Supporting Information

Ene Reaction of Arynes with Alkynes

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Experimental Section

General: All reactions were conducted under nitrogen atmosphere on a dual-manifold Schlenk line unless otherwise mentioned and in oven-dried glass wares. Acetonitrile was dried with CaH_2 and distilled prior to use. Aryne precursors¹ **1a-f** were synthesized according to the literature procedures. Alkyne α,α -dideuteriobenzylethyne ($\text{C}_6\text{H}_5\text{CD}_2\text{CCH}$) (**2l**) was prepared according to the literature procedure.² 18-crown-6 was dried under vacuum at 80°C overnight and recrystallized from acetonitrile. KF was dried at 150°C under vacuum. Other reagents were commercially available and used as purchased.

Density functional theory (DFT) was applied in this study. We chose the three-parameter mixing of the exchange functional of Becke,³ and the correlation functional of Lee, Yang, and Parr (B3LYP).⁴ The geometries of minima and transition states (TSs) fully optimized with analytic gradients at the B3LYP/6-31G* level. Harmonic vibrational frequency calculations and thermal corrections were then performed at the stationary points. The GAUSSIAN 98 suite of programs has been used in this work. Optimized geometries and relative energy diagram of the reaction of benzyne and propyne (Figure 1S) (page S-8).

General procedure for the synthesis of phenylallenes (3): A 25-mL round-bottom side-arm flask containing KF (1.50 mmol) 18-crown-6 (1.75 mmol) was evacuated and purged with nitrogen gas three times. To the flask were then added THF followed by aryne precursor (**1**) (0.50 mmol) and alkyne (**2**) (2.00 mmol) via syringes. The reaction mixture was allowed to stir at room temperature for 6 h. At the end of the reaction, the reaction mixture was diluted with CH_2Cl_2 , filtered through Celite and silica gel. The filtrate was concentrated and the residue was purified through a silica gel column using hexane as eluent to give pure **3**. Compounds **3a-r**, **4** were prepared by following this procedure.

Procedure for the synthesis of 9-tert-butylphenanthrene (5): A 25-mL round-bottom side-arm flask containing KF (1.50 mmol) 18-crown-6 (1.75 mmol) was evacuated and purged with nitrogen gas three times. To the flask were then added THF followed by benzyne precursor (**1**) (0.50 mmol) and 3,3-dimethyl-1-butyne (**2l**) (0.25 mmol) via syringes. The reaction mixture was allowed to stir at room

temperature for 6 h. At the end of the reaction, the reaction mixture was diluted with CH₂Cl₂, filtered through Celite and silica gel. The filtrate was concentrated and the residue was purified through a silica gel column using hexane as eluent to give pure **5**.

Spectral data of **3a-h**, **3k-o**, **3q**, **3r-d**, **3k-d₂**, **4**, **5** and copies ¹H and ¹³C NMR of all compounds (**3a-q**, **3r-d**, **3k-d₂**, **4**, **5**) are given below:

References:

1. (a)Himeshima, Y.; Sonoda, T.; Kobayashi, H. *Chem. Lett.* **1983**, 1211. (b) Peña, D.;Pérez, D.; Guitián, E.; Castedo, L. *J. Am. Chem. Soc.* **1999**, *121*, 5827.
2. Coperet, C.; Sugihara, T.; Wu, G.; Shimoyama, I.; Negishi E.-I. *J. Am. Chem. Soc.* **1995**, *117*, 3422.
3. Becke, A. D., *J. Chem. Phys.*, **1993**, *98*, 5648.
4. Lee, C., Yang, W., and Parr, R. G., *Phys. Rev. B*, **1988**, *37*, 785.

Complete Reference 12:

Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.;Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Zakrzewski, V. J.; Montgomery, Jr. J. A.; Stratmann, R. E.; Burant, J. C.; Daprich, S.; Millam, J. M.; Daniels, A. D.; Kudin, K. N.; Strain, M. C.; Farkas, O.; Tomasi, J.; Barone, V.; Cossi, M.; Cammi, R.; Mennucci, D.; Pomelli, C.; Adamo, C.; Clifford, S.; Ochterski, J.; Petersson, G. A.; Ayala, P. Y.; Cui, Q.; Morokuma, K.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Cioslowski, J.; Ortiz, J. V.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz,T.; Komaromi, I.; Gomperts, R.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Gonzalez, C.; Challacombe M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Andres, J. L.; Gonzalez, C.; Head-Gordon, M.; Replogle, E. S.; Pople, J. A. *Gaussian 98*, revision A.3; Gaussian,Inc.:Pittsburgh, PA, 1998.

1-(Hexa-1,2-dienyl)benzene (3a): colorless oil; $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 7.27-7.24 (m, 4H), 7.15-7.13 (m, 1H), 6.10-6.08 (m, 1H), 5.30 (q, $J = 13.3$, $J = 6.6$ Hz, 1H), 2.10-2.06 (m, 2H), 1.50-1.46 (m, 2H), 0.94 (t, $J = 7.2$ Hz, 3H); $^{13}\text{C NMR}$ (150 MHz, CDCl_3): δ 205.2, 135.1, 128.5, 126.5(2C), 94.9, 94.5, 30.8, 22.4, 13.7; **HRMS** calcd for $\text{C}_{12}\text{H}_{14}$ 158.1096, found 158.1091. **IR** 1951 cm^{-1} **CAS Registry Number:** [13633-27-7]

1-(4-Methylpenta-1,2-dienyl)benzene (3b): colorless oil; $^1\text{H NMR}$ (400 MHz, CDCl_3): δ 7.33-7.29 (m, 4H), 7.24-7.16 (m, 1H), 6.21-6.19 (m, 1H), 5.62 (t, $J = 6.0$ Hz, 1H), 2.50-2.44 (m, 1H), 1.12 (dd, $J = 7.2$ Hz, $J = 3.2$ Hz, 6H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3): δ 203.7, 135.2, 128.5, 126.6, 126.5, 102.4, 95.7, 28.4, 22.6, 22.5; **HRMS** calcd for $\text{C}_{12}\text{H}_{14}$ 158.1096, found 158.1100. **IR** 1947 cm^{-1} **CAS Registry Number:** [141821-03-6]

1-(3-Cyclopentylpropa-1,2-dienyl)benzene (3c): colorless oil; $^1\text{H NMR}$ (400 MHz, CDCl_3): δ 7.27-7.24 (m, 4H), 7.19-7.15 (m, 1H), 6.16-6.13 (m, 1H), 5.62 (t, $J = 6.8$ Hz, 1H), 2.64-2.56 (m, 1H), 1.87-1.80 (m, 2H), 1.64-1.43 (m, 6H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3): δ 204.0, 135.2, 128.5, 126.6, 126.5, 100.0, 95.3, 39.2, 32.9, 32.8, 24.9(2C); **HRMS** calcd for $\text{C}_{14}\text{H}_{16}$ 184.1252, found 184.1257. **IR** 1947 cm^{-1}

1,3-Diphenylpropa-1,2-diene (3d): colorless solid; $^1\text{H NMR}$ (400 MHz, CDCl_3): δ 7.36-7.21 (m, 10H), 6.58 (m, 2H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3): δ 207.8, 133.6, 128.7, 127.3, 127.0, 98.4; **HRMS** calcd for $\text{C}_{15}\text{H}_{12}$ 192.0939, found 192.0933; **IR** 1940 cm^{-1} **CAS Registry Number:** [19753-98-1]

1-(Hepta-1,2-dien-6-ynyl)benzene (3e): colorless oil; $^1\text{H NMR}$ (400 MHz, CDCl_3): δ 7.34-7.28 (m, 4H), 7.22-7.18 (m, 1H), 6.22-6.19 (m, 1H), 5.66 (q, $J = 6.4$, $J = 3.2$ Hz, 1H), 2.41-2.37 (m, 4H), 1.99 (t, $J = 2.4$, 1H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3): δ 205.2, 134.6, 128.5, 126.9, 126.7, 95.6, 93.4, 83.7, 68.9, 28.0, 18.4; **HRMS** calcd for $\text{C}_{13}\text{H}_{12}$, 168.0939 found 168.0943; **IR** 1948 cm^{-1} , 2114 cm^{-1} , 3303 cm^{-1} .

1-(3-Bromopropa-1,2-dienyl)benzene (3f): colorless oil; $^1\text{H NMR}$ (400MHz, CDCl_3): δ 7.35-7.32 (m, 4H), 7.29-7.23 (m, 1H), 6.34 (d, $J = 5.6$ Hz, 1H), 6.30 (d, $J = 6.0$ Hz, 1H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3):

δ 202.9, 131.7, 128.8, 128.6, 127.9, 102.6, 74.8; **HRMS** calcd for C_9H_7Br 193.9731, found 193.9727; **IR** 1943 cm^{-1} **CAS Registry Number**: [33992-52-8]

1-(3-Chloropropa-1,2-dienyl)benzene (3g): colorless oil; **1H NMR** (400MHz, $CDCl_3$): δ 7.35-7.34 (m, 4H), 7.29-7.27 (m, 1H), 6.50 (d, $J = 6.0$ Hz, 1H), 6.41 (d, $J = 6.0$ Hz, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 203.5, 132.2, 128.8, 128.6, 127.9, 103.8, 91.3; **HRMS** calcd for C_9H_7Cl 150.0236, found 150.0233. **IR** 1945 cm^{-1} **CAS Registry Number**: [64788-21-2]

4-(Hexa-3,4-dien-3-yl)-1,2-dimethylbenzene (3h): colorless oil; **1H NMR** (400 MHz, $CDCl_3$): δ 7.15-7.05 (m, 3H), 5.47-5.44 (m, 1H), 2.41-2.34 (m, 2H), 2.22 (s, 3H), 2.18 (s, 3H), 1.74 (d, $J = 5.6$ Hz, 3H), 1.09 (t, $J = 7.2$ Hz, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 204.1, 136.3, 135.1, 134.7, 129.5, 127.2, 123.3, 106.6, 89.7, 22.3, 19.9, 19.4, 14.5, 12.6; **HRMS** calcd for $C_{14}H_{18}$ 186.1409, found 186.1404; **IR** 1942 cm^{-1}

1

5-(3-Phenylpropa-1,2-dienyl)benzo[d][1,3]dioxole (3k): yellow oil; **1H NMR** (400 MHz, $CDCl_3$): δ 7.33-7.27 (m, 4H), 7.22-7.20 (m, 1H), 6.84 (d, $J = 1.6$ Hz, $H6$, 1H), 6.78 (dd, $J = 8.0, 1.6$ Hz, $H2$, 1H), 6.74 (d, $J = 8.0$ Hz, $H3$, 1H), 6.56 (d, $J = 6.4$ Hz, allenyl C-H, 1H), 6.50 (d, $J = 6.4$ Hz, allene C-H, 1H), 5.91 (q, $J = 2.8, 1.6$ Hz, 2H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 207.2, 148.1, 147.1, 133.7, 128.7, 127.5, 127.3, 126.9, 120.8 (C2), 108.4, 106.7, 101.0, 98.6 (allenyl C-H), 98.2 (allenyl C-H); **HRMS** calcd for $C_{16}H_{12}O_2$ 236.0837, found 236.0825.

5-(3-Deutero-3-phenylpropa-1,2-dienyl)-6-deutero benzo[d][1,3]dioxole (3k- d_2): yellow oil; **1H NMR** (400 MHz, $CDCl_3$): δ 7.33-7.27 (m, 4H), 7.22-7.20 (m, 1H), 6.84 (s, $H6$, 1H), 6.75 (s, $H3$, 1H),

6.52 (s, *H*7, 1H), 5.92 (q, *J* = 3.2 Hz, *J* = 1.6 Hz, 2H); ¹³C NMR (150 MHz, CDCl₃): δ 207.2, 148.1, 147.1, 133.7, 128.7, 127.5, 127.3, 126.9, 108.3, 106.7, 101.1, 98.3 (allenyl C-H); HRMS calcd for C₁₆H₁₀D₂O₂ 238.0963, found 238.0956. The coupling patterns (all singlets) of protons H1, H3 and H6 are in agreement with the assigned structure. The ¹³C signals for C2 and C9 were not observed. These observations also support the presence of deuterium at these two carbons. See also **3k** (unlabelled version of **3k-d₂**)

4-(Hexa-1,2-dienyl)-1,2-dimethylbenzene (3l): colorless oil; ¹H NMR (400 MHz, CDCl₃): δ 7.11-7.06 (m, 3H), 6.13-6.10 (m, 1H), 5.58 (q, *J* = 13.2 Hz, *J* = 6.4 Hz, 1H), 2.37-2.21 (m, 6H), 2.18-2.12 (m, 2H), 1.60-1.31 (m, 2H), 1.02 (t, *J* = 7.2 Hz, 3H); ¹³C NMR (150 MHz, CDCl₃): δ 204.9, 136.6, 135.0, 132.5, 129.8, 127.8, 124.1, 94.6, 94.3, 30.9, 22.4, 19.7, 19.4, 13.7; HRMS calcd for C₁₄H₁₈ 186.1409, found 186.1415; IR 1944 cm⁻¹

5-(Hexa-1,2-dienyl)-2,3-dihydro-1H-indene (3m): colorless oil; ¹H NMR (600 MHz, CDCl₃): δ 7.16-7.13 (m, 2H), 7.05 (d, *J* = 7.2 Hz, 1H), 6.11-6.09 (m, 1H), 5.52 (q, *J* = 13.2, *J* = 6.6 Hz, 1H), 2.87-2.85 (m, 4H), 2.11-2.03 (m, 4H), 1.51-1.47 (m, 2H), 0.95 (t, *J* = 7.5 Hz, 3H); ¹³C NMR (100 MHz, CDCl₃): δ 204.9, 144.7, 142.9, 133.0, 124.7, 124.4, 122.4, 94.7, 94.6, 32.8, 32.6, 30.9, 25.5, 22.4, 13.7; HRMS calcd for C₁₅H₁₈, 198.1409 found 198.1412; IR 1947 cm⁻¹

5-(Hepta-1,2-dienyl)benzo[d][1,3]dioxole (3n): colorless oil; ¹H NMR (400 MHz, CDCl₃): δ 6.80 (s, 1H), 6.73-6.68 (m, 2H), 6.05-6.02 (m, 1H), 5.93 (d, *J* = 12.4 Hz, 2H), 5.53 (q, *J* = 13.2, *J* = 6.4 Hz, 1H), 2.13-2.07 (m, 2H), 1.48-1.34 (m, 4H), 0.90 (t, *J* = 7.5 Hz, 3H); ¹³C NMR (100 MHz, CDCl₃): δ 204.5, 148.0, 146.5, 129.3, 120.2, 108.3, 106.5, 100.9, 95.3, 94.4, 31.3, 28.5, 22.2, 13.8; HRMS calcd for C₁₄H₁₆O₂ 216.1150, found 216.1156; IR 1942 cm⁻¹.

1,2-Difluoro-4-(hexa-1,2-dienyl)benzene (3o): colorless oil; ¹H NMR (400 MHz, CDCl₃): δ 7.09-7.03 (m, 2H), 7.01-6.92 (m, 1H), 6.03-6.00 (m, 1H), 5.57 (q, *J* = 13.2, *J* = 6.4 Hz, 1H), 2.12-2.06 (m, 2H), 1.53-1.23 (m, 2H), 0.94 (t, *J* = 7.2 Hz, 3H); ¹³C NMR (150 MHz, CDCl₃): δ 205.2, 150.7(dd), 149.0(dd),

132.4, 122.3, 117.2(d), 114.8(d), 95.7, 93.1, 30.6, 22.3, 13.7; **HRMS** calcd for C₁₂H₁₂F₂, 194.0907 found 194.0911. **IR** 1948 cm⁻¹.

1-(Hexa-1,2-dienyl)-3-methoxybenzene (3q): colorless oil; ¹H NMR (600 MHz, CDCl₃): δ 6.95 (t, 1H), 6.61 (d, *J* = 12.0 Hz, 1H), 6.59 (s, 1H), 6.48 (d, *J* = 10.2 Hz, 1H), 5.85-5.83 (m, 1H), 5.31-5.30 (m, 1H), 3.54 (s, 3H), 1.87-1.83 (m, 2H), 1.31-1.24 (m, 2H), 0.71 (t, *J* = 7.5 Hz, 3H); ¹³C NMR (150 MHz, CDCl₃): δ 205.3, 159.8, 136.6, 129.5, 119.3, 112.4, 111.7, 94.9, 94.4, 55.1, 30.8, 22.4, 13.7; **HRMS** calcd for C₁₃H₁₆O, 188.1201 found 188.1204. **IR** 1943 cm⁻¹.

4-(1-Deutero-hepta-1,2-dienyl)-1,2-dimethylbenzene (3r-d): colorless oil; ¹H NMR (600 MHz, CDCl₃): δ 7.06-7.01 (m, 3H), 5.53 (t, *J* = 1.8 Hz, 3H), 2.24 (s, 3H), 2.23 (s, 3H), 2.13-2.09 (m, 2H), 1.47-1.36 (m, 4H), 0.90 (t, *J* = 7.2 Hz, 3H); ¹³C NMR (150 MHz, CDCl₃): δ 204.8, 136.6, 135.0, 132.5, 129.8, 127.7, 123.9, 94.9, 94.1(t), 31.3, 28.5, 22.2, 19.7, 19.4, 13.9; **HRMS** calcd for C₁₅H₁₉D 201.1628, found 201.1630; **IR** 1951 cm⁻¹

1-(3,3-Dimethylbut-1-ynyl)benzene (4): white solid; ¹H NMR (400 MHz, CDCl₃): δ 7.40-7.38 (m, 2H), 7.27-7.25 (m, 3H), 1.32 (s, 9H); ¹³C NMR (100 MHz, CDCl₃): δ 131.5, 128.1, 127.4, 124.1, 98.4, 79.0, 31.0, 27.9; **HRMS** calcd for C₁₂H₁₄ 158.1096, found 158.1092. **CAS Registry Number:** [4250-82-2]

9-tert-Butylphenanthrene (5): white powder; ¹H NMR (400 MHz, CDCl₃): δ 8.04 (dd, *J* = 5.2, *J* = 2.8 Hz, 1H), 8.64 (d, *J* = 7.2 Hz, 1H), 8.55 (dd, *J* = 7.2, *J* = 4.4 Hz, 1H), 7.87 (d, *J* = 7.6 Hz, 1H), 7.77 (s, 1H), 7.64-7.57 (m, 4H), 1.71 (s, 9H); ¹³C NMR (100 MHz, CDCl₃): δ 144.0, 131.8, 131.7, 130.8, 129.6, 128.7, 127.6, 126.5, 126.2, 125.4, 125.3, 124.1, 123.7, 122.2, 35.9, 31.8; **HRMS** calcd for C₁₈H₁₈, 234.1409 found 234.1414. **CAS Registry Number:** [17024-05-4]

Figure 1S: The optimized geometries (in Å and deg) and the relative energies (in kcal/mol) of the pathways at B3LYP/6-31G* level (Energetics including zero-point vibrational energy ZPVE corrections are included in the parenthesis).

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PROCNO 1

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F2 - Processing parameters
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 1.538
 1.532
 1.521
 1.118
 1.114
 1.103
 1.100
 1.095
 1.084
 1.082
 1.077

Current Data Parameters
NAME J2-185
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060115
Time 18.11
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg30
TD 32768
SFO 500.135090 MHz
CQPC13
AQ 469
RG 0
SM 45945.047 Hz
FIDRES 1.374666 Hz
AQ 0.383748 sec
RG 11.100 usec
RG 11.100 usec
RG 6.50 usec
RG 0.0 K
RG 3.0000000 sec
RG 0.0000000 sec
RG 2.9000010 sec
RG 0.0000000 sec
RG 0.0000000 sec
RG 0.0000000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 4.50 usec
PL1 0.00 dB
SFO1 150.760970 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
P2 92.00 usec
PL2 120.00 dB
PL12 11.00 dB
PL13 11.00 dB
SFO2 500.502975 MHz

F2 - Processing parameters
SI 32768
SF 150.744429 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 0.50

1D NMR 2D parameters
CY 250.00 cm
CY 4.50 cm
P1P 220.0000 ppm
F1 33163.77 Hz
F2P 0.0000 ppm
F2 0.00 Hz
F2PC 11.0000 ppm/cm
F2CN 1658.18895 Hz/cm

13C OBSERVE
207.15

exp3 std13c
date Jan 14 2006
solvent CDCl3
file ACQUISITION
sfrq 100.785
at 0.635
np 32000
fb 13800
bs 4
tpwr 58
pw 6.5
di 2.000
tor 2000.0
nt 100000
wfs
gain not used
proc 4
fn not used
ft
wft

DEC. & VT
dfrq 400.454
dn H1
dpr 42
dof 0
dm yyy
dem w
der PROCESSING 8000
lb wfile
wfile
proc 4
fn not used
ft
wft

flags
11 n
in n
dp y
display -0.2
sp 22152.3
wp 50
vs 0
sc 0
wc 250
hzm 88.61
ls 500.00
rf1 9839.1
thp 7753.3
tms 100.000
nm no ph

146.154
147.116
133.709
128.716
128.442
128.213
127.765
127.678
127.510
127.296
126.960
125.724
125.525
122.197
120.836
108.347
106.775
102.454
101.339
101.232
101.079
100.881
98.636
98.316

77.321
77.000
76.695

Current Data Parameters
NAME J2-110
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20050721
Time 14.23
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg30
TD 32768
SOLVENT CDCl₃
NS 1348
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 2048
IN 11.100 usec
DE 6.50 usec
TE 298.7 K
D1 4.0000000 sec
d11 0.0300000 sec
DELTA 3.9000010 sec
MCREST 0.0000000 sec
PCORR 0.0150000 sec

===== CHANNEL f1 =====
NUC1 ¹³C
P1 9.00 usec
PL1 -2.00 dB
SFO1 150.7876323 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 ¹H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 9.80 dB
PL13 14.00 dB
SFO2 599.6029980 MHz

F2 - Processing parameters
SI 65536
SF 150.7876323 MHz
WDW EM
SSB 0
LB 5.00 Hz
GB 0
PC 0.50

1D NMR plot parameters
CX 20.00 cm
CY 4.50 cm
FIP 220.000 ppm
F1 33189.30 Hz
F2 0.000 ppm
F2 0.00 Hz
PRACH 11.00000 ppm/cm
H2CN 1658.46497 Hz/cm

STANDARD 1H OBSERVE

expl stdih
 SAMPLE
 date Aug 3 2005 dfrq 400.454
 solvent CDCl3 dn H1
 file ACQUISITION exp 42
 sfrq 400.455 dpr 0
 tn 400.455 dm nm
 at 2.664 H1
 np 32016 lb PROCESSING 8000
 sw 6000.6 wffile 0.10
 tb 3400 proc ft
 tpr 58 fn not used
 pw 8.0
 d1 1.000 werr
 nt 500.0 wexp wft
 ct 16 wbs wft
 clock 0 wnt
 gain not used
 flags
 il n
 in n
 dp n
 SP DISPLAY y
 wp -200.4
 vs 4204.5
 sc 100
 wc 250
 hzmm 16.82
 fl 384.62
 rf 384.62
 rfp 2895.3
 th
 ins 10.000
 nm cdc ph

7.240
 7.200
 7.173
 7.163
 7.104
 7.000
 6.996
 6.104
 6.097
 6.089
 6.075
 5.956
 5.947
 5.940
 5.931
 5.928

2.326
 2.320
 2.130
 2.121
 2.112
 2.103
 2.095
 2.066
 2.060
 1.540
 1.532
 1.525
 1.521
 1.514
 1.503
 1.496
 1.490
 1.485
 1.477
 1.466
 0.981
 0.970
 0.963
 0.952
 0.944

Current Data Parameters
NAME J-187
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20051128
Time 17.45
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SNH 8389.262 Hz
FIDRES 0.756020 Hz
AQ 1.9510228 sec
RG 128
DM 59.600 usec
DE 6.50 usec
TE 296.8 K
D1 1.50000000 sec
MCREST 0.00000000 sec
MCWRR 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 11.50 usec
PL1 3.00 dB
SFO1 599.5035970 MHz

F2 - Processing parameters
SI 16384
SF 599.5001711 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 15.00 cm
F1P 9.500 ppm
F1 5695.25 Hz
F2P -0.500 ppm
F2 -299.75 Hz
PPMCM 0.50000 ppm/cm
HZCM 299.75009 Hz/cm