Supplementary Material (ESI) for *Chemical Communications*

Supporting Information

for

Diindeno[1,2,3,4-*defg*;1',2',3',4'-*mnop*]chrysenes: Solution-Phase Synthesis and The Bowl-to-Bowl Inversion Barrier

Hung-Ing Chang,[a] Hsin-Ting Huang,[a] Cheng-Hao Huang,[b] Ming-Yu Kuo,[b] Yao-Ting Wu*[a]

[a]Department of Chemistry, National Cheng-Kung University, No.1 Ta-Hsueh Rd., 70101 Tainan, Taiwan

[b]Department of Applied Chemistry, National Chi Nan University, No. 1 University Rd., 54561 Puli, Nantou, Taiwan

E-mail: ytwuchem@mail.ncku.edu.tw

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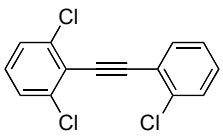
A. Synthetic Procedures and Analytic Data

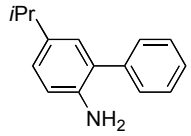
General:

^{1}H and ^{13}C NMR: Bruker 300 (300 and 75.5 MHz) and 500 (500 and 125 MHz). Melting points were determined with a Büchi melting point apparatus B545 and are uncorrected. $PdCl_2(PCy_3)_2$ was purchased from Strem Chemical. 1,3-Dichloro-2-ethynylbenzene was prepared from 1,3-dichloro-2-iodobenznene in 96% yield according to the published procedure.[S1] Other compounds, which are not mentioned in experimental section, are commercially available.

A.1. Synthesis of alkyne 8 and biphenyls 7

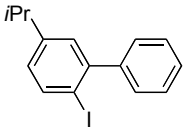


2,2',6-Trichlorodiphenylethyne (**8**): A mixture of 1-chloro-2-iodobenzene (5.02 g, 21.1 mmol), $Pd(PPh_3)_4$ (608.1 mg, 0.82 mmol) and bis(2,6-dichlorophenylethynyl)zinc, which was generated from 1,3-dichloro-2-ethynylbenzene (3.01 g, 17.5 mmol), THF (35 mL), *n*-butyllithium (7.7 mL, 2.50 M in hexane, 19.2 mmol) and $ZnBr_2$ (1.98 g, 8.79 mmol), was stirred at 50 ºC under nitrogen for 20 h. After cooling to room temperature and diluted with NH_4Cl aqueous solution (30 mL), the solution was extracted with CH_2Cl_2 (3 x 20 mL). The combined organic phases were dried over $MgSO_4$ and filtered. The solvents of the filtrate were removed under reduced pressure. The residue was subjected to chromatography on silica gel. Elution with hexane gave alkyne **8** (4.04 g, 82%) as white solids, m. p. 73.6–74.6 ºC. ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ = 7.15–7.39 (m, 5H), 7.45 (dd, *J* = 6.8, *J* = 1.6 Hz, 1H), 7.65 (dd, *J* = 6.8, *J* = 1.6 Hz, 1H). ^{13}C NMR (75.5 MHz, $CDCl_3$, plus DEPT, ppm): δ = 88.3 (C_{quat}), 96.4 (C_{quat}), 122.7 (C_{quat}), 123.0 (C_{quat}), 126.4 (CH), 127.5 (x 2, CH), 129.3 (CH), 129.4 (CH), 129.9 (CH), 133.7 (CH), 136.1 (C_{quat}), 137.4 (x 2, C_{quat}). EI MS (70 eV), *m*/*z* (%): 284/283/282/281/280 (42/20/99/20/100) [M^+], 210 (47), 174 (14). HRMS (EI) cacld for $C_{14}H_7Cl_3$: 279.9613; found: 279.9612.



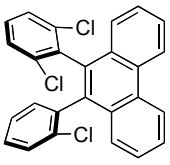
2-Amino-5-isopropylbiphenyl: Similar to Zhang's procedure,[S2] a mixture of $Pd(OAc)_2$ (31.5 mg, 0.14 mmol), Na_2CO_3 (1.48 g, 14.0 mmol), 2-bromo-4-isopropylaniline (1.50 g, 7.01 mmol), phenylbornic acid (1.28 g, 10.5 mmol), water (7 mL), and PEG 600 (7.01 g) in a thick-wall pyrex tube was purged with nitrogen for 5 min. The sealed tube was heated at 50 ºC for 10 h. After cooling to room temperature, the suspension was diluted with water and extracted with CH_2Cl_2 (50 mL). The

combined organic phases were dried over $MgSO_4$ and filtered. The solvents of the filtrate were removed under reduced pressure, and the residue was subjected to chromatography on alumina. Elution with hexane/CH_2Cl_2 (10:1) gave the title compound (1.37 g, 93%) as pale yellow solids, m.p. 39.5–40.4 ºC. ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ = 1.24 (d, *J* = 7.1 Hz, 6H), 2.85 (heptet, *J* = 7.1 Hz, 1H), 6.74 (d, *J* = 8.1 Hz, 1H), 7.01 (d, *J* = 1.8 Hz, 1H), 7.04 (dd, *J* = 8.1, *J* = 1.8 Hz, 1H), 7.34–7.37 (m, 1H), 7.42–7.50 (m, 4H). The signal of NH_2 was not observed. ^{13}C NMR (75.5 MHz, $CDCl_3$, plus DEPT, ppm): δ = 24.2 (x 2, CH_3), 33.3 (CH), 117.3 (CH), 126.4 (CH), 127.3 (CH), 128.5 (CH), 128.8 (x 2, CH), 129.2 (x 2, CH), 138.4 (C_{quat}), 139.2 (C_{quat}), 139.3 (C_{quat}), 141.2 (C_{quat}). EI MS (70 eV), *m*/*z* (%): 211 (37) [M^+], 196 (100), 180 (33), 165 (22), 152 (18). HRMS (EI) cacld for $C_{15}H_{17}N$: 211.1361; found: 211.1365.



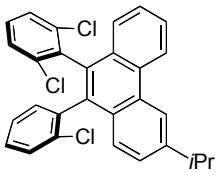
2-Iodo-5-isopropylbiphenyl (**7**-*i*Pr): A solution of 2-amino-5-isopropylbiphenyl (1.42 g, 6.63 mmol) at 0 ºC was treated with water (9 mL), *conc.* hydrochloric acid (1.8 mL), and finally dropwise added an aqueous solution of $NaNO_2$ (0.55 g in 6.5 mL of water), and stirred at the same temperature for 35 min. An aqueous solution of KI (2.20 g, 13.2 mmol) was then added and the mixture was stirred at room temperature for 12 h. The reaction was quenched with $Na_2S_2O_3$ aqueous solution and extracted with CH_2Cl_2. After drying over $MgSO_4$ and filtration, the solvents of the filtrate were removed under reduced pressure, and the residue was subjected to chromatography on silica gel. Elution with hexane gave **7**-*i*Pr (1.64 g, 78%) as colorless liquid. ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ = 1.27 (d, *J* = 6.8 Hz, 6H), 2.90 (heptet, *J* = 6.8 Hz, 1H), 6.93 (dd, *J* = 8.2, *J* = 2.2 Hz, 1H), 7.19 (d, *J* = 2.2 Hz, 1H), 7.35–7.44 (m, 5H), 7.86 (d, *J* = 8.2 Hz, 1H). ^{13}C NMR (75.5 MHz, $CDCl_3$, plus DEPT, ppm): δ = 23.8 (x 2, CH_3), 33.7 (CH), 94.8 (C_{quat}), 127.2 (CH), 127.5 (CH), 127.9 (x 2, CH) 128.5 (CH), 129.3 (x 2, CH), 139.3 (CH), 144.4 (C_{quat}), 146.4 (C_{quat}), 149.1 (C_{quat}). EI MS (70 eV), *m*/*z* (%): 323/322 (47/100) [M^+], 307 (99), 195 (24) [M^+ – I], 180 (75), 165 (62), 152 (44). HRMS (EI) cacld for $C_{15}H_{15}I$: 322.0218; found: 322.0219.

A2. Preparation of Phenanthrenes 3:



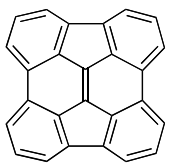
9-(2,6-Dichlorophenyl)-10-(2-chlorophenyl)phenanthrene (**3**-H): A mixture of $Pd(OAc)_2$ (40.8 mg, 0.18 mmol), LiCl (76.1 mg, 1.79 mmol), sodium acetate (590 mg, 7.14 mmol), alkyne **8** (1.21 g, 4.26 mmol), biphenyl **7**-H (1.00 g, 3.57 mmol) and DMF (20 mL) in a thick-wall pyrex tube was purged with nitrogen for 5 min. The sealed tube was heated at 100 ºC for 20 h. After cooling to room temperature, the suspension was diluted with CH_2Cl_2 (50 mL) and filtered through a 3 cm thick layer of Celite, and the Celite was rinsed well with CH_2Cl_2 (30 mL). The solvents of the filtrate were removed

under reduced pressure, and the residue was subjected to chromatography on alumina. Elution with hexane/CH_2Cl_2 (20:1) gave **3**-H (972 mg, 63%) as white solids, m. p. 257.7–258.4 ºC. ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ = 7.11–7.39 (m, 6H), 7.44–7.53 (m, 5H), 7.73 (t, *J* = 7.5 Hz, 2H), 8.86 (d, *J* = 8.2 Hz, 2H). ^{13}C NMR (75.5MHz, $CDCl_3$, plus DEPT, ppm): δ = 122.8 (CH), 123.0 (CH), 126.0 (CH), 126.2 (CH), 126.8 (CH), 127.03 (CH), 127.05 (CH), 127.2 (CH), 127.4 (CH), 127.5 (CH), 128.0 (CH), 129.0 (CH), 129.2 (CH), 129.6 (CH), 130.0 (C_{quat}), 130.3 (C_{quat}), 130.4 (C_{quat}), 130.6 (C_{quat}), 131.0 (CH), 132.7 (C_{quat}), 134.6 (C_{quat}), 134.9 (C_{quat}), 136.4 (x 2, C_{quat}), 137.0 (x 2, C_{quat}). EI MS (70 eV), *m*/*z* (%): 434/433/432 (99/28/100) [M^+], 326 (81), 324 (57), 322 (66), 280 (83), 162 (78). HRMS (EI) cacld for $C_{26}H_{15}Cl_3$: 432.0239; found: 432.0244.



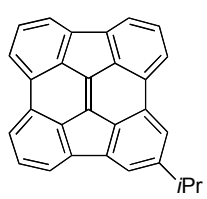
10-(2,6-Dichlorophenyl)-10-(2-chlorophenyl)-3-isopropylphenanthrene (**3**-*i*Pr): Similar to the synthesis of **3**-H, **7**-*i*Pr (104 mg, 0.32 mmol) was conducted in this reaction. After chromatographic purification, a mixture of **3**-*i*Pr and **3**'-*i*Pr (102 mg, 65%; ratio 10:1) was obtained as white solids. **3**-*i*Pr: m. p. 219.4–220.6 ºC. ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ = 1.43 (d, *J* = 6.9 Hz, 6H), 3.22 (heptet, *J* = 6.9 Hz, 1H), 7.10–7.34 (m, 6H), 7.38–7.54 (m, 5H), 7.71 (dd, *J* = 7.6, *J* = 2.0 Hz, 1H), 8.67 (s, 1H), 8.87 (d, *J* = 8.3 Hz, 1H). ^{13}C NMR (75.5MHz, $CDCl_3$, plus DEPT, ppm): δ = 24.1 (CH_3), 24.2 (CH_3), 34.6 (CH), 120.0 (CH), 122.9 (CH), 125.97 (CH), 126.02 (CH), 126.2 (CH), 126.8 (CH), 127.0 (CH), 127.4 (CH), 127.6 (CH), 128.0 (CH), 128.88 (CH), 128.94 (C_{quat}), 129.2 (CH), 129.6 (CH), 130.2 (C_{quat}), 130.32 (C_{quat}), 130.35 (C_{quat}), 131.0 (CH), 131.9 (C_{quat}), 134.6 (C_{quat}), 134.8 (C_{quat}), 136.53 (C_{quat}), 136.55 (C_{quat}), 137.1 (C_{quat}), 137.2 (C_{quat}), 147.6 (C_{quat}). EI MS (70 eV), *m*/*z* (%): 476/475/474 (35/11/35) [M^+], 404 (100), 389 (97), 289 (23), 263 (27). HR MS (EI) cacld for $C_{29}H_{21}Cl_3$: 474.0709; found: 474.0712.

A.3. Synthesis of bulkybowls 2



Diindeno[1,2,3,4-*defg*:1',2',3',4'-*mnop*]chrysene (**2**-H): A mixture of Cs_2CO_3 (67.6 mg, 0.21 mmol), $PdCl_2(PCy_3)_2$ (30.6 mg, 0.04 mmol), DBU (31.5 mg, 0.21 mmol), phenanthrene **3**-H (30.0 mg, 0.07 mmol) and NMP (1 mL) in a thick-wall pyrex tube was purged with nitrogen for 5 min. The sealed tube was heated at 150 ºC for 2 d. After cooling to room temperature, the suspension was diluted with CH_2Cl_2 (10 mL) and filtered through a 3 cm thick layer of Celite, and the Celite was rinsed well with CH_2Cl_2 (10 mL). The solvents of the filtrate were removed under reduced pressure, and the residue was subjected to chromatography on silica gel. Elution with hexane/CH_2Cl_2 (20:1) gave **2**-H (4.70 mg, 21%) as yellow solids. ^{1}H-NMR spectrum of **2**-H in $CDCl_3$ is identical to that reported in ref. S3. ^{1}H NMR (300 MHz, CD_2Cl_2, ppm): δ = 7.63 (dd, *J* = 7.8, *J* = 6.8 Hz, 4H),

7.90 (d, J = 6.8 Hz, 4H), 8.27 (d, J = 7.8 Hz, 4H).



2-Isopropyldiindeno[1,2,3,4-*defg*:1',2',3',4'-*mnop*]chrysene (**2**-*i*Pr): Similar to the synthesis of **2**-H, a mixture of **3**-*i*Pr and **3'**-*i*Pr (30.0 mg, 0.06 mmol) was conducted in this reaction. Elution with cyclohexane gave **2**-*i*Pr (4.50 mg, 19%) as yellow solids, m. p. 287.3–288.1 ºC. *Note: When 90.0 mg of the starting material was divided into three equal portions and conducted under the same conditions, 13.2 mg (18%) of **2**-iPr was obtained.* ^{1}H NMR (300 MHz, CD_2Cl_2, ppm): δ = 1.42 (d, J = 6.9 Hz, 6H), 3.18 (heptet, J = 6.9 Hz, 1H), 7.55–7.62 (m, 3H), 7.80 (s, 1H), 7.86 (dd, J = 7.1, J = 2.3 Hz, 3H), 8.10 (s, 1H), 8.22 (d, J = 8.0 Hz, 2H), 8.26 (d, J = 8.0 Hz, 1H). ^{13}C NMR (75.5MHz, CD_2Cl_2, plus DEPT, ppm): δ = 24.7 (x 2, CH_3), 35.9 (CH), 121.6 (CH), 122.0 (CH), 122.27 (x 2, CH), 122.33 (CH), 124.36 (x 3, CH), 128.45 (CH), 128.49 (CH), 128.6 (CH), 133.1 (C_{quat}), 133.34 (C_{quat}), 133.38 (C_{quat}), 133.43 (C_{quat}), 136.8 (C_{quat}), 137.5 (C_{quat}), 137.7 (C_{quat}), 139.02 (C_{quat}), 139.06 (C_{quat}), 139.14 (C_{quat}), 141.2 (C_{quat}), 141.3 (C_{quat}), 141.4 (C_{quat}), 141.5 (C_{quat}), 150.7 (C_{quat}). EI MS (70 eV), *m*/*z* (%): 366 (2) [M^+], 248 (69), 205 (100). HRMS (EI) cacld for $C_{29}H_{18}$: 366.1409; found: 366.1413.

B. Computational Results

B.1 Summary of computational data

2-H:

B3LYP/cc-pVDZ

Reactant HF = -998.0577637 au = -626291.227299387 Kcal/mol
Freq = 77.3923 bowl depth = 1.334 Å
Product HF = -998.0577636 au = -626291.227236636 Kcal/mol
Freq = 77.4648 bowl depth = 1.334 Å
TS HF = -998.0484708 au = -626285.395911708 Kcal/mol
Freq = -66.4910
ΔG = 5.831324928 Kcal/mol

M06-2X/cc-pVDZ

Reactant HF = -997.7225698 au = -626080.889775198 Kcal/mol
Freq = 77.8425 bowl depth = 1.384 Å
Product HF = -997.7225698 au = -626080.889775198 Kcal/mol
Freq = 77.8425 bowl depth = 1.384 Å
TS HF = -997.7115511 au = -626073.975430761 Kcal/mol
Freq = -70.7027
QST3 HF = -997.7115515 au = -626073.975430761 Kcal/mol
Freq = -70.7027
ΔG = 6.914344437 Kcal/mol

2-*i*Pr :

B3LYP/cc-pVDZ

Reactant HF = -1116.0016101 au = -700302.170353851 Kcal/mol
Freq = 28.5353 bowl depth = 1.358 and 1.360 Å
Product HF = -1116.0019844 au = -700302.405230844 Kcal/mol
Freq = 28.4303 bowl depth = 1.354 and 1.359 Å
QST3 HF = -1115.9920573 au = -700296.175876323 Kcal/mol
Freq = -60.9805
ΔG^{1} = 5.994477528 Kcal/mol

ΔG^2 = 6.229354521 Kcal/mol

M062X/cc-pVDZ

Reactant HF = -1115.6103753 au = -700056.666604503 Kcal/mol
Freq = 19.6767 bowl depth = 1.408 and 1.413Å
Product HF = -1115.6108527 au = -700056.966177777 Kcal/mol
Freq = 34.0495 bowl depth = 1.408 and 1.409 Å
TS HF = -1115.5992004 au = -700049.654243004 Kcal/mol
Freq = -64.0132
QST3 HF = -1115.5992004 au = -700049.654243004 Kcal/mol
Freq = -64.0090

ΔG^1 = 7.012361499 Kcal/mol
ΔG^2 = 7.311934773 Kcal/mol

9-H:

B3LYP/cc-pVDZ

Reactant HF = -768.1950128 au = -482050.052482128 Kcal/mol
Freq = 140.3729 bowl depth = 0.874 Å
Product HF = -768.1950209 au = -482050.057564959 Kcal/mol
Freq = 140.5197 bowl depth = 0.874 Å
TS HF = -768.1804884 au = -482040.938275884 Kcal/mol
Freq = -108.2674
QST3 HF = -768.1804951 au = -482040.942480201 Kcal/mol
Freq = -107.6895

ΔG^1 = 9.119289075 Kcal/mol
ΔG^2 = 9.110001927 Kcal/mol

M062X/cc-pVDZ

Reactant HF = -767.9319213 au = -481884.959934963 Kcal/mol
Freq = 138.2912 bowl depth = 0.886 Å
Product HF = -767.9319514 au = -481884.978823014 Kcal/mol
Freq = 139.0536 bowl depth = 0.886 Å
TS HF = -767.916182 au = -481875.08336682 Kcal/mol
Freq = -111.1554

ΔG^1 = 9.876568143 Kcal/mol
ΔG^2 = 9.895456194 Kcal/mol

10

B3LYP/cc-pVDZ

Reactant HF = -807.4761593 au = -506699.364722343 Kcal/mol
Freq = 130.6002 bowl depth = 1.142 Å

Product HF = -807.4761407 au = -506699.353050657 Kcal/mol
Freq = 130.5313 bowl depth = 1.142 Å

QST2 HF = -807.4471558 au = -506681.164736058 eV
Freq = -120.6124

ΔG^1 = 18.199986285 Kcal/mol

ΔG^2 = 18.188314599 Kcal/mol

M062X/cc-pVDZ

Reactant HF = -807.200978 au = -506526.68570478 Kcal/mol
Freq = 129.9096 bowl depth = 1.156 Å

Product HF = -807.200872 au = -506526.61918872 Kcal/mol
Freq = 129.5655 bowl depth = 1.156 Å

B.2. Cartesian coordinates

Compound 2-H:

2-H-reactant
#p b3lyp/cc-pVDZ opt freq=noraman
HF = -998.0577637

0 1

C	1.39604200	-1.16619900	0.54190300
C	0.74943500	-2.39628000	0.27795200
C	-0.74950200	-2.39625900	0.27795500
C	-1.39607500	-1.16616000	0.54190900
C	-0.67018200	0.00001000	0.85369400

C	0.67018200	-0.00000900	0.85369200
C	1.39607400	1.16616000	0.54190300
C	0.74950200	2.39625900	0.27795300
C	-0.74943400	2.39628000	0.27795100
C	-1.39604200	1.16619900	0.54190500
C	2.70562300	-0.76132500	0.14402100
C	2.70564600	0.76125000	0.14402600
C	-2.70564500	-0.76125100	0.14402900
C	-2.70562200	0.76132500	0.14402200
C	-1.63213000	3.39277800	-0.21390300
C	-2.97134000	3.07881800	-0.48025400
C	-3.51865000	1.77221600	-0.35944300
C	-1.63222600	-3.39273300	-0.21389600
C	-2.97142800	-3.07873700	-0.48024400
C	-3.51870200	-1.77212000	-0.35943200
C	1.63213000	-3.39277900	-0.21390100
C	2.97133800	-3.07882000	-0.48025300
C	3.51864900	-1.77221700	-0.35944500
C	3.51870300	1.77212100	-0.35943000
C	2.97142800	3.07873900	-0.48024000
C	1.63222700	3.39273500	-0.21389600
H	-1.27271000	4.39907700	-0.44142900
H	-3.61635900	3.86961400	-0.87091900
H	-4.53641400	1.58563800	-0.71053600
H	-1.27283500	-4.39904300	-0.44142100
H	-3.61646900	-3.86951500	-0.87090800
H	-4.53646000	-1.58551400	-0.71052800
H	1.27270700	-4.39907900	-0.44141900
H	3.61635900	-3.86961500	-0.87091800
H	4.53641200	-1.58564400	-0.71054200
H	4.53646200	1.58551900	-0.71052500
H	3.61647200	3.86951600	-0.87090300
H	1.27283400	4.39904400	-0.44141800

2-H-porduct

#p b3lyp/cc-pVDZ opt freq=noraman

HF = -998.0577636

0 1

C	-1.39623700	-1.16606900	0.54184600
C	-0.74962300	-2.39626600	0.27792300
C	0.74923000	-2.39638800	0.27792700
C	1.39605100	-1.16630500	0.54186900
C	0.67026600	-0.00005500	0.85351600
C	-0.67026700	0.00005600	0.85352000
C	-1.39605300	1.16630600	0.54187600
C	-0.74923100	2.39639000	0.27793600
C	0.74962200	2.39626800	0.27792600
C	1.39623700	1.16606900	0.54183900
C	-2.70580200	-0.76101400	0.14401000
C	-2.70567600	0.76145700	0.14401800
C	2.70568000	-0.76145900	0.14402800
C	2.70579800	0.76101100	0.14399700
C	1.63262800	3.39274700	-0.21381000
C	2.97174100	3.07864700	-0.48006300
C	3.51890900	1.77183900	-0.35949100
C	1.63206100	-3.39300300	-0.21385200
C	2.97121900	-3.07911300	-0.48013400
C	3.51861000	-1.77240500	-0.35951400
C	-1.63262800	-3.39274400	-0.21381700
C	-2.97174200	-3.07864500	-0.48006700
C	-3.51891400	-1.77184000	-0.35947700
C	-3.51860400	1.77240200	-0.35953300
C	-2.97121800	3.07911300	-0.48013300
C	-1.63205800	3.39300000	-0.21385600
H	1.27319700	4.39904700	-0.44134200
H	3.61704300	3.86931300	-0.87052200
H	4.53664900	1.58543400	-0.71073000
H	1.27246000	-4.39923900	-0.44140000
H	3.61637500	-3.86987000	-0.87065400
H	4.53636200	-1.58614600	-0.71079500
H	-1.27319500	-4.39904300	-0.44135200
H	-3.61704200	-3.86930800	-0.87053600
H	-4.53665200	-1.58543200	-0.71071700
H	-4.53636000	1.58614700	-0.71080100
H	-3.61637700	3.86987400	-0.87063600

H	-1.27245500	4.39923200	-0.44141600

2-H-TS

#p b3lyp/cc-pVDZ opt=(calcfc,ts,noeigen) freq scfcyc=1000

HF = -998.0484708

0 1

C	-1.40043000	-1.16876900	-0.00028700
C	-0.75972200	-2.43025900	-0.00014500
C	0.75972100	-2.43025900	-0.00014600
C	1.40042900	-1.16877000	-0.00029200
C	0.65851500	-0.00000100	-0.00047100
C	-0.65851600	0.00000000	-0.00046700
C	-1.40042900	1.16876900	-0.00028700
C	-0.75971900	2.43025900	-0.00014500
C	0.75972100	2.43025900	-0.00014600
C	1.40043000	1.16876800	-0.00029200
C	-2.77091200	-0.77674400	-0.00007200
C	-2.77091100	0.77674600	-0.00007300
C	2.77091100	-0.77674500	-0.00007700
C	2.77091100	0.77674200	-0.00007800
C	1.71665400	3.47936800	0.00012200
C	3.09067800	3.17428900	0.00025400
C	3.64862900	1.86001600	0.00018700
C	1.71665400	-3.47936900	0.00012200
C	3.09067600	-3.17429000	0.00025500
C	3.64862700	-1.86001700	0.00018900
C	-1.71665500	-3.47936900	0.00011700
C	-3.09067900	-3.17428900	0.00025000
C	-3.64862900	-1.86001500	0.00018900
C	-3.64862700	1.86001800	0.00018800
C	-3.09067600	3.17429100	0.00025100
C	-1.71665200	3.47937000	0.00011800
H	1.41512900	4.52976100	0.00026100
H	3.79111800	4.01316600	0.00047200
H	4.73572600	1.74923700	0.00037900
H	1.41512800	-4.52976200	0.00026000
H	3.79111700	-4.01316700	0.00047200

H	4.73572500	-1.74923900	0.00038100
H	-1.41513000	-4.52976200	0.00025000
H	-3.79112000	-4.01316500	0.00046300
H	-4.73572700	-1.74923700	0.00038200
H	-4.73572500	1.74924100	0.00037800
H	-3.79111500	4.01316900	0.00046700
H	-1.41512600	4.52976200	0.00025400

2-H-reactant

#p M062X/cc-pVDZ opt freq=noraman

HF = -997.7225698

0 1

C	-1.39293300	1.16615400	0.56225900
C	-0.74736700	2.38574000	0.29035900
C	0.74746000	2.38571200	0.29036200
C	1.39297800	1.16610000	0.56226200
C	0.66741900	-0.00001300	0.88348700
C	-0.66741900	0.00001300	0.88348700
C	-1.39297800	-1.16610000	0.56226200
C	-0.74745900	-2.38571200	0.29036200
C	0.74736700	-2.38574000	0.29035900
C	1.39293300	-1.16615400	0.56225900
C	-2.69284200	0.76018300	0.15378000
C	-2.69287300	-0.76008000	0.15378700
C	2.69287300	0.76008000	0.15378700
C	2.69284200	-0.76018300	0.15378000
C	1.61839400	-3.37583100	-0.22366000
C	2.94932100	-3.06191300	-0.50030200
C	3.49635100	-1.75911400	-0.37234400
C	1.61852500	3.37577000	-0.22365100
C	2.94944200	3.06180200	-0.50028800
C	3.49642300	1.75898300	-0.37232800
C	-1.61839400	3.37583100	-0.22366000
C	-2.94932100	3.06191300	-0.50030200
C	-3.49635100	1.75911400	-0.37234300
C	-3.49642300	-1.75898300	-0.37232800
C	-2.94944200	-3.06180200	-0.50028800

C	-1.61852500	-3.37577000	-0.22365100
H	1.25175400	-4.37621900	-0.46081700
H	3.58765500	-3.84564500	-0.91090500
H	4.50564600	-1.56551900	-0.73946900
H	1.25192500	4.37617300	-0.46080800
H	3.58780700	3.84551100	-0.91088800
H	4.50571100	1.56534900	-0.73945300
H	-1.25175500	4.37621900	-0.46081700
H	-3.58765500	3.84564500	-0.91090500
H	-4.50564700	1.56551800	-0.73946800
H	-4.50571100	-1.56534900	-0.73945200
H	-3.58780700	-3.84551100	-0.91088800
H	-1.25192500	-4.37617300	-0.46080800

2-H-product

#p M062X/cc-pVDZ opt freq=noraman

HF = -997.7225698

0 1

C	-1.39291200	-1.16618000	0.56226000
C	-0.74732700	-2.38575500	0.29035900
C	0.74750900	-2.38569900	0.29036400
C	1.39300100	-1.16607400	0.56226200
C	0.66741900	0.00002500	0.88349100
C	-0.66741900	-0.00002600	0.88349100
C	-1.39300100	1.16607400	0.56226600
C	-0.74750900	2.38570000	0.29037600
C	0.74732700	2.38575600	0.29037100
C	1.39291300	1.16617900	0.56226400
C	-2.69282600	-0.76023500	0.15377500
C	-2.69288300	0.76003200	0.15377800
C	2.69288600	-0.76003300	0.15378600
C	2.69282300	0.76023400	0.15376800
C	1.61832700	3.37586600	-0.22364400
C	2.94925800	3.06197000	-0.50031000
C	3.49630400	1.75918000	-0.37237800
C	1.61858900	-3.37574500	-0.22363700
C	2.94950300	-3.06175200	-0.50027800

C	3.49645300	-1.75892300	-0.37233300
C	-1.61832900	-3.37586400	-0.22365400
C	-2.94926400	-3.06197000	-0.50030600
C	-3.49631100	-1.75918200	-0.37236100
C	-3.49644500	1.75892100	-0.37235000
C	-2.94949800	3.06175300	-0.50028200
C	-1.61858700	3.37574700	-0.22362700
H	1.25167100	4.37624800	-0.46080100
H	3.58756800	3.84571900	-0.91092000
H	4.50560000	1.56559300	-0.73950700
H	1.25201200	-4.37615600	-0.46079400
H	3.58787600	-3.84545400	-0.91087900
H	4.50573600	-1.56526000	-0.73945700
H	-1.25167400	-4.37624600	-0.46081300
H	-3.58757500	-3.84571800	-0.91091500
H	-4.50560800	-1.56559400	-0.73948700
H	-4.50572800	1.56526000	-0.73947600
H	-3.58786900	3.84545500	-0.91088400
H	-1.25200900	4.37615800	-0.46078100

2-H-TS

#p M062X/cc-pVDZ opt=(calcfc,ts,noeigen) freq scfcyc=1000

HF = -997.7115511

0 1

C	-1.40027800	1.16867400	0.00004900
C	-0.75976200	2.43030500	-0.00018300
C	0.75984100	2.43038700	0.00001500
C	1.40045800	1.16879300	-0.00039000
C	0.65861600	-0.00000100	-0.00053100
C	-0.65841200	0.00000000	-0.00019400
C	-1.40028300	-1.16867100	0.00004800
C	-0.75977000	-2.43030300	-0.00018300
C	0.75983300	-2.43038900	0.00001400
C	1.40045400	-1.16879700	-0.00039100
C	-2.77081100	0.77683700	0.00009100
C	-2.77081500	-0.77682800	0.00009100
C	2.77102000	0.77691700	-0.00005100

C	2.77101800	-0.77692500	-0.00005200
C	1.71665000	-3.47956200	0.00018600
C	3.09066300	-3.17458000	0.00022900
C	3.64863900	-1.86036000	0.00005400
C	1.71666000	3.47955700	0.00018800
C	3.09067200	3.17457100	0.00023100
C	3.64864400	1.86035000	0.00005500
C	-1.71679800	3.47933900	-0.00003900
C	-3.09085800	3.17418900	0.00008300
C	-3.64874200	1.85992200	0.00013900
C	-3.64874800	-1.85991200	0.00014200
C	-3.09086700	-3.17418100	0.00008600
C	-1.71680800	-3.47933500	-0.00003800
H	1.41504600	-4.52993200	0.00036800
H	3.79105600	-4.01349500	0.00043500
H	4.73574300	-1.74968300	0.00022900
H	1.41505900	4.52992800	0.00037100
H	3.79106700	4.01348400	0.00043800
H	4.73574800	1.74967000	0.00023100
H	-1.41535400	4.52975500	-0.00016000
H	-3.79131500	4.01305600	0.00007700
H	-4.73582400	1.74902800	0.00010200
H	-4.73583000	-1.74901500	0.00010800
H	-3.79132700	-4.01304500	0.00008200
H	-1.41536800	-4.52975100	-0.00015800

2-H-QST3

#p M062X/cc-pVDZ opt=qst3 freq scfcyc=1000

HF = -997.7115515

0 1

C	1.39761200	-1.16922500	0.00000700
C	0.75780800	-2.42237200	-0.00015700
C	-0.75781100	-2.42236900	-0.00027400
C	-1.39761600	-1.16922300	-0.00016200
C	-0.65540300	0.00000000	-0.00013600
C	0.65540100	0.00000000	0.00003200
C	1.39761200	1.16922500	0.00000400

C	0.75780900	2.42237200	-0.00016200
C	-0.75781000	2.42236900	-0.00027100
C	-1.39761600	1.16922300	-0.00016100
C	2.76236700	-0.77601000	0.00017800
C	2.76236700	0.77600900	0.00017300
C	-2.76237300	-0.77600800	0.00006000
C	-2.76237300	0.77600900	0.00006700
C	-1.71083400	3.46985500	-0.00040100
C	-3.07936800	3.16582700	0.00009700
C	-3.63711200	1.85494500	0.00058800
C	-1.71083400	-3.46985400	-0.00041100
C	-3.07936900	-3.16582700	0.00008000
C	-3.63711200	-1.85494400	0.00057200
C	1.71083800	-3.46985200	-0.00044400
C	3.07937200	-3.16582200	-0.00002200
C	3.63711500	-1.85493700	0.00049900
C	3.63711500	1.85493600	0.00048500
C	3.07937200	3.16582200	-0.00003800
C	1.71083900	3.46985200	-0.00045500
H	-1.40849400	4.51879000	-0.00044800
H	-3.77804000	4.00392200	0.00027100
H	-4.72253800	1.74397700	0.00089500
H	-1.40849400	-4.51878900	-0.00046000
H	-3.77804000	-4.00392200	0.00024800
H	-4.72253800	-1.74397700	0.00087500
H	1.40850900	-4.51879100	-0.00062300
H	3.77803700	-4.00392300	0.00001400
H	4.72253900	-1.74396200	0.00070100
H	4.72253900	1.74396200	0.00068600
H	3.77803700	4.00392200	-0.00000600
H	1.40851000	4.51879000	-0.00063600

Compound **2**-*i*Pr:

2-*i*Pr-reactant

#p b3lyp/cc-pVDZ opt freq=noraman

HF = -1116.0016101

0 1

C	-0.94638700	0.35640900	-0.78410400
C	-1.50407200	-0.92369600	-0.56584200
C	-0.55130900	-2.07960200	-0.49183700
C	0.82633000	-1.79299300	-0.63995100
C	1.28828500	-0.48900700	-0.90873300
C	0.43608600	0.54383700	-0.97680800
C	0.84031700	1.84387600	-0.61371200
C	2.17089900	2.12792800	-0.22689600
C	3.12467100	0.97399800	-0.15384300
C	2.61605500	-0.30645200	-0.47498800
C	-1.50462200	1.61336900	-0.41403700
C	-0.33880400	2.58732800	-0.30432000
C	1.93423500	-2.54562100	-0.14604100
C	3.10225700	-1.57555900	-0.03871200
C	4.40566300	0.92618700	0.45502100
C	4.99326000	-0.30723300	0.76554100
C	4.34955700	-1.56090400	0.57834100
C	-0.79716900	-3.39587900	-0.02245900
C	0.27135400	-4.22947400	0.33330500
C	1.63194100	-3.81794400	0.32976100
C	-2.86642100	-0.88334300	-0.17874100
C	-3.52672000	0.33829800	0.05376100
C	-2.83659800	1.58588200	-0.01329400
C	-0.12615100	3.85110600	0.23773500
C	1.21284900	4.26309200	0.48076900
C	2.32929100	3.43664500	0.29905100
H	4.92773000	1.84319100	0.73814700
H	5.97494100	-0.30244600	1.24545600
H	4.82144300	-2.46629300	0.96760700
H	-1.81735300	-3.76032200	0.11894300
H	0.04049500	-5.23159800	0.70274800
H	2.39189600	-4.48373000	0.74587100
H	-3.41060100	-1.81416200	-0.00222400
C	-4.99921100	0.33987700	0.46363800
H	-3.36212800	2.49055800	0.30484400

H	-0.94807100	4.50915700	0.52995100
H	1.37361400	5.25882300	0.90121100
H	3.30922400	3.79875500	0.61877000
C	-5.90298400	-0.19605600	-0.66134800
C	-5.24481400	-0.41604000	1.78171300
H	-5.01690800	-1.49040000	1.68181100
H	-4.61958100	-0.01563500	2.59534600
H	-6.30092100	-0.32977800	2.08674200
H	-5.68893300	-1.25657700	-0.87563600
H	-5.75678700	0.36917400	-1.59533500
H	-6.96584900	-0.12058700	-0.37731300
H	-5.27894300	1.39369900	0.63525300

2-*i*Pr-product

#p b3lyp/cc-pVDZ opt freq=noraman

HF = -1116.0019844

0 1

C	1.11294200	-1.77135900	-0.61603100
C	-0.20579400	-2.26395600	-0.47035000
C	-1.32285700	-1.26984700	-0.56849200
C	-0.96748400	0.07607200	-0.80313600
C	0.37036000	0.47158500	-0.99266200
C	1.37111800	-0.41680500	-0.90467500
C	2.65190200	-0.02542200	-0.46706500
C	2.95459000	1.32268600	-0.16321200
C	1.83548500	2.31500900	-0.25984400
C	0.56709300	1.82392200	-0.64848100
C	2.31926100	-2.33710000	-0.10335200
C	3.32358800	-1.19760500	-0.00594300
C	-1.71636700	1.23881400	-0.45531700
C	-0.71422000	2.38193600	-0.35614100
C	1.78711100	3.64025900	0.24558000
C	0.55575800	4.28795800	0.40916300
C	-0.70213100	3.67108000	0.16716200
C	-2.68198300	-1.43058500	-0.19196600
C	-3.52161300	-0.32348500	0.01967800
C	-3.02923900	1.01701500	-0.05970800
C	-0.25052800	-3.59510000	0.01987400

C	0.93032900	-4.24855900	0.39551000
C	2.21184700	-3.63287300	0.39242000
C	4.54747400	-0.98145600	0.62014100
C	4.98906100	0.35897700	0.79099300
C	4.22194300	1.48216100	0.45500500
H	2.69743500	4.15371800	0.56375800
H	0.55877900	5.30290400	0.81403900
H	-1.61737600	4.19912500	0.44556100
H	-3.08949300	-2.42811800	-0.00711900
C	-4.97506300	-0.56068900	0.42462500
H	-3.67996900	1.84082100	0.24336200
H	-1.20395700	-4.10952500	0.16117100
H	0.85329300	-5.26820700	0.78080700
H	3.06145300	-4.16720200	0.82441900
H	5.14869900	-1.79734000	1.02858300
H	5.95338200	0.52224200	1.27828700
H	4.59392600	2.47301400	0.72605800
C	-5.27743200	-0.04339700	1.84268500
C	-5.95716700	0.02957200	-0.60326400
H	-5.12739900	-1.65368900	0.43535800
H	-5.16912700	1.05224800	1.90680500
H	-4.59772200	-0.49112500	2.58485600
H	-6.31227700	-0.28986000	2.13294400
H	-5.76701700	-0.36918800	-1.61221700
H	-5.87256700	1.12805400	-0.65621600
H	-6.99797800	-0.21071400	-0.32964800

2-*i*Pr-QST3

#p b3lyp/cc-pVDZ opt=qst3 freq scfcyc=1000

HF= -1115.9920573

0 1

C	-0.94638700	0.35640900	-0.78410400
C	-1.50407200	-0.92369600	-0.56584200
C	-0.55130900	-2.07960200	-0.49183700
C	0.82633000	-1.79299300	-0.63995100
C	1.28828500	-0.48900700	-0.90873300
C	0.43608600	0.54383700	-0.97680800

C	0.84031700	1.84387600	-0.61371200
C	2.17089900	2.12792800	-0.22689600
C	3.12467100	0.97399800	-0.15384300
C	2.61605500	-0.30645200	-0.47498800
C	-1.50462200	1.61336900	-0.41403700
C	-0.33880400	2.58732800	-0.30432000
C	1.93423500	-2.54562100	-0.14604100
C	3.10225700	-1.57555900	-0.03871200
C	4.40566300	0.92618700	0.45502100
C	4.99326000	-0.30723300	0.76554100
C	4.34955700	-1.56090400	0.57834100
C	-0.79716900	-3.39587900	-0.02245900
C	0.27135400	-4.22947400	0.33330500
C	1.63194100	-3.81794400	0.32976100
C	-2.86642100	-0.88334300	-0.17874100
C	-3.52672000	0.33829800	0.05376100
C	-2.83659800	1.58588200	-0.01329400
C	-0.12615100	3.85110600	0.23773500
C	1.21284900	4.26309200	0.48076900
C	2.32929100	3.43664500	0.29905100
H	4.92773000	1.84319100	0.73814700
H	5.97494100	-0.30244600	1.24545600
H	4.82144300	-2.46629300	0.96760700
H	-1.81735300	-3.76032200	0.11894300
H	0.04049500	-5.23159800	0.70274800
H	2.39189600	-4.48373000	0.74587100
H	-3.41060100	-1.81416200	-0.00222400
C	-4.99921100	0.33987700	0.46363800
H	-3.36212800	2.49055800	0.30484400
H	-0.94807100	4.50915700	0.52995100
H	1.37361400	5.25882300	0.90121100
H	3.30922400	3.79875500	0.61877000
C	-5.90298400	-0.19605600	-0.66134800
C	-5.24481400	-0.41604000	1.78171300
H	-5.01690800	-1.49040000	1.68181100
H	-4.61958100	-0.01563500	2.59534600
H	-6.30092100	-0.32977800	2.08674200
H	-5.68893300	-1.25657700	-0.87563600
H	-5.75678700	0.36917400	-1.59533500

H	-6.96584900	-0.12058700	-0.37731300
H	-5.27894300	1.39369900	0.63525300

2-*i*Pr-reactant

#p M062X/cc-pVDZ opt freq=noraman

HF= -1115.6103753

0 1

C	-0.94471200	0.36433000	-0.81904400
C	-1.50476200	-0.90598700	-0.59541100
C	-0.56208900	-2.06399400	-0.51696500
C	0.80993200	-1.79139600	-0.66639800
C	1.28242200	-0.49058900	-0.94224000
C	0.44057900	0.54331300	-1.01436000
C	0.85098400	1.84002800	-0.63950100
C	2.17176100	2.10971900	-0.23826700
C	3.11496600	0.95308900	-0.16090000
C	2.60765900	-0.31634500	-0.49200300
C	-1.48997500	1.61782900	-0.43902600
C	-0.32029900	2.58230000	-0.32315500
C	1.90365900	-2.54265400	-0.15555900
C	3.07526400	-1.58129300	-0.04186100
C	4.37721500	0.90171500	0.47692300
C	4.94862900	-0.32858200	0.80234800
C	4.30099600	-1.57513200	0.60467600
C	-0.82319100	-3.36514000	-0.02656200
C	0.23155300	-4.19932800	0.34524900
C	1.59208700	-3.79805600	0.34179700
C	-2.85708700	-0.86178700	-0.18989800
C	-3.50298600	0.35829200	0.05185100
C	-2.81055700	1.59896700	-0.01902400
C	-0.10810500	3.82832300	0.24474300
C	1.22806700	4.22949800	0.50233100
C	2.33556500	3.40298100	0.31356000
H	4.89383600	1.81709900	0.77128000
H	5.91497900	-0.32845900	1.30895700
H	4.75036200	-2.48218500	1.01227000
H	-1.84732400	-3.71368500	0.11871800

H	-0.00867200	-5.19037300	0.73334800
H	2.34454100	-4.45761300	0.77723000
H	-3.40327700	-1.78987200	-0.00340600
C	-4.96079300	0.35819100	0.48659700
H	-3.32454400	2.50377100	0.31431900
H	-0.93013500	4.47822600	0.54920000
H	1.38994800	5.21296200	0.94618000
H	3.31489500	3.74852300	0.64938500
C	-5.86761600	-0.19660000	-0.61588000
C	-5.16688300	-0.40150300	1.80042400
H	-4.93123900	-1.47042200	1.67927100
H	-4.52191600	-0.00163900	2.59586100
H	-6.21431500	-0.32669100	2.12940000
H	-5.63397300	-1.25407500	-0.81641600
H	-5.73785400	0.36022900	-1.55486100
H	-6.92496200	-0.13588600	-0.31691100
H	-5.24403200	1.40895700	0.65951400

2-*i*Pr-product

#p M062X/cc-pVDZ opt freq=noraman

HF= -1115.6108527

0 1

C	1.11068300	-1.77016300	-0.64035200
C	-0.20114400	-2.25787800	-0.49370200
C	-1.31611300	-1.26884700	-0.59669100
C	-0.96700000	0.06974400	-0.83534400
C	0.37130000	0.46753200	-1.02736400
C	1.36928100	-0.41544000	-0.93658400
C	2.64588000	-0.02199300	-0.48355600
C	2.93826500	1.31834100	-0.17150100
C	1.82137600	2.30597400	-0.27328300
C	0.56378500	1.81981500	-0.67346900
C	2.30696900	-2.32650300	-0.10960200
C	3.30746500	-1.18681400	-0.00709800
C	-1.71234600	1.22648100	-0.47884900
C	-0.71367200	2.36885500	-0.37479500
C	1.77143100	3.61841800	0.25351700

C	0.54390900	4.25896500	0.42387900
C	-0.70852500	3.64227300	0.17110000
C	-2.66644800	-1.43522300	-0.20462600
C	-3.49971600	-0.33433900	0.01490200
C	-3.01382200	1.00450100	-0.06690300
C	-0.25320300	-3.57626600	0.01825800
C	0.91887200	-4.22221400	0.41154700
C	2.19701800	-3.60692200	0.40919900
C	4.50945700	-0.97101300	0.64827700
C	4.94566200	0.36663800	0.82696600
C	4.18617400	1.48294200	0.47479700
H	2.68055600	4.12457500	0.58346900
H	0.54319700	5.26443700	0.84751900
H	-1.62573300	4.15746800	0.46127700
H	-3.06899100	-2.43320100	-0.01397000
C	-4.93964700	-0.56384100	0.44413300
H	-3.66102900	1.82551000	0.25051400
H	-1.20950300	-4.08200300	0.16334200
H	0.83735700	-5.23169600	0.81726700
H	3.04152700	-4.12740700	0.86392500
H	5.09528000	-1.78595800	1.07686000
H	5.89533000	0.53164900	1.33794100
H	4.54424500	2.47492100	0.75623300
C	-5.19906000	-0.04237500	1.86084800
C	-5.92285300	0.05177400	-0.55603700
H	-5.10316800	-1.65331200	0.45158400
H	-5.07729100	1.05107800	1.90841700
H	-4.50256300	-0.49185200	2.58291600
H	-6.22734600	-0.27653300	2.17510000
H	-5.75408300	-0.33956200	-1.56938400
H	-5.81074300	1.14682100	-0.59344900
H	-6.96091100	-0.16947800	-0.26557300

2-*i*Pr-TS

#p M062X/cc-pVDZ opt=(calcfc,ts,noeigen) freq scfcyc=1000

HF = -1115.5992004

0 1

C	-1.10919300	-1.76799700	-0.00003000
C	0.19440200	-2.29986300	-0.00002600
C	1.34271000	-1.31019600	-0.00003900
C	1.00668500	0.05316300	-0.00006800
C	-0.31675100	0.45609300	-0.00008000
C	-1.31058400	-0.39822400	-0.00005400
C	-2.63538200	0.00367600	-0.00002400
C	-2.96699200	1.37150900	-0.00001700
C	-1.81697500	2.36007000	-0.00002800
C	-0.51474800	1.82682400	-0.00006000
C	-2.40004900	-2.36074300	0.00000700
C	-3.41292400	-1.18469300	0.00000900
C	1.78862300	1.23759800	-0.00003700
C	0.77724600	2.41693400	-0.00003500
C	-1.77615300	3.77591500	0.00001200
C	-0.53978100	4.43634000	0.00002400
C	0.73764400	3.80529200	0.00000600
C	2.74976700	-1.47969000	0.00000100
C	3.61090900	-0.36909600	0.00002700
C	3.15236700	0.98896700	0.00001400
C	0.15520000	-3.71576300	0.00000800
C	-1.08007200	-4.37819300	0.00003500
C	-2.35840800	-3.74907800	0.00003800
C	-4.77980200	-0.93669100	0.00004500
C	-5.21185600	0.42100300	0.00004500
C	-4.37272500	1.54424200	0.00001600
H	-2.68849600	4.37510900	0.00003800
H	-0.55504900	5.52737600	0.00005900
H	1.63301500	4.42878400	0.00003200
H	3.19795300	-2.47633300	0.00002600
C	5.11358500	-0.61155200	0.00006200
H	3.89316300	1.79201600	0.00005300
H	1.06848200	-4.31355600	0.00001600
H	-1.06315400	-5.46920400	0.00006200
H	-3.25296700	-4.37373100	0.00006900
H	-5.53073500	-1.72864100	0.00007800
H	-6.28821600	0.59996300	0.00007400
H	-4.82711300	2.53692800	0.00002100
C	5.77533800	-0.04969400	-1.26207300

C	5.77533600	-0.04948200	1.26210300
H	5.26395500	-1.70281500	0.00015300
H	5.67221700	1.04583700	-1.30830600
H	5.31966100	-0.47020200	-2.16991000
H	6.85044700	-0.28399100	-1.27107800
H	5.31960400	-0.46977000	2.17001300
H	5.67230400	1.04606600	1.30812000
H	6.85042700	-0.28385500	1.27118600

2-*i*Pr-QST3

#p M062X/cc-pVDZ opt=qst3 freq scfcyc=1000

HF= -1115.5992004

0 1

C	-1.10920000	-1.76799800	0.00010200
C	0.19438500	-2.29988000	0.00003700
C	1.34271300	-1.31020400	0.00002200
C	1.00668300	0.05315700	0.00010800
C	-0.31675500	0.45609500	0.00022500
C	-1.31059200	-0.39822100	0.00021000
C	-2.63538600	0.00368800	0.00015700
C	-2.96699200	1.37151700	0.00012500
C	-1.81697400	2.36007400	0.00008200
C	-0.51475400	1.82682600	0.00017900
C	-2.40006600	-2.36072900	-0.00001400
C	-3.41293400	-1.18468600	0.00002200
C	1.78861400	1.23759600	0.00003900
C	0.77725100	2.41693300	0.00008100
C	-1.77614100	3.77592500	-0.00011000
C	-0.53977300	4.43634100	-0.00015200
C	0.73765600	3.80528600	-0.00007100
C	2.74977100	-1.47967900	-0.00008200
C	3.61091500	-0.36906600	-0.00010100
C	3.15236300	0.98897900	-0.00005300
C	0.15516600	-3.71578500	-0.00007600
C	-1.08011400	-4.37819700	-0.00015800
C	-2.35844200	-3.74906000	-0.00014500
C	-4.77980600	-0.93668400	-0.00011100

C	-5.21185900	0.42101700	-0.00007800
C	-4.37273100	1.54424900	0.00003800
H	-2.68848500	4.37511700	-0.00018600
H	-0.55502800	5.52737600	-0.00027800
H	1.63302600	4.42878000	-0.00017600
H	3.19797300	-2.47631400	-0.00013100
C	5.11359900	-0.61149200	-0.00013300
H	3.89315100	1.79203800	-0.00009100
H	1.06844200	-4.31358700	-0.00013400
H	-1.06330300	-5.46920900	-0.00023100
H	-3.25300900	-4.37370100	-0.00021200
H	-5.53074500	-1.72862900	-0.00022900
H	-6.28821900	0.59997200	-0.00018300
H	-4.82711000	2.53693800	-0.00001300
C	5.77546200	-0.04932900	-1.26209100
C	5.77530700	-0.04992800	1.26220500
H	5.26398800	-1.70274800	-0.00047700
H	5.67156100	1.04610500	-1.30868500
H	5.32056000	-0.47042200	-2.17004300
H	6.85075400	-0.28282800	-1.27029400
H	5.31970900	-0.47083200	2.16989300
H	5.67207800	1.04557400	1.30883000
H	6.85044700	-0.28409000	1.27110400

Compound 9:

9-H-reactant
#p b3lyp/cc-pVDZ opt freq=noraman
HF= -768.1950128

0 1

C	-1.20724700	-0.01539300	0.61921300
C	-0.35840300	-1.15288000	0.61908700
C	0.98583400	-0.69722400	0.61916300
C	0.96775000	0.72204500	0.61939100
C	-0.38763800	1.14344400	0.61933600
C	-2.49179300	-0.03169900	0.09527800

C	-2.97627500	-1.35255600	-0.25418700
C	-2.14397600	-2.46785700	-0.25433700
C	-0.73983900	-2.37948500	0.09502200
C	0.36664900	-3.24838100	-0.25439500
C	1.68463400	-2.80161700	-0.25444200
C	2.03454000	-1.43893200	0.09493800
C	1.99705800	1.49016000	0.09488700
C	3.18504100	0.73646500	-0.25439600
C	3.20286600	-0.65508000	-0.25437800
C	-3.00972500	1.27637900	-0.25414400
C	-2.20598100	2.41246600	-0.25441800
C	-0.80007700	2.35983500	0.09502100
C	0.28385600	3.25680000	-0.25429000
C	1.61272200	2.84350200	-0.25460800
H	-4.00136100	-1.47010300	-0.61669200
H	-2.54845100	-3.41706000	-0.61687800
H	0.16162600	-4.25972000	-0.61660700
H	2.46235000	-3.47985300	-0.61659800
H	4.10143400	-1.16252400	-0.61642800
H	-4.03753300	1.36776700	-0.61646100
H	-2.63449800	3.35112700	-0.61679700
H	0.05311600	4.26259200	-0.61643900
H	4.07027200	1.26678900	-0.61652600
H	2.37306800	3.54103500	-0.61699900

9-H-product

#p b3lyp/cc-pVDZ opt freq=noraman

HF= -768.1950209

0 1

C	-0.28574400	1.17297700	0.61962600
C	-1.20406600	0.09061500	0.61988100
C	-0.45821700	-1.11708300	0.61983200
C	0.92090700	-0.78109200	0.61972700
C	1.02741500	0.63435900	0.61946500
C	-0.58993300	2.42093900	0.09529900
C	-1.98565400	2.59662700	-0.25459700
C	-2.88600200	1.53545900	-0.25438700

C	-2.48497400	0.18706900	0.09552000
C	-3.08360200	-1.08613200	-0.25391100
C	-2.35208700	-2.27003300	-0.25463000
C	-0.94565200	-2.30503100	0.09474800
C	1.90031000	-1.61191500	0.09504600
C	1.43222100	-2.93851000	-0.25477700
C	0.08012200	-3.26781700	-0.25476700
C	0.56852600	3.21911100	-0.25451200
C	1.85601800	2.69096500	-0.25496600
C	2.12024200	1.30921900	0.09484600
C	3.23735300	0.45403500	-0.25435300
C	3.13278500	-0.93365800	-0.25459600
H	-2.32986800	3.56907700	-0.61778100
H	-3.90158400	1.71663000	-0.61744100
H	-4.11512900	-1.11326400	-0.61616800
H	-2.83808800	-3.18022100	-0.61709700
H	-0.21303200	-4.25719800	-0.61702000
H	0.42689100	4.24105600	-0.61733600
H	2.67441700	3.31911900	-0.61781400
H	4.16582400	0.90444200	-0.61645500
H	2.14748200	-3.68222900	-0.61708900
H	3.98328700	-1.51803400	-0.61675500

9-H-TS

#p b3lyp/cc-pVDZ opt=(calcfc,ts,noeigen) freq scfcyc=1000

HF = -768.1804884

0 1

C	-1.09490300	0.46831100	-0.00000100
C	0.10709800	1.18606600	-0.00000100
C	1.16110800	0.26465400	0.00000000
C	0.61050800	-1.02247800	0.00000000
C	-0.78376900	-0.89664100	0.00000000
C	-2.35427700	1.00692700	-0.00000200
C	-2.29373600	2.46974600	-0.00000300
C	-1.08648100	3.19068600	-0.00000400
C	0.23011800	2.55028000	-0.00000200
C	1.64012100	2.94470000	-0.00000300

C	2.69877600	2.01927100	-0.00000100
C	2.49657300	0.56916500	0.00000000
C	1.31282400	-2.19847100	0.00000200
C	2.75443200	-1.94267600	0.00000300
C	3.30748000	-0.64987500	0.00000200
C	-3.37030400	-0.04726800	-0.00000200
C	-3.05777000	-1.41821600	0.00000000
C	-1.68525400	-1.92793600	0.00000200
C	-0.99650600	-3.21994700	0.00000400
C	0.40396100	-3.34628700	0.00000400
H	-3.21959300	3.05154500	-0.00000200
H	-1.15973400	4.28171700	-0.00000300
H	1.90750200	4.00497700	-0.00000400
H	3.71383500	2.42592600	0.00000000
H	4.39850100	-0.57653500	0.00000500
H	-4.43050300	0.22043800	-0.00000400
H	-3.89728800	-2.11889000	0.00000200
H	-1.57855800	-4.14564400	0.00000900
H	3.45488900	-2.78238400	0.00000600
H	0.81095200	-4.36121900	0.00000700

9-H-QST3

#p b3lyp/cc-pVDZ opt=qst3 freq scfcyc=1000

HF= -768.1804951

0 1

C	0.50361600	-1.07914200	-0.00008400
C	-0.87070900	-0.81247800	0.00009600
C	-1.04175600	0.57698100	0.00001700
C	0.22685700	1.16906500	-0.00015400
C	1.18197300	0.14552300	-0.00023800
C	1.08306300	-2.32044000	0.00000100
C	0.06242300	-3.37014200	0.00019700
C	-1.31819300	-3.10230600	0.00029400
C	-1.87224200	-1.74708800	0.00027500
C	-3.18601100	-1.10080200	0.00047400
C	-3.35784400	0.29501200	0.00037300
C	-2.24009800	1.24068300	0.00003100

C	0.48773100	2.51389100	-0.00012900
C	-0.75708900	3.28461900	-0.00007200
C	-2.03143800	2.68981000	0.00006400
C	2.54314700	-2.21228900	-0.00020500
C	3.22458000	-0.98208800	-0.00035600
C	2.54161400	0.31293000	-0.00025500
C	2.88993800	1.73502600	-0.00022900
C	1.93044200	2.76323200	-0.00019700
H	0.36433100	-4.42113700	0.00006000
H	-1.99119100	-3.96417000	0.00025600
H	-4.09229600	-1.71267900	0.00057100
H	-4.38544900	0.66885100	0.00051300
H	-2.89344800	3.36262000	0.00031200
H	3.15482700	-3.11871200	-0.00028600
H	4.31743500	-1.01982700	-0.00047000
H	3.94100400	2.03667000	-0.00018700
H	-0.71922500	4.37746300	-0.00005200
H	2.30398600	3.79093900	-0.00013400

9-H-reactant

#p M062X/cc-pVDZ opt freq=noraman

HF= -767.9319213

0 1

C	0.17624800	1.19340800	0.62772700
C	-1.08059500	0.53629900	0.62794700
C	-0.84406300	-0.86215500	0.62808800
C	0.55896800	-1.06928300	0.62800400
C	1.18956100	0.20114500	0.62786600
C	0.36239300	2.45386400	0.09742800
C	-0.86112900	3.14094400	-0.25856900
C	-2.08748700	2.49979500	-0.25828900
C	-2.22179600	1.10300900	0.09766300
C	-3.25334600	0.15174100	-0.25816100
C	-3.02259800	-1.21277600	-0.25818100
C	-1.73560500	-1.77221000	0.09753300
C	1.14915600	-2.19821200	0.09743200
C	0.21945700	-3.24940000	-0.25856300

C	-1.14957400	-3.04717100	-0.25861500
C	1.73237000	2.75782900	-0.25832100
C	2.72114800	1.78957600	-0.25833700
C	2.44578400	0.41363700	0.09762200
C	3.15833900	-0.79531000	-0.25803600
C	2.54291700	-2.03484000	-0.25840000
H	-0.81110500	4.16773600	-0.62745600
H	-2.95998900	3.04449400	-0.62570200
H	-4.21448200	0.51706400	-0.62648600
H	-3.81058600	-1.87383500	-0.62553400
H	-1.79416200	-3.84818300	-0.62709100
H	1.98115300	3.75586600	-0.62570900
H	3.71333500	2.05941400	-0.62669400
H	4.18443000	-0.72376300	-0.62528600
H	0.60452400	-4.20295600	-0.62633700
H	3.10597700	-2.89516900	-0.62674300

9-H-product

#p M062X/cc-pVDZ opt freq=noraman

HF= -767.9319514

0 1

C	1.20588500	-0.04279900	0.62797800
C	0.41307800	1.13337900	0.62783200
C	-0.95025200	0.74313600	0.62757300
C	-1.00054300	-0.67412300	0.62795000
C	0.33210700	-1.16007500	0.62805700
C	2.47910600	-0.08773100	0.09766500
C	3.02598700	1.20460500	-0.25822600
C	2.25261600	2.35221700	-0.25803100
C	0.84948100	2.33050800	0.09773200
C	-0.21048900	3.24994800	-0.25851600
C	-1.54095800	2.86919500	-0.25856500
C	-1.95400500	1.52816100	0.09747300
C	-2.05718500	-1.38605900	0.09773000
C	-3.20507600	-0.57889500	-0.25809500
C	-3.15615700	0.80415500	-0.25812700
C	2.93331000	-1.41544800	-0.25821900

C	2.08062300	-2.50560500	-0.25845200
C	0.68259800	-2.38482000	0.09755800
C	-0.43988300	-3.22693200	-0.25851300
C	-1.74005700	-2.75296400	-0.25826100
H	4.05208000	1.26887000	-0.62674500
H	2.69726800	3.27915000	-0.62663000
H	0.04574300	4.24572700	-0.62693400
H	-2.28512300	3.57870500	-0.62694500
H	-4.02443100	1.35537500	-0.62587500
H	3.95244400	-1.55192600	-0.62649000
H	2.45847200	-3.46169500	-0.62721400
H	-0.25500000	-4.23809400	-0.62742100
H	-4.11013600	-1.06754300	-0.62564900
H	-2.53243900	-3.40769200	-0.62736500

9-H-TS

#p M062X/cc-pVDZ opt=(calcfc,ts,noeigen) freq scfcyc=1000

HF = -767.916182

0 1

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C	1.02793100	-0.60017800	-0.00009400
C	0.88876400	0.79184100	-0.00008400
C	-0.47836700	1.08968100	-0.00006600
C	-1.18399100	-0.11850100	-0.00007800
C	-0.54344000	-2.49502600	-0.00000900
C	0.68286900	-3.29204900	0.00003300
C	1.96279000	-2.72985700	0.00003100
C	2.20504300	-1.28767100	-0.00001400
C	3.34236400	-0.36787100	0.00004700
C	3.20328000	1.02318900	0.00003600
C	1.90632000	1.69925700	-0.00001400
C	-1.02729900	2.33789600	0.00000600
C	0.01642300	3.36222700	0.00004200
C	1.38249900	3.06478500	0.00003100
C	-1.98994700	-2.71035300	0.00005200
C	-2.92016100	-1.66686900	0.00004000
C	-2.54078400	-0.25433000	-0.00001900

C	-3.19303800	1.05467200	0.00002300
C	-2.48801900	2.26191600	0.00003700
H	0.62008500	-4.38221000	0.00003100
H	2.80805600	-3.42091300	0.00004400
H	4.35967400	-0.76489400	0.00009400
H	4.12170300	1.61362300	0.00005200
H	2.07354100	3.91006300	0.00004000
H	-2.38632300	-3.72794700	0.00010900
H	-3.97648800	-1.94319400	0.00005800
H	-4.28325500	1.11696600	0.00000800
H	-0.26035300	4.41847700	0.00005700
H	-3.07808300	3.18057200	0.00005200

Compound 10:

10-reactant
#p b3lyp/cc-pVDZ opt freq=noraman
HF= -807.4761593

0 1

C	0.47360000	1.33074600	-0.69528400
C	1.39397700	0.22907600	-0.69565700
C	0.91574500	-1.07543100	-0.69562600
C	-0.49854300	-1.32155300	-0.69580400
C	-1.38930900	-0.25530000	-0.69576900
C	-0.89516700	1.09262200	-0.69554300
C	2.59537900	0.58620100	-0.06814600
C	3.36141800	-0.46897100	0.44696400
C	2.86845400	-1.81437600	0.44650700
C	1.60186200	-2.12441700	-0.06842800
C	1.03888300	2.44942100	-0.06782000
C	0.13708800	3.39106800	0.44741800
C	-1.27464200	3.14560300	0.44688700
C	-1.80527500	1.95459500	-0.06831300
C	2.53460500	2.11705800	0.18799600
C	-2.64078400	-0.32498200	-0.06857400
C	-3.00554300	-1.57692400	0.44636600

C	-2.08697300	-2.67664500	0.44628500
C	-0.79008600	-2.54068000	-0.06868300
C	0.56616800	-3.25354800	0.18741900
C	-3.10079500	1.13649500	0.18718400
H	4.29713300	-0.27458800	0.97873600
H	3.45694300	-2.56765700	0.97790800
H	0.49513400	4.27709200	0.97930600
H	-1.91096600	3.85863000	0.97869000
H	3.20350200	2.67597500	-0.49055800
H	2.83800500	2.37020800	1.21578300
H	-3.95210100	-1.70996100	0.97782100
H	-2.38664600	-3.58450600	0.97743600
H	0.63362000	-3.64199800	1.21554000
H	0.71592100	-4.11281900	-0.49044600
H	-3.91907400	1.43667200	-0.49144400
H	-3.47184500	1.27260000	1.21496100

10-product

#p b3lyp/cc-pVDZ opt freq=noraman

HF= -807.4761407

0 1

C	1.40523300	-0.14371200	-0.69517800
C	0.80521800	1.16037700	-0.69544500
C	-0.57822300	1.28841400	-0.69518500
C	-1.40782800	0.11692400	-0.69523900
C	-0.82707700	-1.14522100	-0.69504200
C	0.60230900	-1.27753700	-0.69508100
C	1.64355200	2.09244800	-0.06860900
C	1.01949900	3.23749900	0.44615500
C	-0.40723100	3.36962500	0.44630000
C	-1.23093400	2.35866100	-0.06839700
C	2.65849100	-0.11325600	-0.06847100
C	3.12198800	-1.33214500	0.44641600
C	2.29399800	-2.50161000	0.44640700
C	0.99028200	-2.46957800	-0.06824100
C	3.00030900	1.38039900	0.18707100
C	-1.42729600	-2.24560600	-0.06801200

C	-2.71462500	-2.03743000	0.44684100
C	-3.31353700	-0.73567500	0.44680100
C	-2.63410200	0.37726300	-0.06837000
C	-2.69545100	1.90830500	0.18733100
C	-0.30469200	-3.28838100	0.18793300
H	1.59684400	3.99932300	0.97758200
H	-0.83495300	4.22449800	0.97766700
H	4.07613800	-1.38928700	0.97786400
H	2.66509200	-3.38251900	0.97782600
H	3.35987300	1.54595200	1.21461500
H	3.79184300	1.74484000	-0.49182800
H	-3.24122200	-2.83513600	0.97833100
H	-4.26188300	-0.61654000	0.97835900
H	-3.40679200	2.41211900	-0.49120700
H	-3.01805300	2.13654600	1.21513000
H	-0.34088200	-3.68162800	1.21583900
H	-0.38529500	-4.15675700	-0.49007700

10-QST2

#p b3lyp/cc-pVDZ opt=qst3 freq scfcyc=1000

HF= -807.4471558

0 1

C	-1.34594700	0.32673100	0.00017500
C	-0.37168600	1.33417900	0.00017000
C	0.95597900	1.00220100	-0.00002600
C	1.34136300	-0.34521400	-0.00018100
C	0.38995800	-1.32894200	-0.00016300
C	-0.96969500	-0.98901700	-0.00000900
C	-0.88750100	2.61258900	0.00030800
C	0.14655100	3.58646700	0.00022000
C	1.55885500	3.23335900	0.00001000
C	2.01279900	1.88740100	-0.00011900
C	-2.64092800	0.79946900	0.00042500
C	-3.57964400	-0.26666900	0.00036100
C	-3.17933800	-1.66632100	0.00005700
C	-1.81889000	-2.07495600	-0.00006900
C	-2.46810400	2.38673300	0.00056600

C	0.62814300	-2.68673800	-0.00029200
C	2.02076600	-2.96664100	-0.00045200
C	3.03276500	-1.92018200	-0.00043300
C	2.70641900	-0.53773600	-0.00029600
C	3.30100000	0.94410400	-0.00021800
C	-0.83286700	-3.33079800	-0.00018600
H	-0.07620800	4.65721400	0.00041100
H	2.25925400	4.07333700	0.00007800
H	-4.65727700	-0.08008800	0.00043300
H	-3.99531000	-2.39455000	0.00012700
H	-2.94105100	2.84402200	-0.88346900
H	-2.94061300	2.84370800	0.88500800
H	2.39787100	-3.99324000	-0.00049300
H	4.07139700	-2.26279000	-0.00055400
H	3.93326900	1.12491400	0.88403600
H	3.93326500	1.12505200	-0.88442600
H	-0.99239400	-3.96891800	-0.88433800
H	-0.99219700	-3.96878400	0.88408900

10-reactant

#p M062X/cc-pVDZ opt freq=noraman

HF= -807.200978

0 1

C	0.81574100	-1.15043900	-0.70367100
C	-0.61623400	-1.26848700	-0.70337500
C	-1.40425800	-0.13131800	-0.70360600
C	-0.79037900	1.16769100	-0.70326200
C	0.58844500	1.28142700	-0.70323900
C	1.40687400	0.10057600	-0.70374800
C	-1.01001300	-2.44926300	-0.06800500
C	-2.30673200	-2.46592500	0.45214900
C	-3.11971100	-1.29276100	0.45181700
C	-2.64832300	-0.08485600	-0.06873700
C	1.39758000	-2.25075400	-0.06855600
C	2.67946800	-2.05493600	0.45192600
C	3.28925800	-0.76448400	0.45188400
C	2.62645500	0.34998000	-0.06876400

C	0.27038900	-3.27796200	0.18843700
C	1.25033300	2.33542400	-0.06768300
C	0.44001500	3.34742800	0.45304700
C	-0.98240600	3.23030800	0.45274000
C	-1.61605500	2.09925400	-0.06810600
C	-2.97447900	1.40524300	0.18678300
C	2.70412800	1.87342700	0.18685500
H	-2.67978200	-3.33828300	0.99297900
H	-4.06738500	-1.33497400	0.99288500
H	3.18992000	-2.85426700	0.99350200
H	4.23073400	-0.65085400	0.99347800
H	0.34171300	-4.14366500	-0.48908600
H	0.30223200	-3.66235200	1.21737600
H	0.87730500	4.18911900	0.99421400
H	-1.55182700	3.98926900	0.99347300
H	-3.32583100	1.57093200	1.21471300
H	-3.75779600	1.77583100	-0.49350700
H	3.41574600	2.36729400	-0.49382800
H	3.02439900	2.09451800	1.21449700

10-product

#p M062X/cc-pVDZ opt freq=noraman

HF= -807.200872

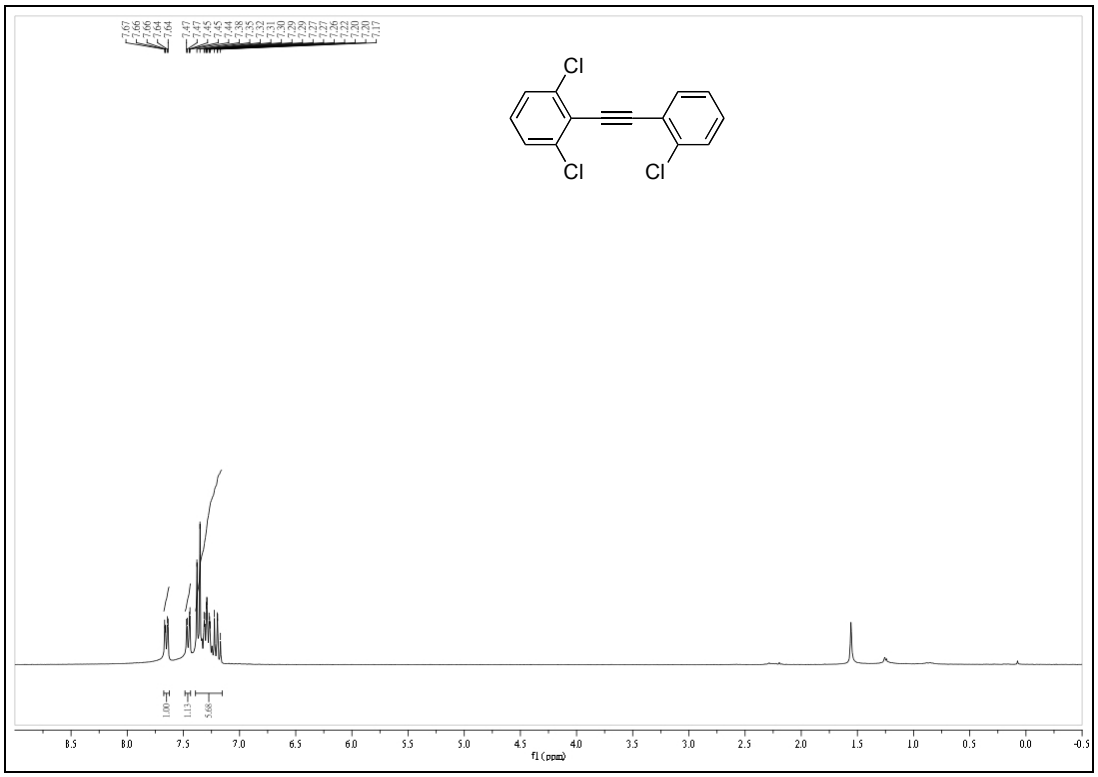
0 1

C	-0.76375600	-1.18540700	-0.70314700
C	0.67188000	-1.23987800	-0.70360600
C	1.40854500	-0.06866200	-0.70398200
C	0.73785900	1.20199800	-0.70418700
C	-0.64483000	1.25438900	-0.70419400
C	-1.40974600	0.03807600	-0.70367300
C	1.11776400	-2.40181000	-0.06806800
C	2.41375200	-2.36115400	0.45269700
C	3.17353500	-1.15311600	0.45215500
C	2.64912500	0.03250600	-0.06879300
C	-1.29635600	-2.31044600	-0.06755200
C	-2.58575400	-2.17162200	0.45243100
C	-3.25211100	-0.90946300	0.45146100

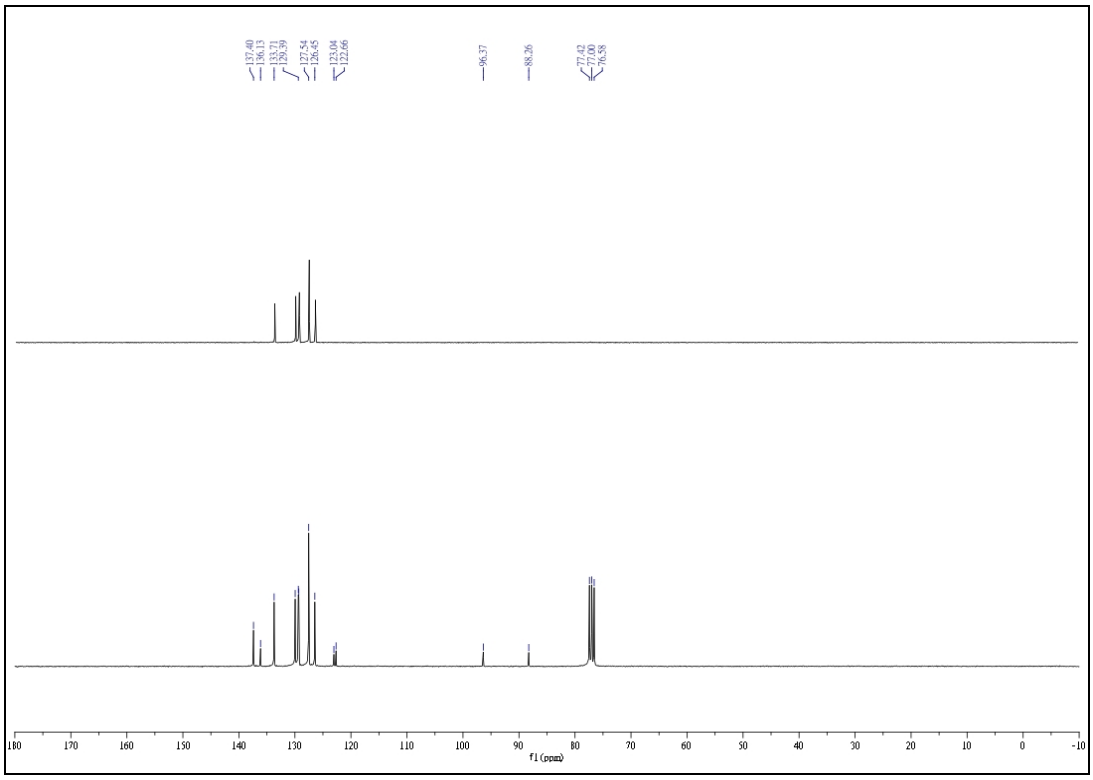
C	-2.63919700	0.23317200	-0.06886300
C	-0.12442700	-3.28696900	0.18768300
C	-1.35285300	2.27797300	-0.06890700
C	-0.58794500	3.32469200	0.45271800
C	0.83812200	3.27022400	0.45329600
C	1.52141000	2.16867600	-0.06823400
C	2.90901800	1.53553000	0.18701400
C	-2.78422800	1.75138000	0.18779700
H	2.82386500	-3.21580900	0.99495300
H	4.12242800	-1.15268600	0.99277500
H	-3.06009000	-2.99303200	0.99358900
H	-4.19873600	-0.83764900	0.99130000
H	-0.13915100	-3.67529700	1.21554400
H	-0.15716300	-4.15289500	-0.49259100
H	-1.06184700	4.14619000	0.99435000
H	1.37301600	4.05246600	0.99611700
H	3.67521700	1.94058500	-0.49315000
H	3.25283500	1.71665600	1.21482900
H	-3.10953800	1.95646100	1.21720500
H	-3.51968600	2.21448700	-0.48920700

C. NMR spectra and VT-NMR Experiments

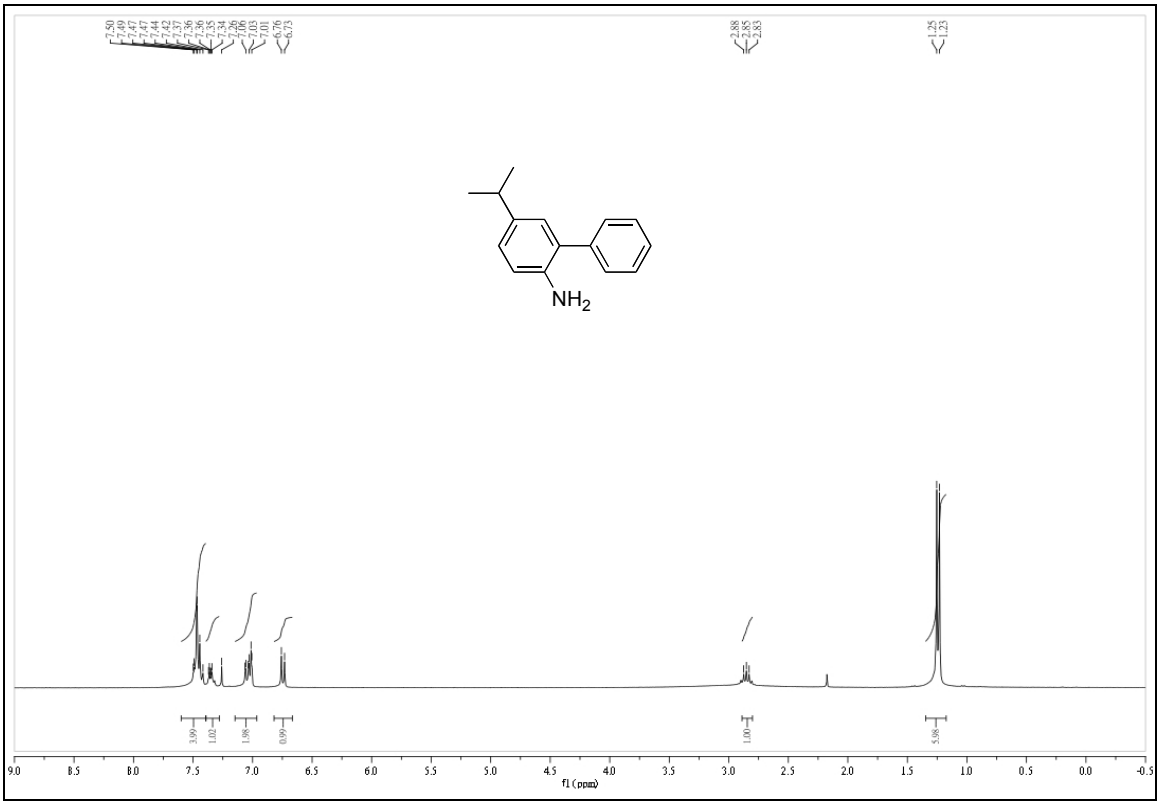
^{1}H-NMR spectrum of alkyne **8** (300 MHz, $CDCl_3$):



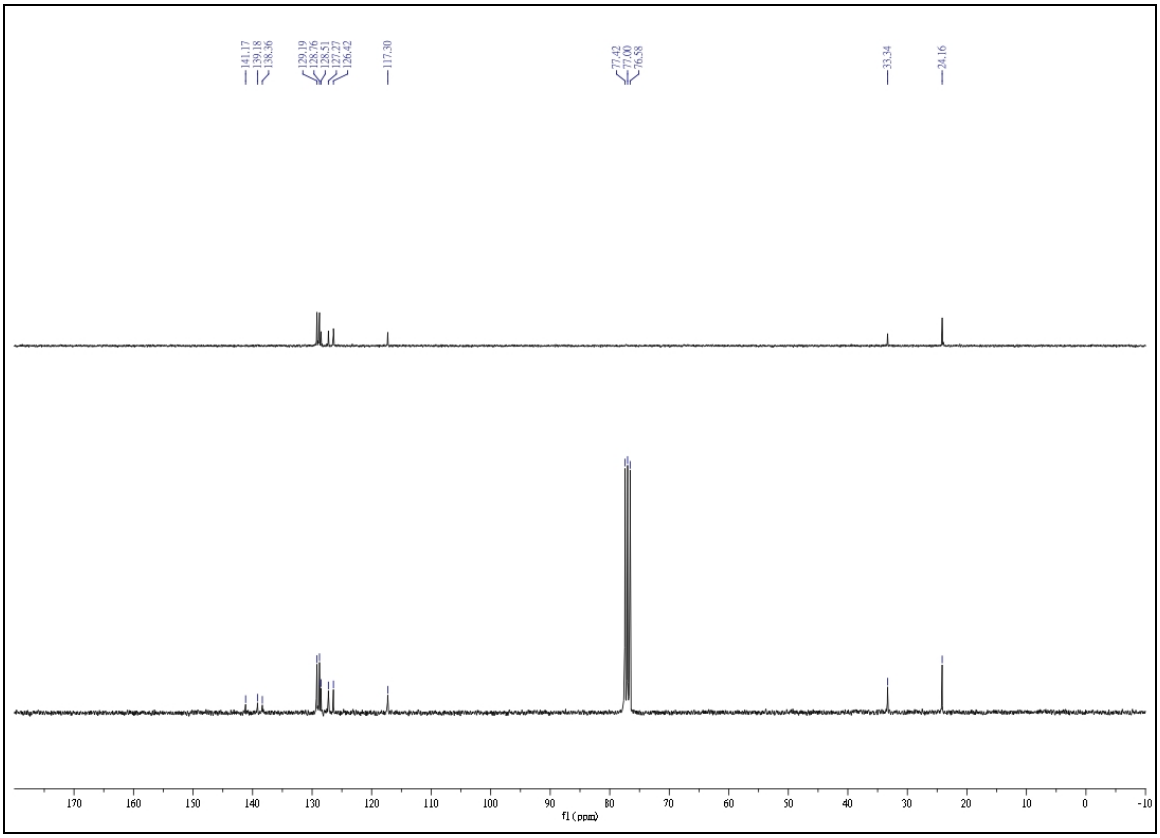
^{13}C-NMR spectrum of 2,2',6-trichlorodiphenylethyne (75.5 MHz, $CDCl_3$):



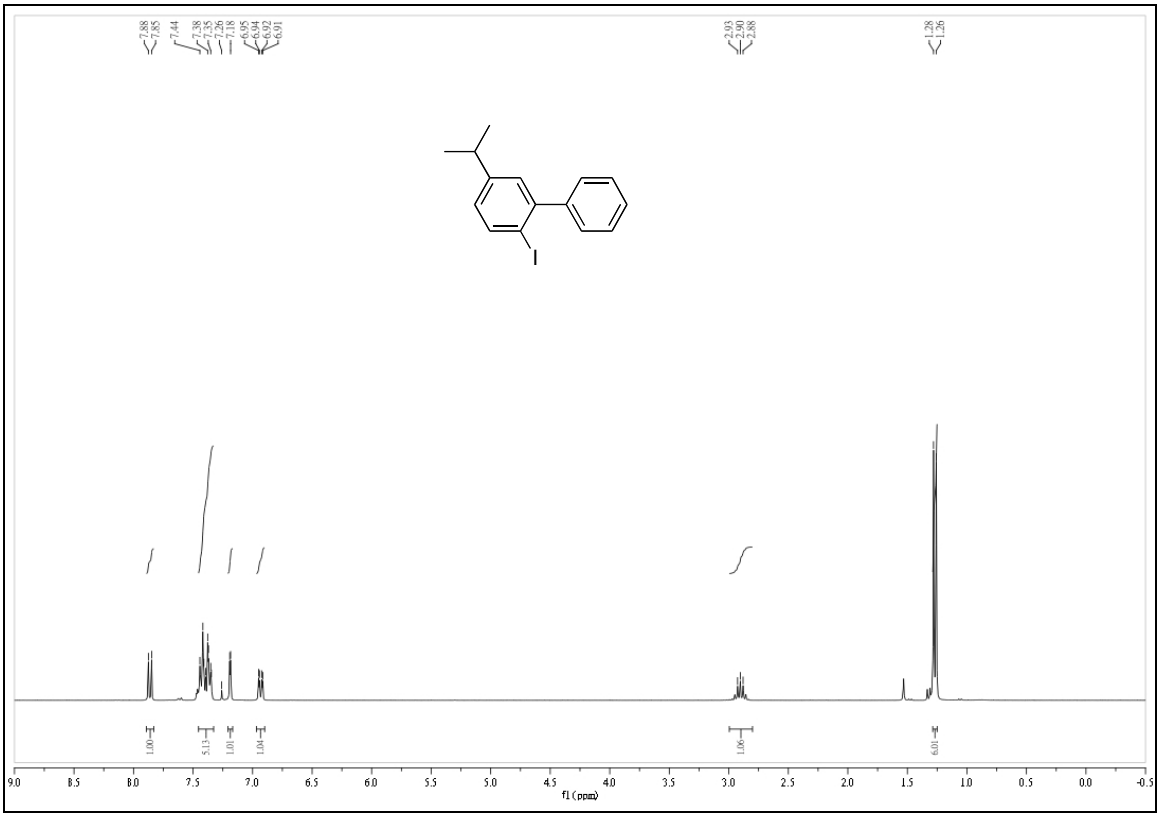
^{1}H-NMR spectrum of 3-isopropyl-2-phenylaniline (300 MHz, $CDCl_3$):



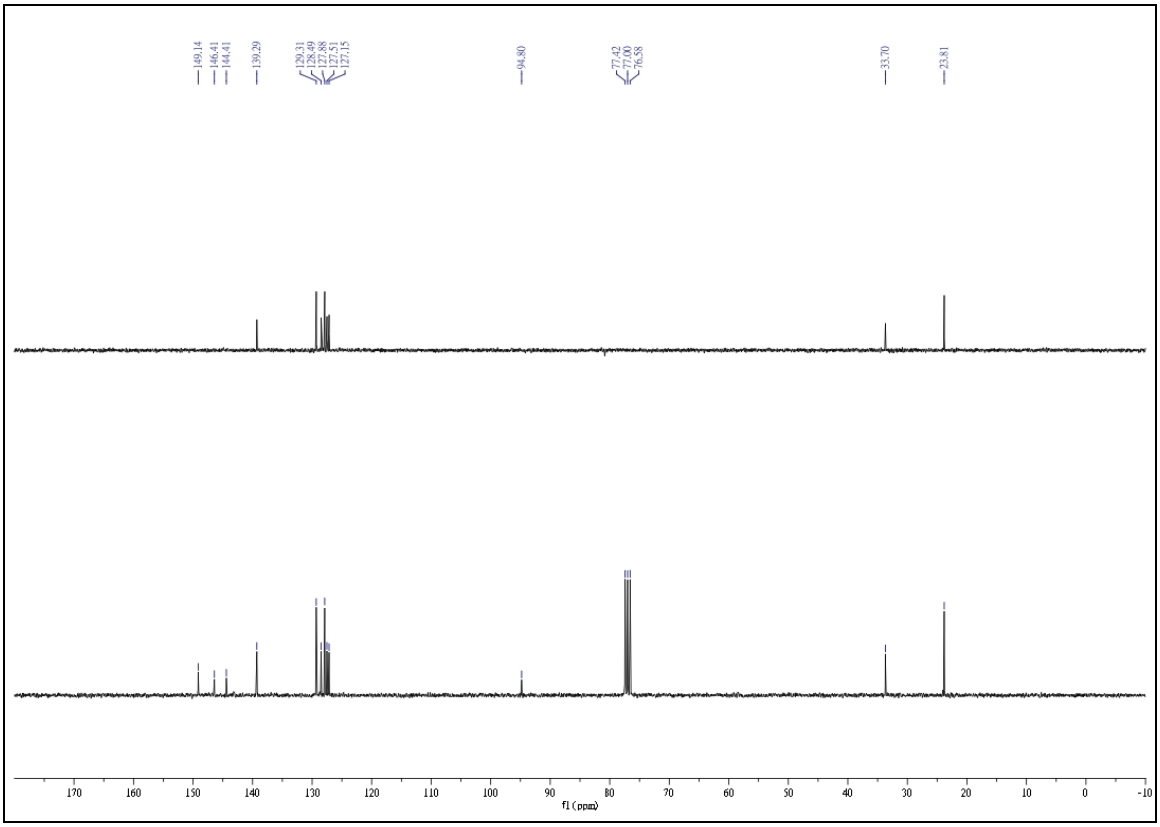
^{13}C-NMR spectrum of 2-phenyl-4-isopropylaniline (75.5 MHz, $CDCl_3$):



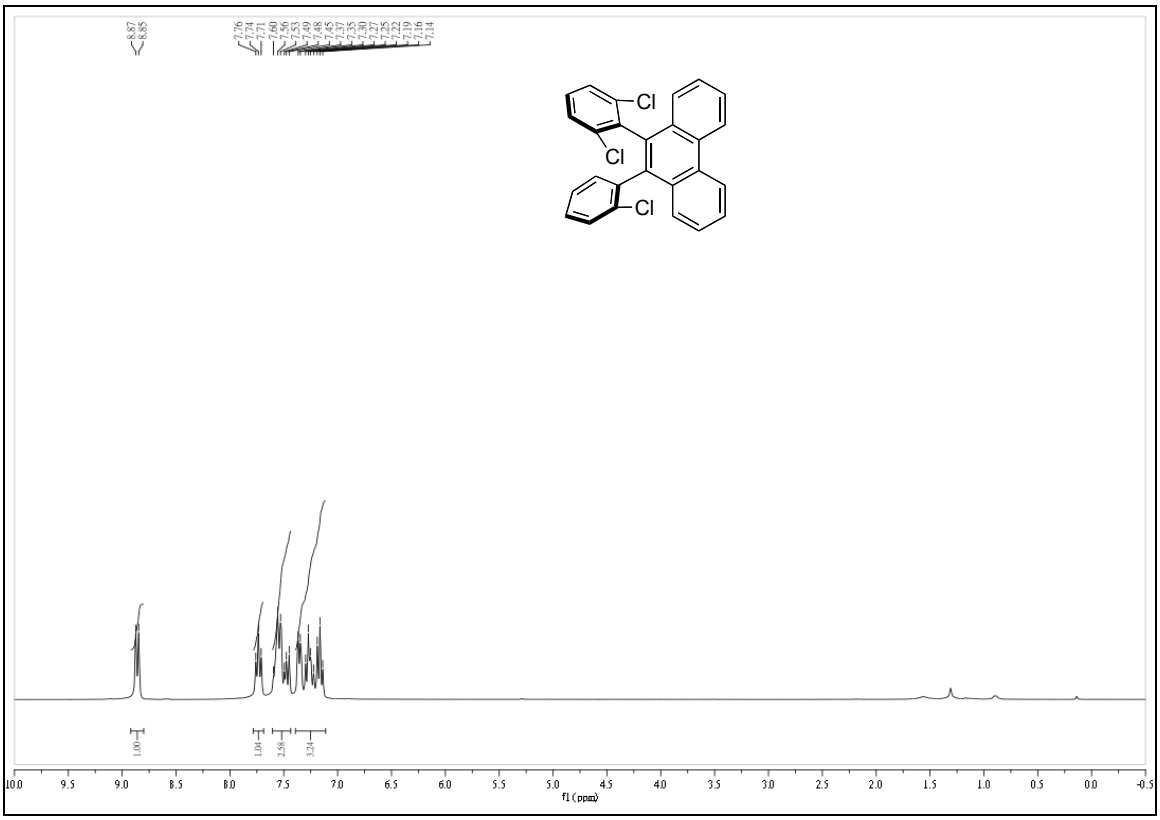
^{1}H-NMR spectrum of biphenyl **7**-*i*Pr (300 MHz, $CDCl_3$):



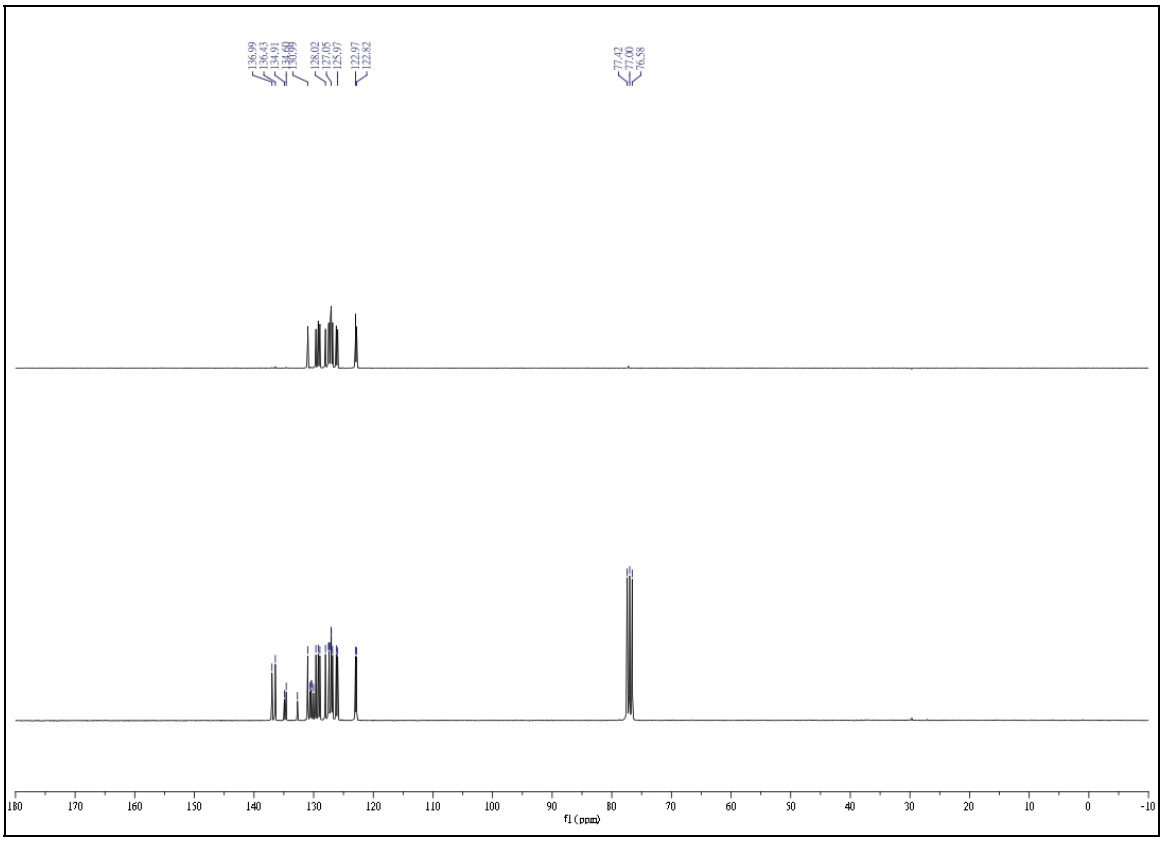
^{13}C-NMR spectrum of biphenyl **7**-*i*Pr (75.5 MHz, $CDCl_3$):



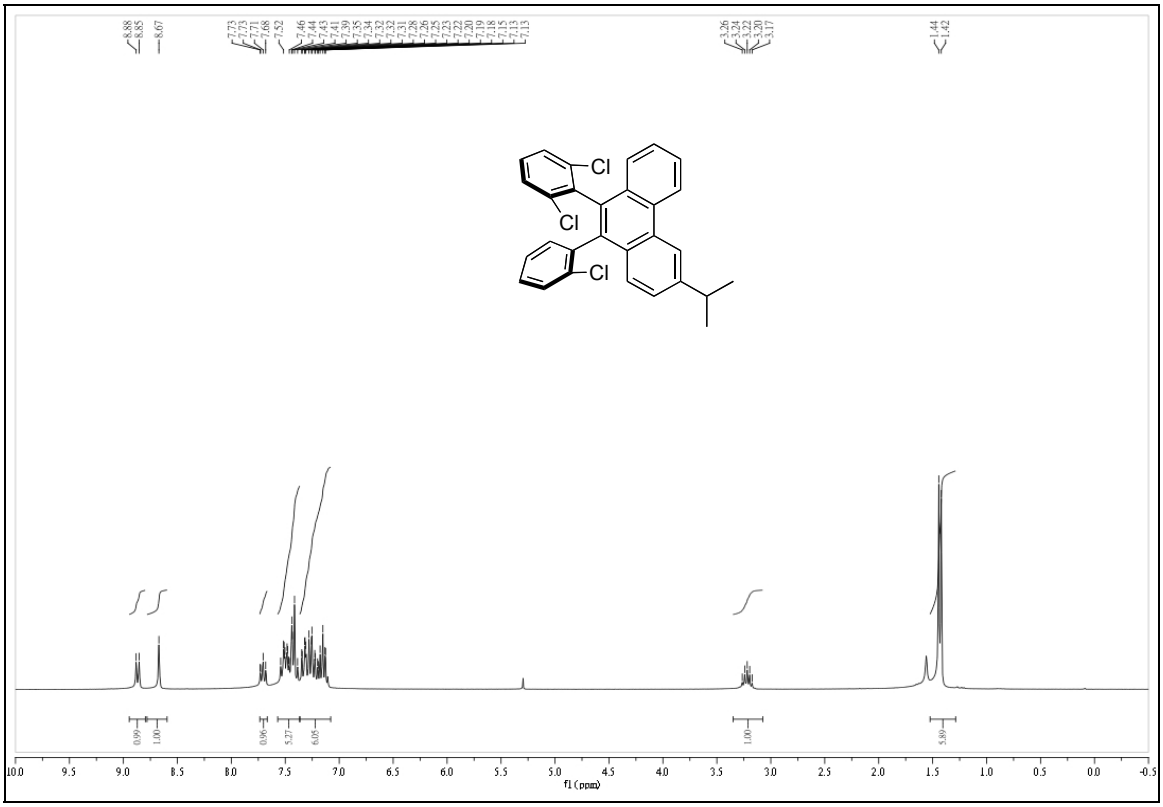
^{1}H-NMR spectrum of phenanthrene **3**-H (300 MHz, $CDCl_3$):



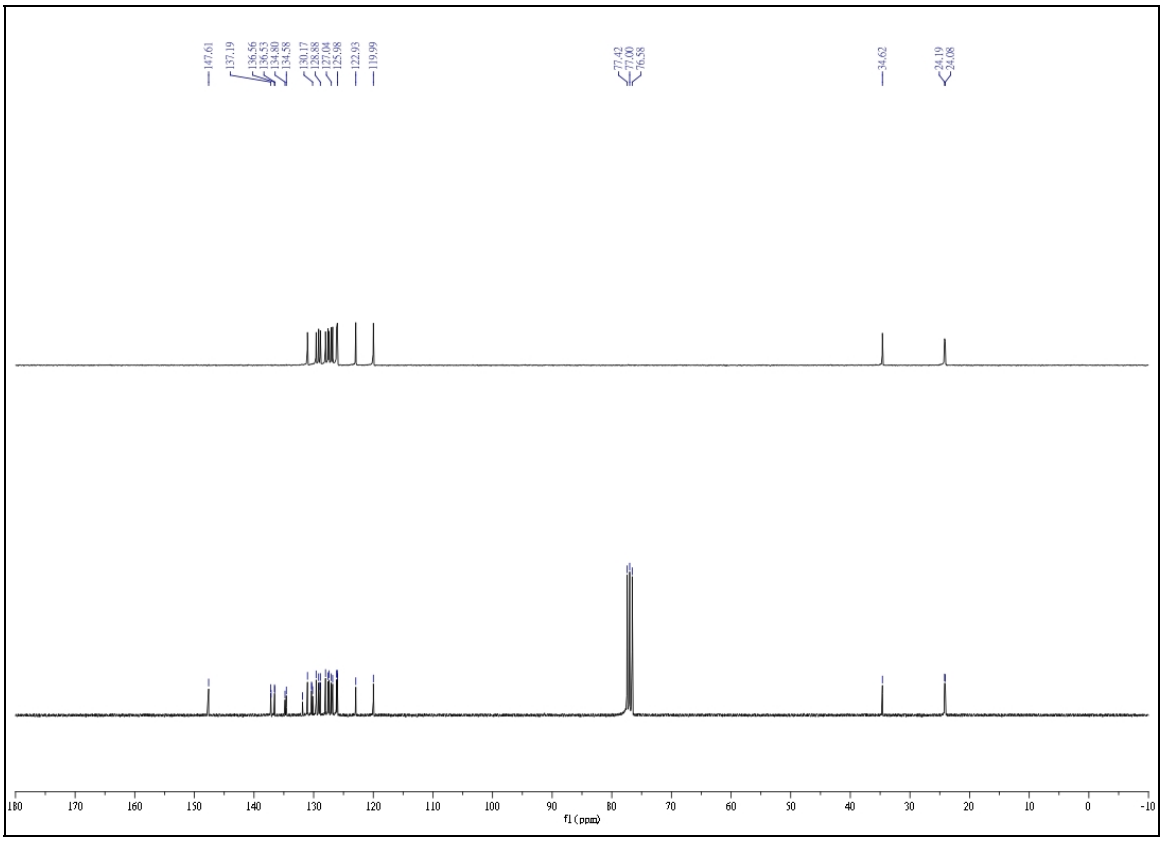
^{13}C-NMR spectrum of phenanthrene **3**-H (75.5 MHz, $CDCl_3$):



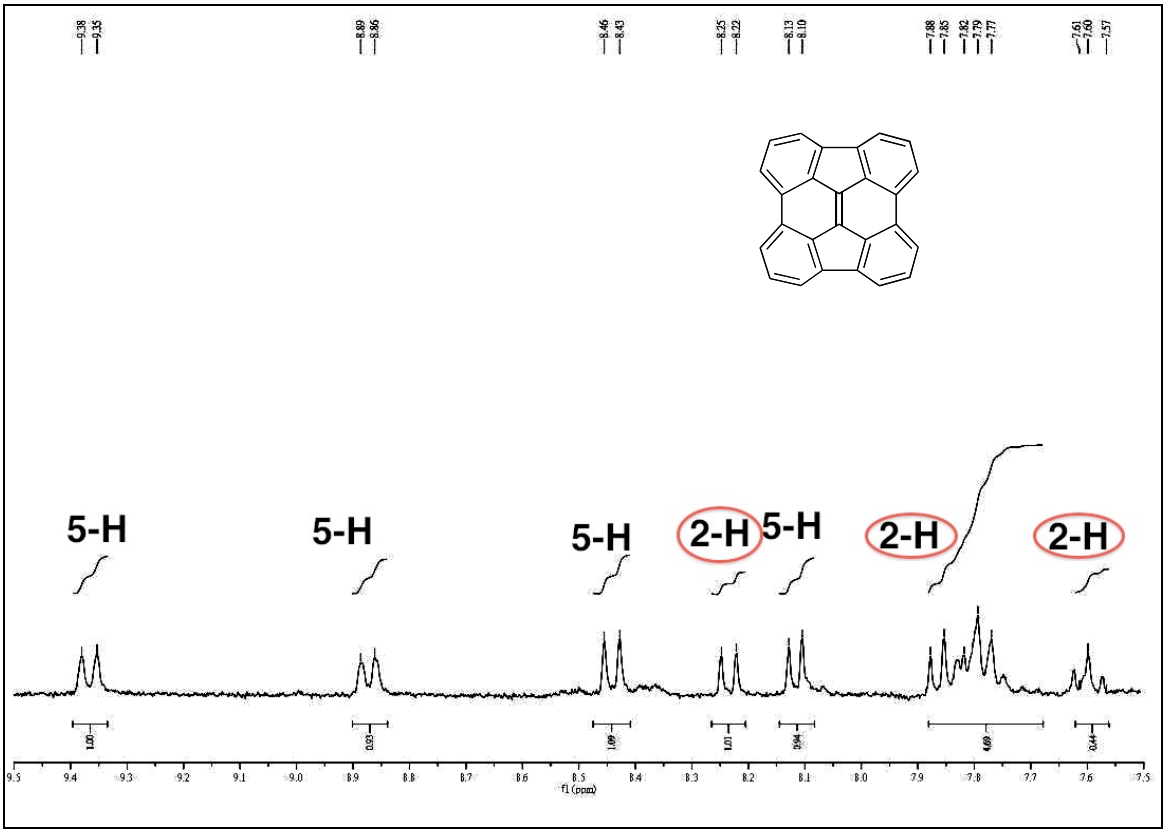
^{1}H-NMR spectrum of phenanthrene **3**-*i*Pr (300 MHz, $CDCl_3$):



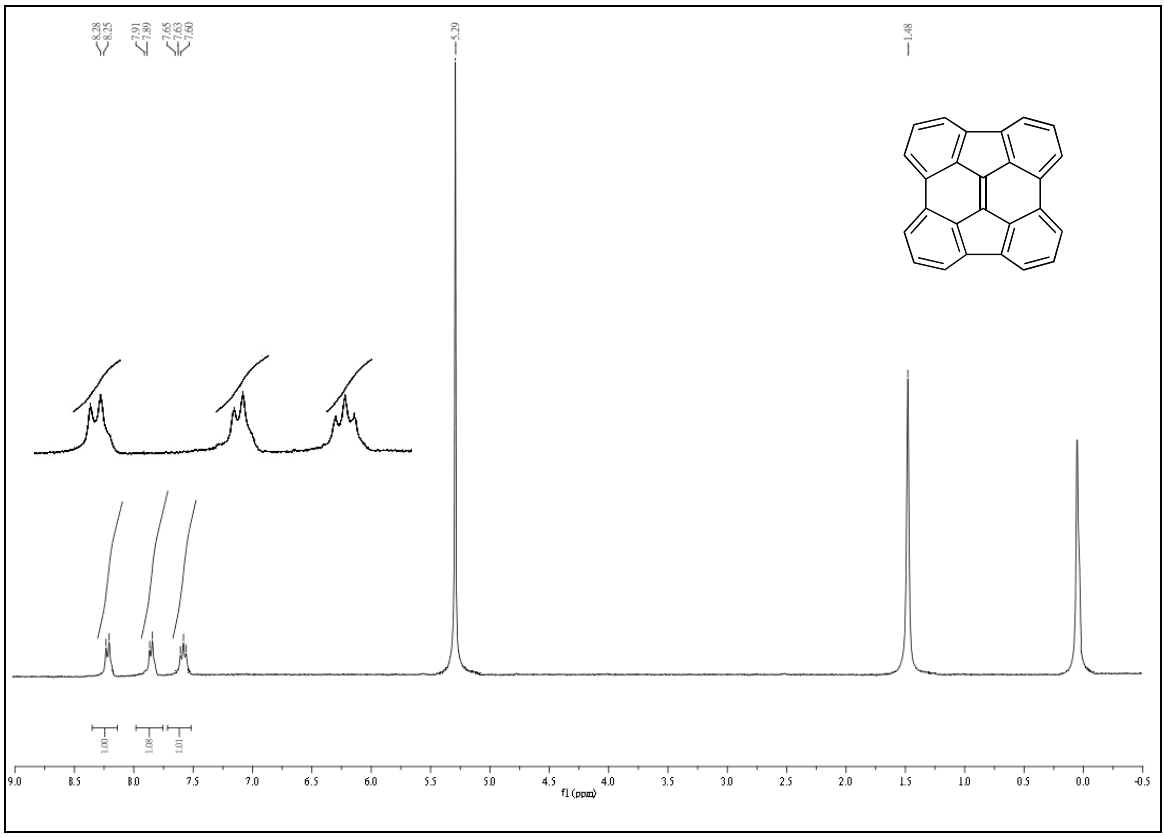
^{13}C-NMR spectrum of phenanthrene **3**-*i*Pr (75.5 MHz, $CDCl_3$):



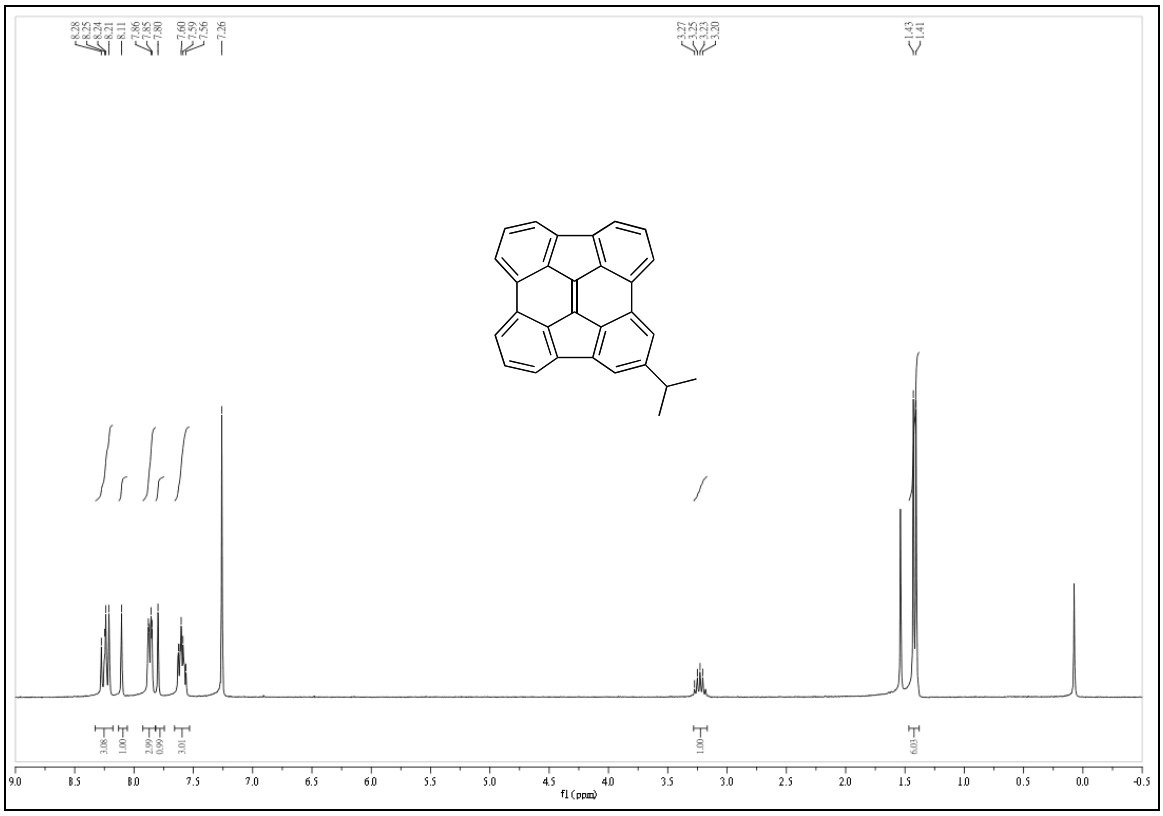
^{1}H-NMR spectrum of **crude** bulkybowl **2**-H (300 MHz, $CDCl_3$):



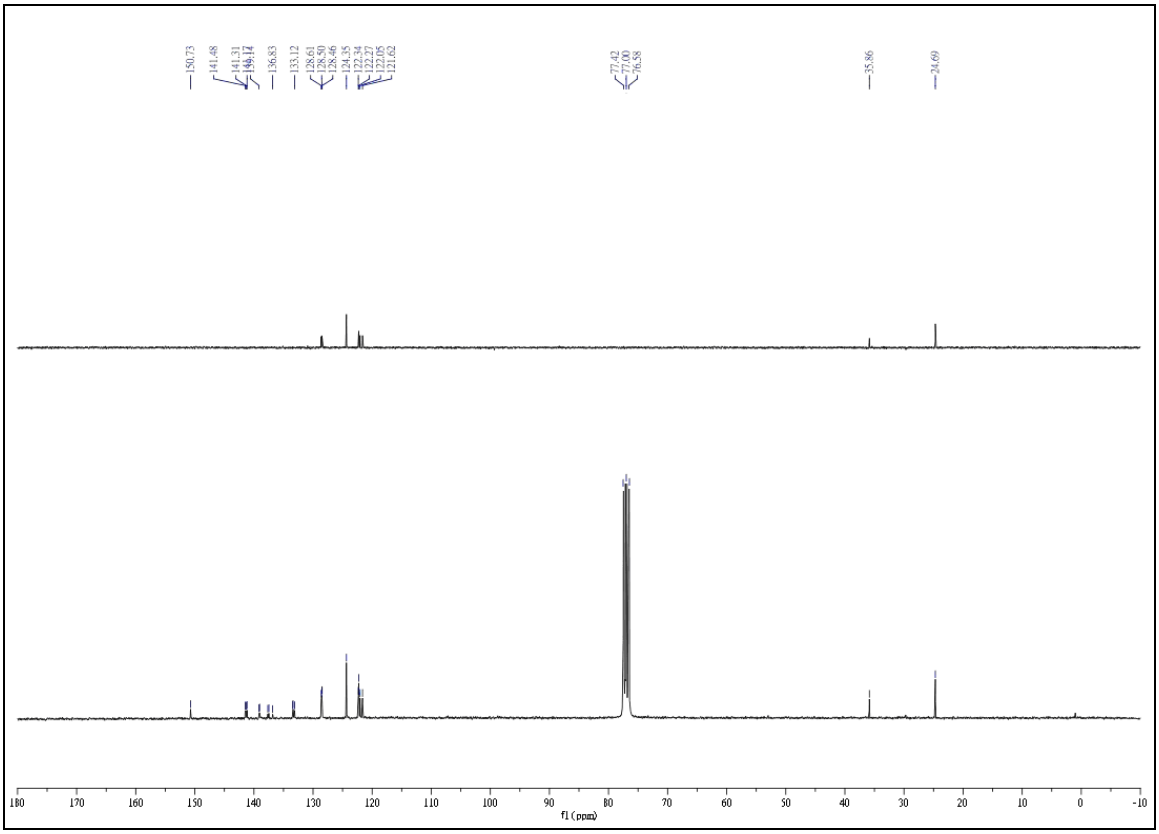
^{1}H-NMR spectrum of bulkybowl **2**-H (300 MHz, CD_2Cl_2):



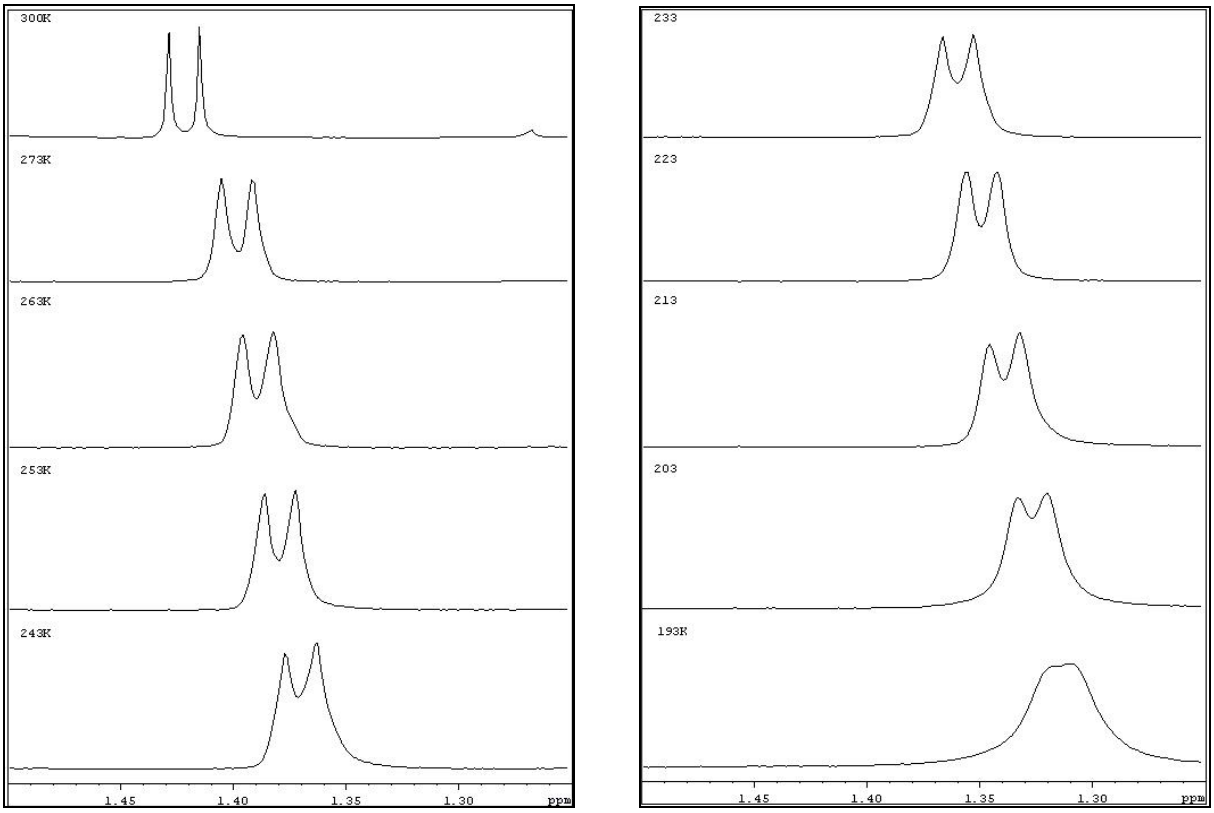
^{1}H-NMR spectrum of bulkybowl **2**-*i*Pr (300 MHz, CD_2Cl_2):



^{13}C-NMR spectrum of bulkybowl **2**-*i*Pr (75.5 MHz, CD_2Cl_2):



Variable temperature ^{1}H-NMR spectra of bulkybowl **2**-*i*Pr (500 MHz, CD_2Cl_2):
Signals of the aryl and benzylic protons do not show significant difference.



D. Reference

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S2. L. Liu, Y. Zhang, Y. Wang, *J. Org. Chem.*, 2005, **70**, 6122.

S3. H. E. Bronstein, N. Choi and L. T. Scott, *J. Am. Soc. Chem.*, 2001, **124**, 8870.