	1	0	5.602823	2.390001	-0.857706
39	6	0	4.691037	2.424777	-2.807968
40	1	0	5.479841	3.012371	-3.262326
41	6	0	3.599633	2.015741	-3.559811
42	1	0	3.532611	2.280662	-4.608376
43	6	0	2.576859	1.266654	-2.982013
44	1	0	1.730429	0.975664	-3.585627
45	6	0	4.900257	-3.513606	0.688413
46	1	0	5.653390	-3.364284	-0.088949
47	1	0	4.894498	-4.571498	0.954143
48	1	0	5.218038	-2.946553	1.568054
49	6	0	-0.662102	1.087595	0.137987
50	6	0	0.853891	0.788197	0.401524
51	6	0	0.768519	-0.191422	1.544633
52	6	0	-0.558372	-0.513362	1.822482
53	6	0	-0.884568	-1.501395	2.742342
54	1	0	-1.912492	-1.754393	2.944822
55	6	0	0.160200	-2.147080	3.396582
56	1	0	-0.077516	-2.932223	4.106450
57	6	0	1.496435	-1.813525	3.178070
58	6	0	1.785780	-0.812024	2.253513
59	1	0	2.819343	-0.542774	2.067513
60	6	0	-2.791065	0.434404	1.317171
61	6	0	-4.665723	1.921694	0.941695
62	6	0	-4.838066	3.043809	-0.072709

63	1	0	-5.789850	3.551006	0.096585
64	1	0	-4.826535	2.644434	-1.088226
65	1	0	-4.024696	3.764713	0.021251
66	6	0	-4.615083	2.478276	2.360358
67	1	0	-5.542597	3.017486	2.563705
68	1	0	-3.782685	3.178743	2.457248
69	1	0	-4.505896	1.682942	3.096380
70	6	0	-5.756851	0.869292	0.781121
71	1	0	-6.725748	1.345061	0.950771
72	1	0	-5.632582	0.057826	1.495970
73	1	0	-5.751271	0.463370	-0.232048
74	6	0	1.462367	2.147400	0.755151
75	6	0	2.037622	2.392453	2.000536
76	1	0	2.041146	1.623406	2.761387
77	6	0	2.609110	3.630563	2.286492
78	1	0	3.057065	3.797906	3.259022
79	6	0	2.597548	4.642702	1.338185
80	1	0	3.046145	5.604132	1.558502
81	6	0	1.991175	4.417605	0.105017
82	1	0	1.962475	5.203715	-0.639864
83	6	0	1.426685	3.185448	-0.184018
84	1	0	0.960883	3.018792	-1.146590
85	6	0	2.610169	-2.556114	3.869499
86	1	0	3.469424	-1.905897	4.045253
87	1	0	2.946830	-3.392428	3.248600
88	1	0	2.283406	-2.958800	4.829366

Cartesian coordinates (in Å) and energy of DFT-*dl*-2aI

E(RM062X) =: –2108.98893808 au

Center number	Atomic number	Atomic type	Coordinates (Angstroms) X	Y	Z
1	8	0	2.596035	1.291029	0.122791
2	7	0	2.192305	-0.670136	-1.053181
3	6	0	1.028027	-1.329227	-1.522210
4	6	0	0.921363	-2.601998	-2.064925
5	1	0	1.783518	-3.245161	-2.149579
6	6	0	-0.340217	-3.030963	-2.460305
7	6	0	-1.470829	-2.226183	-2.324831
8	6	0	-1.326785	-0.947908	-1.784823
9	1	0	-2.211113	-0.330681	-1.670168
10	6	0	-0.075884	-0.492050	-1.383496
11	6	0	0.339421	0.798606	-0.695707
12	6	0	1.854485	0.574470	-0.486530
13	8	0	-2.554642	1.482167	0.004571
14	7	0	-2.252825	-0.525023	1.129862
15	6	0	-1.146775	-1.207081	1.696119
16	6	0	-1.125829	-2.460676	2.286129
17	1	0	-2.038550	-3.013261	2.447356
18	6	0	0.110503	-2.978121	2.660755
19	1	0	0.149561	-3.963924	3.111350
20	6	0	1.295183	-2.273566	2.466140
21	6	0	1.232645	-0.997699	1.900613
22	1	0	2.155462	-0.443792	1.766775

23	6	0	0.014603	-0.458491	1.507263
24	6	0	-0.318258	0.835928	0.778855
25	6	0	-1.844305	0.697035	0.564443
26	6	0	-0.034959	2.116650	1.572951
27	6	0	0.889710	2.130802	2.618375
28	6	0	-0.702803	3.308310	1.265516
29	6	0	1.156078	3.298843	3.322592
30	1	0	1.409838	1.227178	2.898677
31	6	0	-0.439050	4.473728	1.974691
32	1	0	-1.426945	3.329624	0.463390
33	6	0	0.494934	4.477550	3.002719
34	1	0	1.881100	3.280717	4.127475
35	1	0	-0.968216	5.382434	1.713439
36	1	0	0.702004	5.387970	3.552756
37	6	0	0.135216	2.076538	-1.516495
38	6	0	-0.787540	2.131429	-2.561981
39	6	0	0.880483	3.226673	-1.229115
40	6	0	-0.975538	3.301841	-3.287619
41	1	0	-1.365636	1.258504	-2.826564
42	6	0	0.694591	4.393565	-1.959238
43	1	0	1.603025	3.213776	-0.424817
44	6	0	-0.237056	4.439531	-2.988738
45	1	0	-1.700502	3.318214	-4.092596
46	1	0	1.281857	5.270477	-1.713534
47	1	0	-0.382984	5.351516	-3.555459
48	6	0	3.434035	-1.313932	-0.889510
49	8	0	3.543074	-2.511493	-0.854534
50	8	0	4.401773	-0.424096	-0.808778
51	6	0	5.754031	-0.815563	-0.409575
52	6	0	6.457928	0.529004	-0.297697
53	6	0	5.711320	-1.516846	0.943551
54	6	0	6.382734	-1.680758	-1.494486
55	1	0	7.495833	0.381377	0.006420
56	1	0	6.439653	1.044511	-1.259163
57	1	0	5.950318	1.154595	0.438142
58	1	0	6.729393	-1.620091	1.324550
59	1	0	5.138593	-0.914419	1.653387
60	1	0	5.264509	-2.506993	0.868279
61	1	0	7.431442	-1.860044	-1.246775
62	1	0	5.871317	-2.638152	-1.579527
63	1	0	6.340466	-1.163198	-2.455110
64	6	0	-3.546566	-1.073418	1.072441
65	8	0	-3.935745	-1.891022	1.861537
66	8	0	-4.210229	-0.591763	0.036265
67	6	0	-5.662809	-0.754974	-0.064759
68	6	0	-5.994742	0.072768	-1.298247
69	6	0	-6.018882	-2.221989	-0.272144
70	6	0	-6.325155	-0.167221	1.175893
71	1	0	-7.073829	0.080001	-1.462145
72	1	0	-5.641511	1.096344	-1.164739
73	1	0	-5.510689	-0.348811	-2.181739
74	1	0	-7.086808	-2.299709	-0.489149
75	1	0	-5.467055	-2.627717	-1.122736
76	1	0	-5.793362	-2.812033	0.614197
77	1	0	-7.407853	-0.164100	1.034759
78	1	0	-6.092048	-0.751529	2.065326
79	1	0	-5.991689	0.862599	1.321715
80	6	0	2.631807	-2.881613	2.802982

81	1	0	3.099073	-3.279099	1.897078
82	1	0	2.527190	-3.698033	3.518541
83	1	0	3.309762	-2.138638	3.228242
84	1	0	-0.447271	-4.026951	-2.877595
85	6	0	-2.830224	-2.731720	-2.735366
86	1	0	-3.118298	-3.601510	-2.138788
87	1	0	-3.587549	-1.959346	-2.592923
88	1	0	-2.839821	-3.032738	-3.785718

Cartesian coordinates (in Å) and energy of DFT-radical-1aI

E(UM062X) = –1054.46183895 au

Center number	Atomic number	Atomic type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.522694	-1.966766	-0.059379
2	8	0	2.812940	1.553007	0.153726
3	8	0	2.841933	-0.695507	-0.022600
4	7	0	0.867679	0.367130	-0.000311
5	6	0	0.086751	-0.843940	-0.046892
6	6	0	-1.318386	-0.411621	-0.048325
7	6	0	-1.338592	1.002665	-0.042852
8	6	0	0.000205	1.471550	-0.001974
9	6	0	0.280570	2.830379	0.003519
10	1	0	1.297019	3.187122	0.044045
11	6	0	-0.793749	3.712059	-0.051588
12	1	0	-0.588579	4.777672	-0.049007
13	6	0	-2.131219	3.284551	-0.131866
14	6	0	-2.396560	1.927530	-0.132166
15	1	0	-3.415798	1.573504	-0.229784
16	6	0	2.262895	0.486426	0.053658
17	6	0	4.297668	-0.821056	0.044852
18	6	0	4.493314	-2.326610	-0.065035
19	1	0	5.556989	-2.568109	-0.018667
20	1	0	4.084833	-2.691163	-1.008821
21	1	0	3.974151	-2.832247	0.750527
22	6	0	4.805539	-0.304549	1.386455
23	1	0	5.867111	-0.543813	1.479918
24	1	0	4.270784	-0.796576	2.201908
25	1	0	4.679619	0.773425	1.471522
26	6	0	4.940001	-0.100362	-1.134900
27	1	0	6.007791	-0.329928	-1.152510
28	1	0	4.811990	0.977959	-1.058163
29	1	0	4.498921	-0.451036	-2.070589
30	6	0	-2.428049	-1.344010	-0.001727
31	6	0	-3.612509	-1.012400	0.677744
32	1	0	-3.673516	-0.072766	1.212825
33	6	0	-4.675926	-1.900600	0.721028
34	1	0	-5.576492	-1.634561	1.261391
35	6	0	-4.581223	-3.135881	0.086570
36	1	0	-5.413574	-3.828521	0.119137
37	6	0	-3.407981	-3.482668	-0.577271
38	1	0	-3.325995	-4.446706	-1.064867
39	6	0	-2.336664	-2.603608	-0.618074

40	1	0	-1.422564	-2.878286	-1.126115
41	6	0	-3.238927	4.302070	-0.221704
42	1	0	-4.209046	3.819400	-0.343380
43	1	0	-3.084425	4.973314	-1.069573
44	1	0	-3.276469	4.915987	0.681703

Cartesian coordinates (in Å) and energy of DFT-*meso*-2cI

E(RM062X) = –1725.59386620 au

Center number	Atomic number	Atomic type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.770085	-0.345911	-1.677560
2	8	0	-1.746409	2.915320	-0.946123
3	8	0	0.385838	2.167554	-0.891558
4	8	0	1.449097	-3.188663	0.098255
5	8	0	3.228047	0.412958	1.307696
6	8	0	3.486944	-1.503274	0.145789
7	7	0	-1.268624	0.693043	-1.187565
8	7	0	1.503272	-1.068986	1.090372
9	6	0	-0.371703	-0.394662	-1.324459
10	6	0	-1.127229	-1.672357	-0.919644
11	6	0	-2.553800	-1.191947	-0.901823
12	6	0	-2.588224	0.199415	-1.013805
13	6	0	-3.785720	0.895185	-0.949216
14	1	0	-3.805895	1.971247	-1.025108
15	6	0	-4.954413	0.153321	-0.780408
16	1	0	-5.900205	0.682039	-0.723125
17	6	0	-4.954909	-1.238974	-0.704517
18	6	0	-3.729244	-1.909645	-0.770270
19	1	0	-3.705104	-2.993647	-0.716915
20	6	0	-0.920034	2.042505	-1.005471
21	6	0	1.016822	3.488005	-0.826480
22	6	0	2.495254	3.131158	-0.782930
23	1	0	3.095455	4.041695	-0.726051
24	1	0	2.770580	2.576910	-1.682359
25	1	0	2.706849	2.503150	0.085359
26	6	0	0.592066	4.210821	0.445481
27	1	0	1.150289	5.146808	0.522187
28	1	0	0.825999	3.595157	1.315239
29	1	0	-0.473948	4.433551	0.438006
30	6	0	0.678029	4.280402	-2.083952
31	1	0	1.277730	5.193038	-2.098814
32	1	0	-0.376186	4.552825	-2.111752
33	1	0	0.924274	3.693895	-2.971916
34	6	0	-0.860003	-2.796084	-1.917977
35	6	0	-6.248163	-2.004891	-0.592309
36	1	0	-6.673576	-2.192900	-1.582080
37	1	0	-6.987094	-1.446347	-0.015689
38	1	0	-6.095794	-2.970640	-0.108024
39	6	0	0.896112	-2.215101	0.513624
40	6	0	-0.629844	-2.007939	0.559200
41	6	0	-0.755512	-0.791367	1.440740
42	6	0	0.505956	-0.239604	1.673287

43	6	0	0.646494	0.938283	2.390860
44	1	0	1.620499	1.363577	2.576609
45	6	0	-0.516146	1.559572	2.848046
46	1	0	-0.424638	2.492270	3.395183
47	6	0	-1.785916	1.028791	2.631387
48	6	0	-1.893185	-0.178179	1.933795
49	1	0	-2.873008	-0.611380	1.753247
50	6	0	2.817903	-0.633179	0.871725
51	6	0	4.830605	-1.193340	-0.340510
52	6	0	5.145678	-2.408362	-1.201757
53	1	0	6.151910	-2.319768	-1.615793
54	1	0	4.426974	-2.483873	-2.019285
55	1	0	5.083218	-3.318462	-0.603122
56	6	0	5.796272	-1.087708	0.833705
57	1	0	6.812198	-0.969780	0.449903
58	1	0	5.758772	-1.999668	1.433425
59	1	0	5.555024	-0.232098	1.462450
60	6	0	4.797361	0.076008	-1.185656
61	1	0	5.734355	0.156847	-1.741295
62	1	0	4.675815	0.964652	-0.568193
63	1	0	3.971092	0.021208	-1.898614
64	6	0	-1.292827	-3.259925	1.126505
65	6	0	-3.027084	1.754191	3.079472
66	1	0	-3.763255	1.060301	3.489974
67	1	0	-3.490054	2.264274	2.229350
68	1	0	-2.798590	2.502750	3.839026
69	1	0	-2.375767	-3.138026	1.169379
70	1	0	-1.040367	-4.134282	0.525842
71	1	0	-0.931597	-3.430712	2.142350
72	1	0	-1.424246	-3.690840	-1.651216
73	1	0	-1.180476	-2.478135	-2.911771
74	1	0	0.199841	-3.044266	-1.947915

Cartesian coordinates (in Å) and energy of DFT-*dl*-2c

E(RM062X) = –1725.59444943 au

Center number	Atomic number	Atomic type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.582421	-0.292328	2.324505
2	7	0	-2.106423	-1.101380	0.189601
3	6	0	-0.944953	-1.641855	-0.427814
4	6	0	-0.811760	-2.243325	-1.671031
5	1	0	-1.663127	-2.380593	-2.319618
6	6	0	0.459960	-2.672482	-2.040413
7	6	0	1.570091	-2.532420	-1.206351
8	6	0	1.400002	-1.930859	0.041962
9	1	0	2.254047	-1.805545	0.701880
10	6	0	0.147218	-1.473521	0.418337
11	6	0	-0.274956	-0.743971	1.670942
12	6	0	-1.799469	-0.656692	1.493298
13	8	0	2.582203	0.292165	2.324882
14	7	0	2.106459	1.101299	0.189900
15	6	0	0.945051	1.641899	-0.427538
16	6	0	0.811964	2.243595	-1.670644

17	1	0	1.663370	2.381061	-2.319123
18	6	0	-0.459758	2.672743	-2.040087
19	1	0	-0.588501	3.140859	-3.010766
20	6	0	-1.569992	2.532407	-1.206231
21	6	0	-1.400027	1.930576	0.041975
22	1	0	-2.254196	1.804876	0.701681
23	6	0	-0.147246	1.473334	0.418428
24	6	0	0.274826	0.743780	1.671011
25	6	0	1.799393	0.656608	1.493582
26	6	0	-0.049074	1.493281	2.964424
27	6	0	0.048696	-1.493724	2.964289
28	6	0	-3.360451	-1.040272	-0.435897
29	8	0	-3.652003	-1.736119	-1.371279
30	8	0	-4.112254	-0.108543	0.126077
31	6	0	-5.557035	-0.070452	-0.113858
32	6	0	-6.012530	1.027695	0.836143
33	6	0	-5.845173	0.299050	-1.563772
34	6	0	-6.169528	-1.410837	0.275156
35	1	0	-7.096699	1.142264	0.781465
36	1	0	-5.726583	0.777250	1.858928
37	1	0	-5.546577	1.978273	0.568651
38	1	0	-6.919743	0.456049	-1.683393
39	1	0	-5.332995	1.227561	-1.823487
40	1	0	-5.523371	-0.488295	-2.242761
41	1	0	-7.257798	-1.332455	0.230782
42	1	0	-5.849960	-2.203641	-0.400182
43	1	0	-5.882511	-1.667316	1.297453
44	6	0	3.360426	1.040236	-0.435685
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57	1	0	7.257723	1.332973	0.230841
58	1	0	5.849722	2.203939	-0.400055
59	1	0	5.882357	1.667434	1.297518
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61	1	0	-3.245072	2.494285	-2.557862
62	1	0	-2.912940	4.085193	-1.870987
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64	1	0	0.588853	-3.140376	-3.011180
65	6	0	2.926889	-3.015064	-1.650934
66	1	0	3.245152	-2.494656	-2.558079
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69	1	0	-0.258951	-2.536434	2.867019
70	1	0	1.118928	-1.457690	3.169845
71	1	0	-0.494529	-1.050118	3.799414
72	1	0	-1.119336	1.457130	3.169763
73	1	0	0.494075	1.049441	3.799476
74	1	0	0.258555	2.536022	2.867447

Cartesian coordinates (in Å) and energy of DFT-radical-1c

E(UM062X) = –862.752563917

Center number	Atomic number	Atomic type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.854919	2.430776	-0.011969
2	8	0	1.260244	-1.775027	-0.004748
3	8	0	2.330135	0.211952	0.000075
4	7	0	0.091121	0.185572	-0.005739
5	6	0	-0.042888	1.625083	-0.006529
6	6	0	-1.477497	1.889216	-0.002103
7	6	0	-2.152758	0.658607	-0.000022
8	6	0	-1.190716	-0.386331	-0.003405
9	6	0	-1.589650	-1.714715	-0.004263
10	1	0	-0.865308	-2.513478	-0.007120
11	6	0	-2.956960	-1.976452	-0.001644
12	1	0	-3.283655	-3.011452	-0.002540
13	6	0	-3.936925	-0.964752	0.001972
14	6	0	-3.526806	0.354667	0.002984
15	1	0	-4.254280	1.159659	0.006358
16	6	0	1.268602	-0.570774	-0.003752
17	6	0	3.678120	-0.355230	0.003644
18	6	0	4.549643	0.892860	0.006024
19	1	0	5.604322	0.611083	0.008900
20	1	0	4.336216	1.496091	0.889682
21	1	0	4.340948	1.496089	-0.878755
22	6	0	3.903486	-1.174553	-1.262132
23	1	0	4.956399	-1.459982	-1.318223
24	1	0	3.663747	-0.573649	-2.142197
25	1	0	3.293121	-2.076014	-1.265163
26	6	0	3.896345	-1.174333	1.270818
27	1	0	4.948633	-1.460915	1.332369
28	1	0	3.285096	-2.075215	1.271146
29	1	0	3.652838	-0.572900	2.149491
30	6	0	-2.030150	3.265307	0.006762
31	6	0	-5.396918	-1.337082	0.004568
32	1	0	-6.029463	-0.448879	0.005070
33	1	0	-5.646575	-1.931580	0.886714
34	1	0	-5.649291	-1.932472	-0.876201
35	1	0	-1.218471	3.986787	-0.086276
36	1	0	-2.735349	3.412295	-0.816166
37	1	0	-2.568727	3.464810	0.938678

References

Full author information for ref 14:

M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian 09, Revision E.01 (Gaussian, Inc.: Wallingford, CT, 2009).

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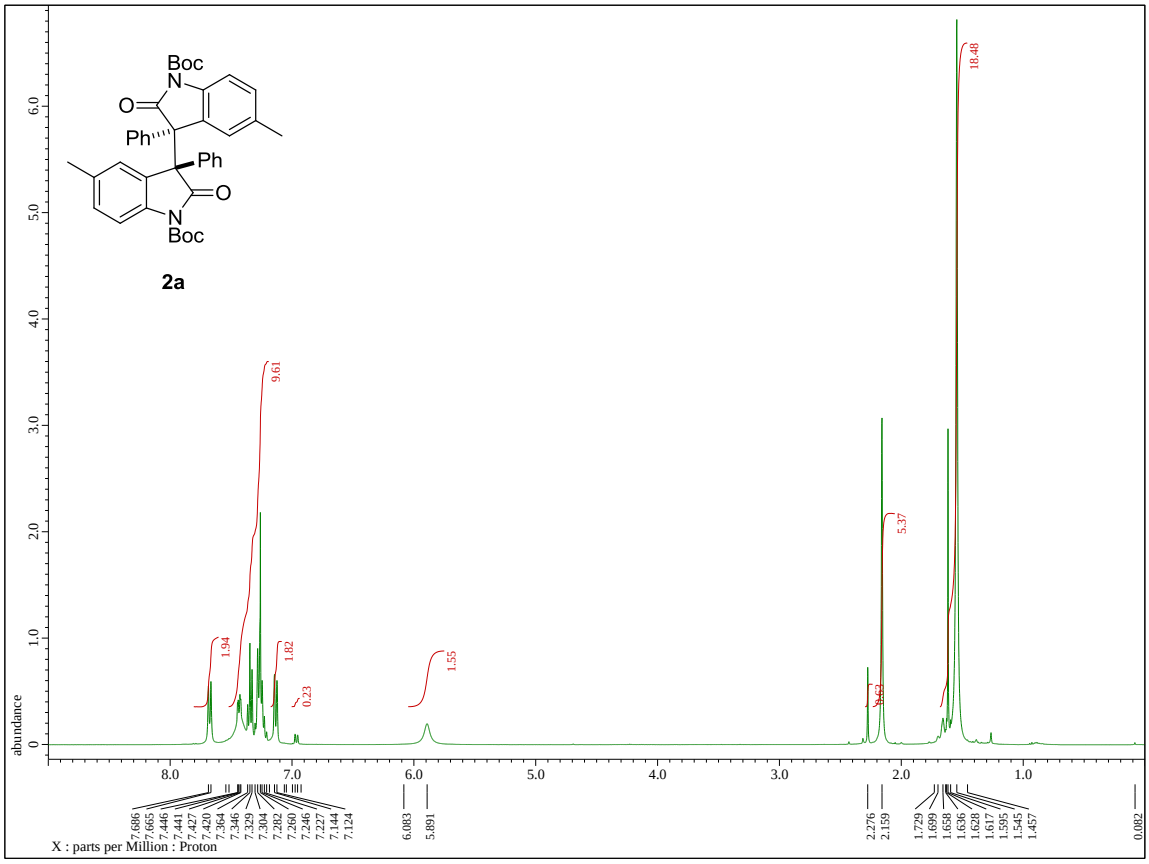
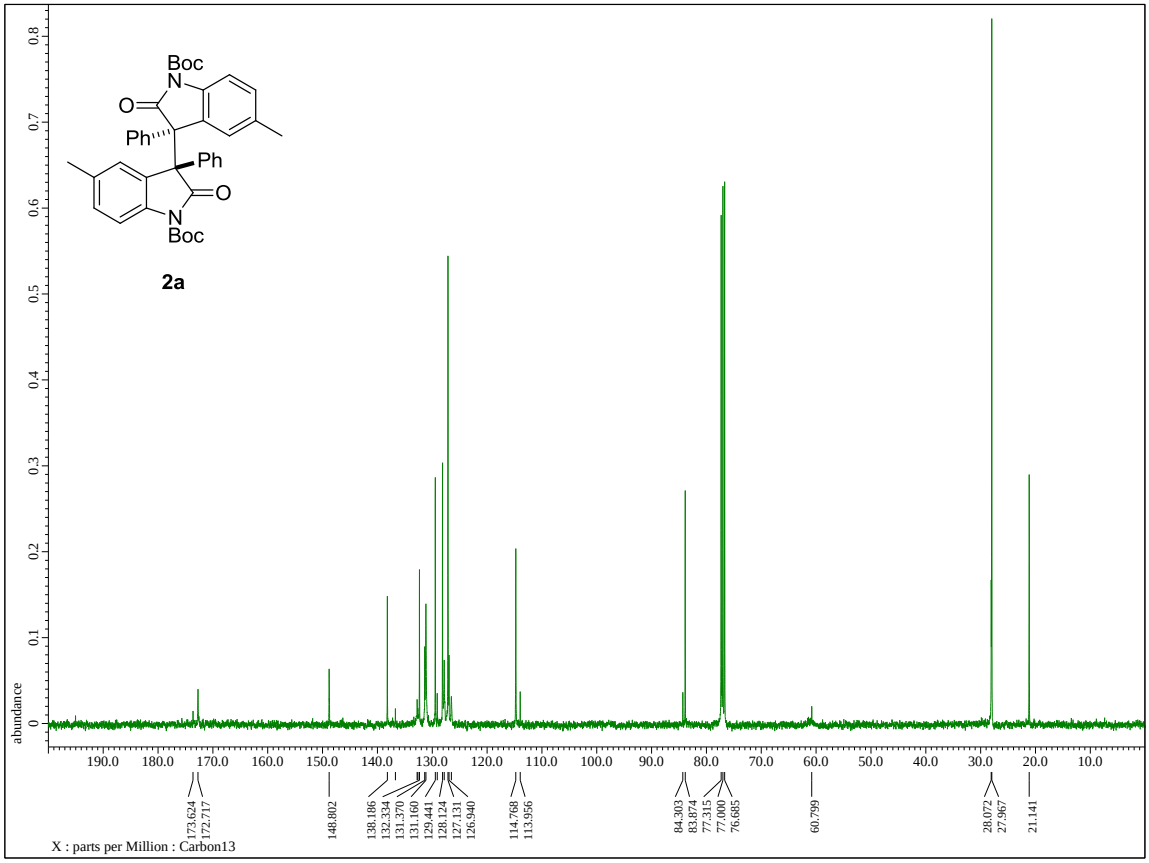
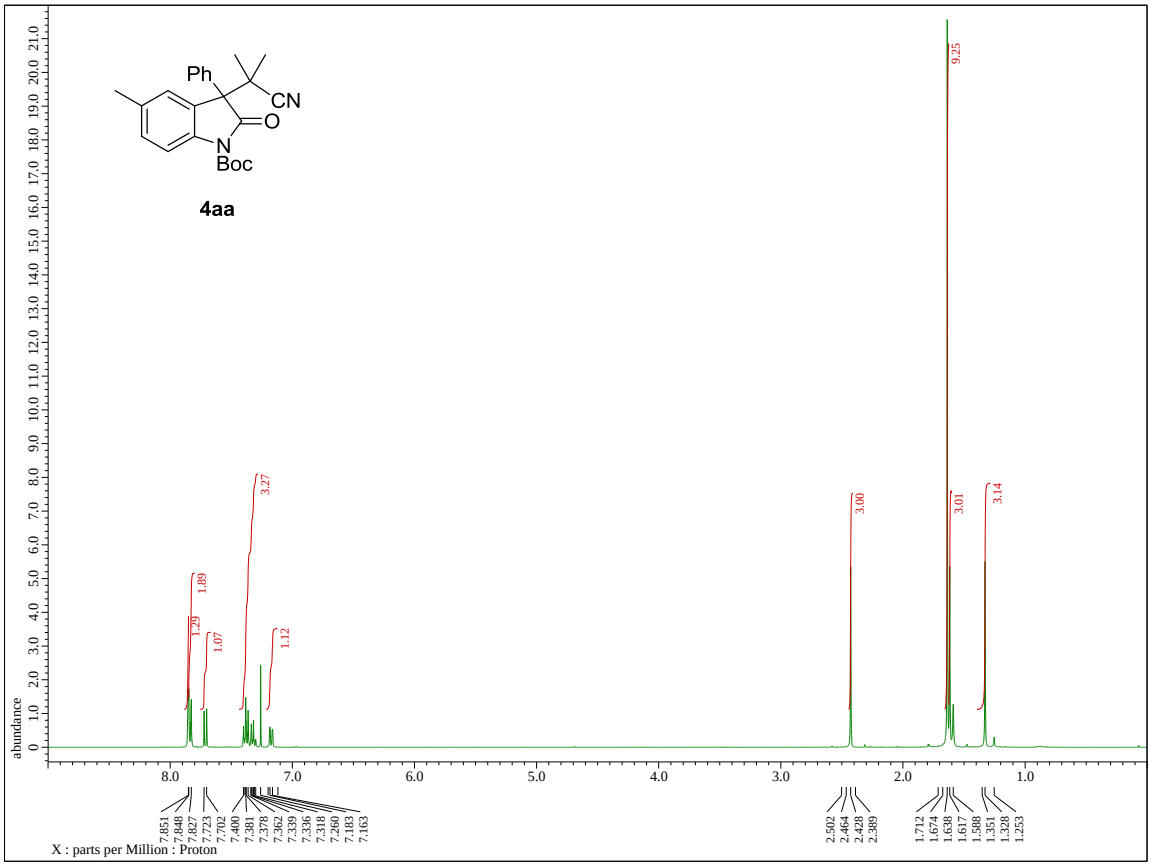
8. ^{1}H and ^{13}C NMR spectra



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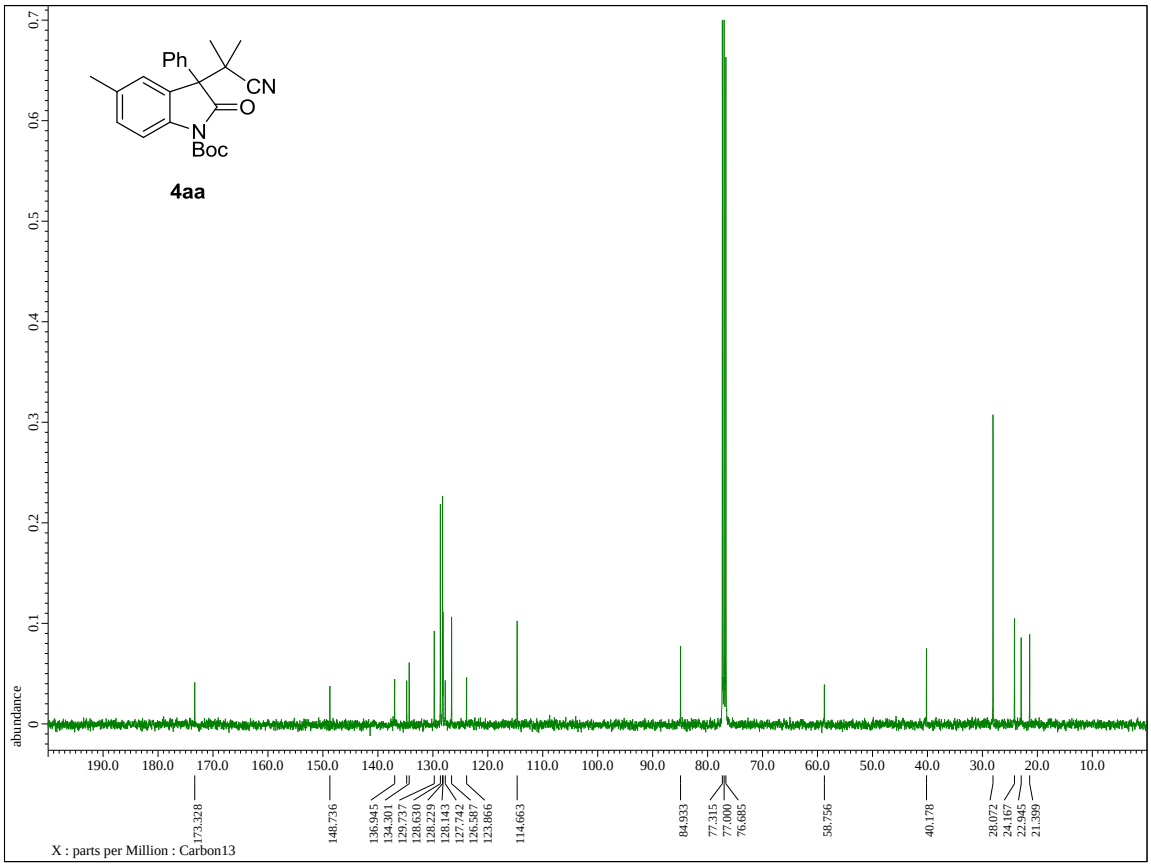
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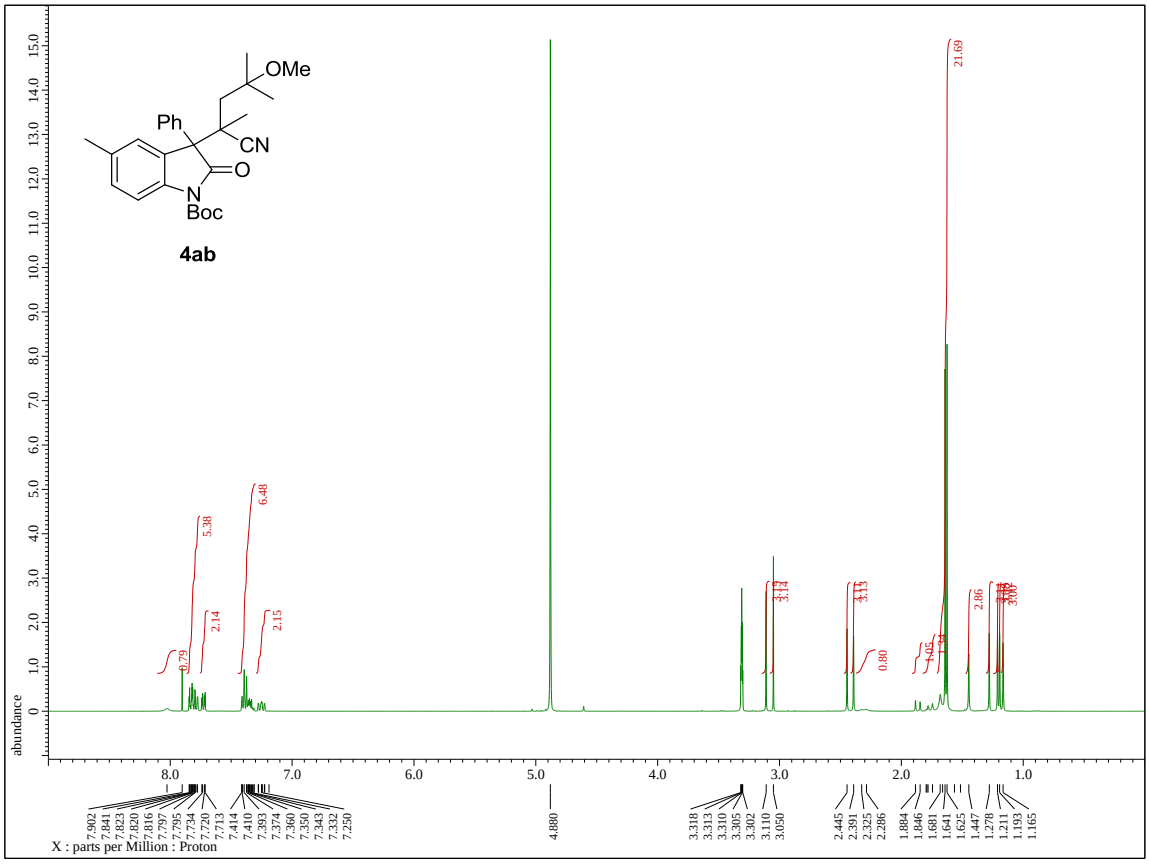
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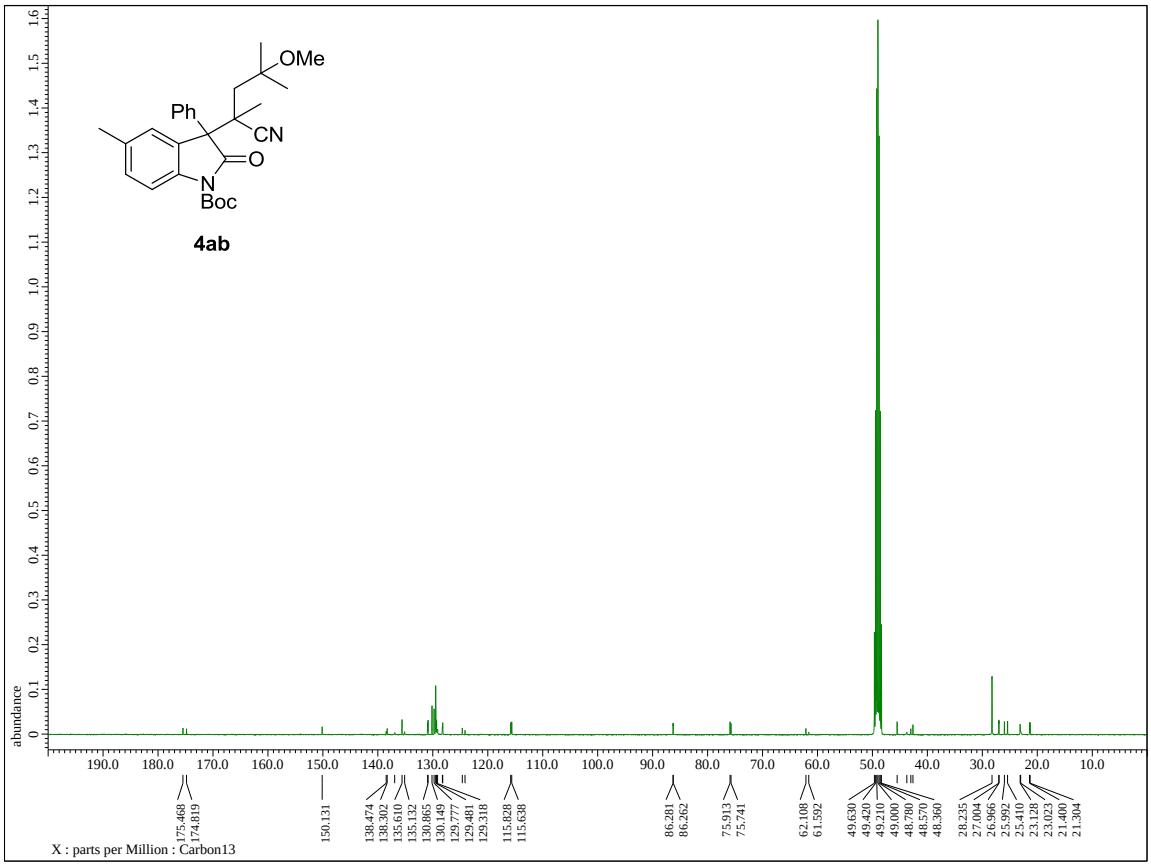
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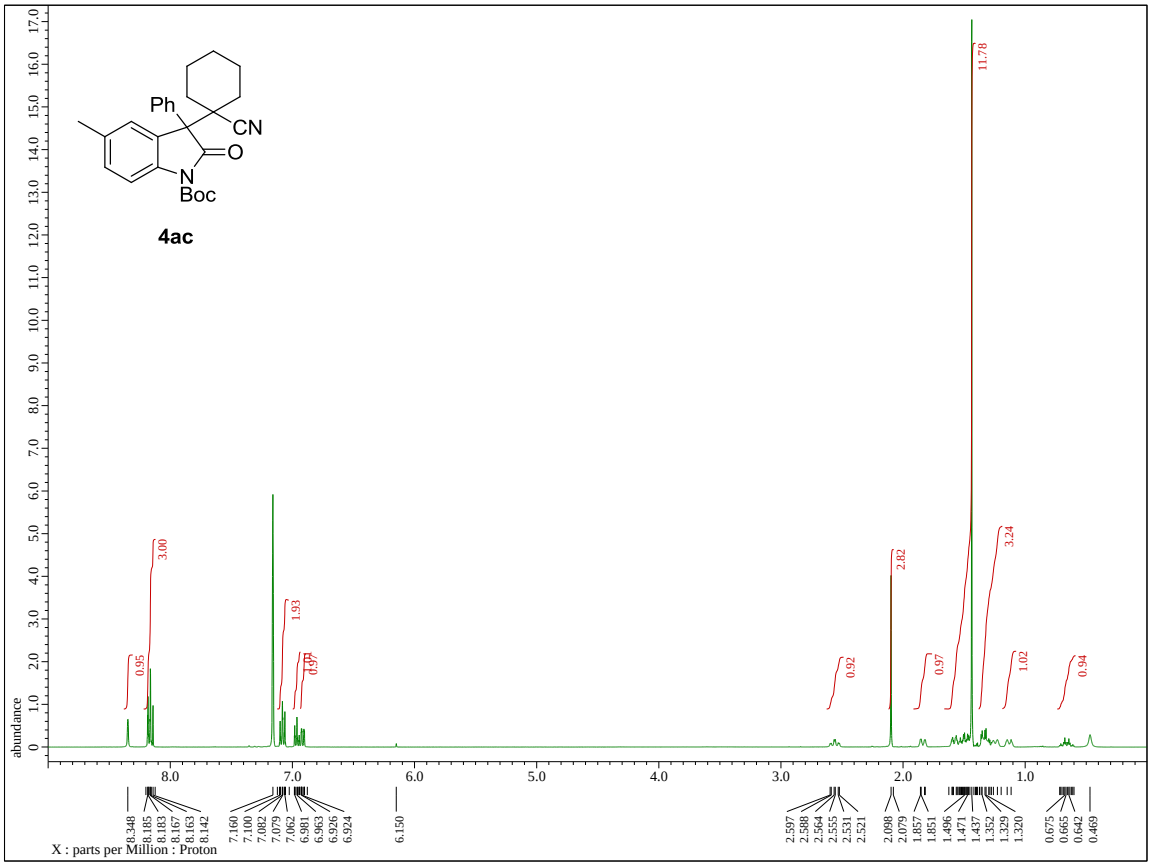
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O
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Boc
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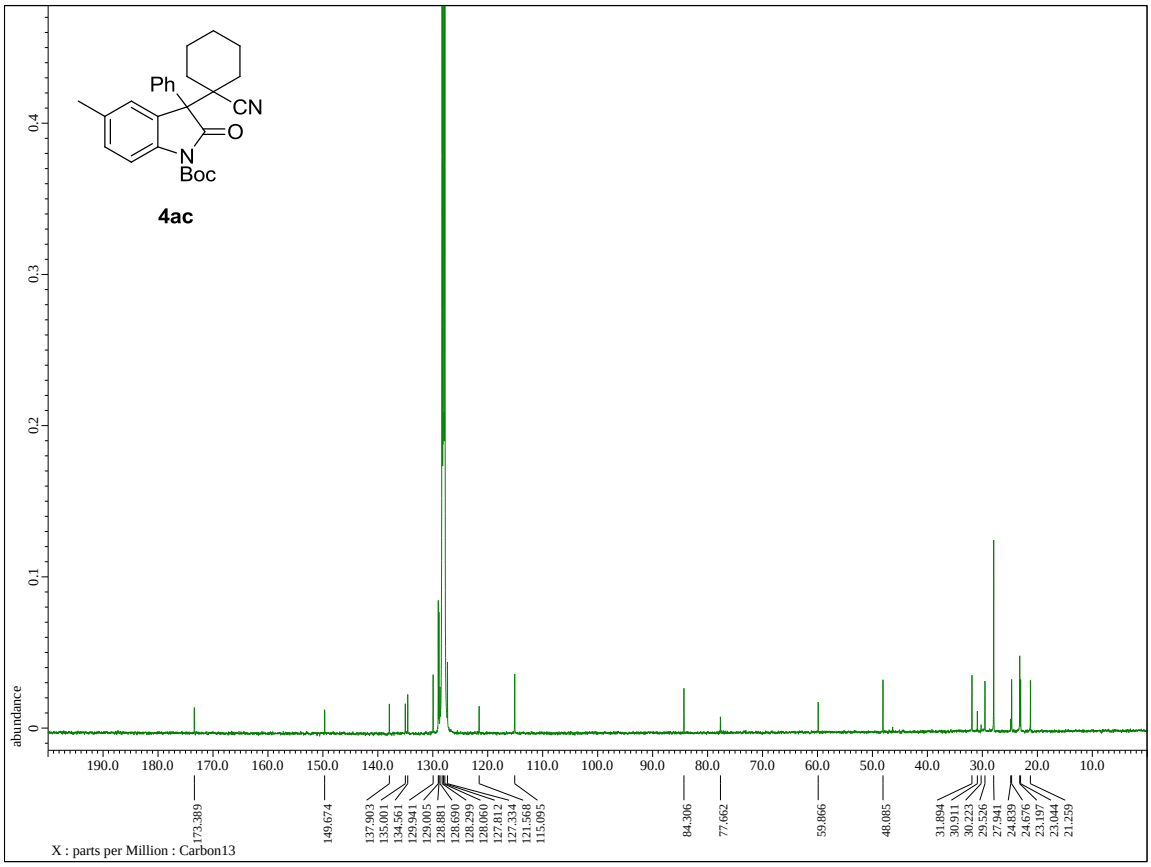
abundance
X : parts per Million : Proton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