

SUPPORTING INFORMATION

Exploiting the π -Acceptor Properties of Carbene-Stabilized Phosphorus Centered Trications $[L_3P]^{3+}$: Applications in Pt(II) Catalysis

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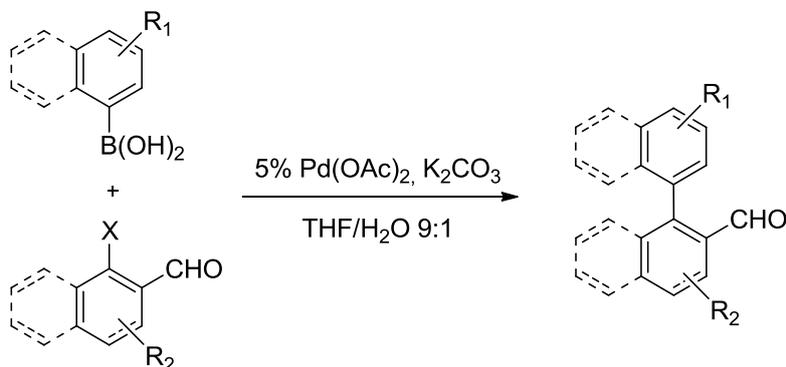
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Experimental procedures:

General: All reactions were carried out in flame-dried glassware under Ar. All solvents were purified by distillation over the drying agents indicated and were transferred under Ar. IR: Nicolet FT-7199 spectrometer, wavenumbers in cm^{-1} . MS (EI): Finnigan MAT 8200 (70 eV), ESIMS: Finnigan MAT 95, accurate mass determinations: Bruker APEX III FT-MS (7 T magnet). NMR: Spectra were recorded on a Bruker AV 400; ^1H and ^{13}C chemical shifts (δ) are given in ppm relative to TMS, coupling constants (J) in Hz. The solvent signals were used as references and the chemical shifts converted to the TMS scale. All flash chromatography was performed on Merck 60 silica gel (40-63 μm). Thin-layer chromatography (TLC) analysis was performed using Merck silica gel 60 F254 TLC plates, and visualized by UV and/or phosphomolybdic acid 10% in EtOH.

All commercially available compounds (Acros, ABCR, Alfa Aesar, Aldrich) were used as received. 1-Chloro-3,4-dihydro-naphthalene-2-carbaldehyde, compounds **4**, **6**, **9a**, **9b**, **10a**, **10b** and Ohira-Bestmann reagent were prepared according to literature procedures.¹

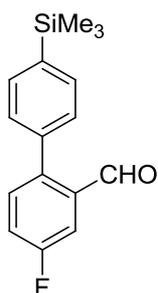
General Procedure for the Suzuki coupling



A suspension of the corresponding aldehyde, the boronic acid (1.1 eq.), Pd(OAc)_2 (0.02 eq.) and K_2CO_3 (2.5 eq.) in degassed mixture of THF and water (9:1) was vigorously stirred overnight at room temperature. The mixture was diluted with water, the aqueous phase was extracted with EtOAc, the combined organic layers were dried over Na_2SO_4 and evaporated, and the crude product was purified by flash chromatography.

¹(a) Mamane, V.; Fürstner, A. *J. Org. Chem.* **2002**, *67*, 6264-6267; (b) Mamane, V.; Hannen, P.; Fürstner, A. *Chem Eur. J.* **2004**, *10*, 4556-4575.; (c) Müller, S.; Liepold, B.; Roth, G. J.; Bestmann, H. J. *Synlett* **1996**, 521-522; (d) Callant, P.; D'Haenens, L.; Vandewalle, M. *Synth. Commun.* **1984**, *14*, 155-161.

Compound 9c:



Prepared from 2-bromo-5-fluorobenzaldehyde (406 mg, 2.00 mmol) and 4-(trimethylsilyl)phenylboronic acid (407 mg, 2.10 mmol) following the general procedure and purified by flash chromatography (hexanes/EtOAc, 15/1). White solid (418 mg, 77%).

¹H NMR (400 MHz, CDCl₃) δ = 0.33 (s, 9H), 7.31 - 7.38 (m, 3H), 7.45 (dd, *J* = 8.5, 5.2 Hz, 1H), 7.61 - 7.65 (m, 2H), 7.70 (dd, *J* = 8.9, 2.8 Hz, 1H), 9.93 (d, *J* = 3.3 Hz, 1H) ppm.

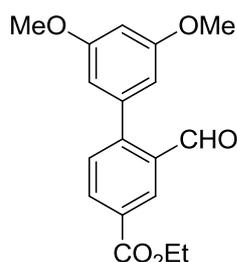
¹³C NMR (101 MHz, CDCl₃) δ = -1.0, 113.8 (d, *J* = 22.4 Hz), 121.0 (d, *J* = 22.0 Hz), 129.6, 132.9 (d, *J* = 7.3 Hz), 133.7, 135.5 (d, *J* = 6.4 Hz), 137.2, 140.9, 142.3 (d, *J* = 3.2 Hz), 162.4 (d, *J* = 249.2 Hz), 191.4 ppm.

¹⁹F NMR (376 MHz, CDCl₃) δ = -113.2 ppm.

HRMS calcd. for C₁₆H₁₇O₁F₁Si₁: 272.103275; found 272.103039.

IR (neat) $\bar{\nu}$ = 655, 692, 733, 759, 776, 815, 834, 887, 968, 1005, 1087, 1112, 1147, 1206, 1248, 1262, 1392, 1415, 1481, 1505, 1581, 1605, 1688, 2956 cm⁻¹.

Compound 9e:



Prepared from ethyl 4-bromo-3-formylbenzoate (364 mg, 2.00 mmol) and (3,5-dimethoxyphenyl)boronic acid (512 mg, 2.00 mmol) following the general procedure and purified by flash chromatography (hexanes/EtOAc, 15/1). White solid (475 mg, 75%).

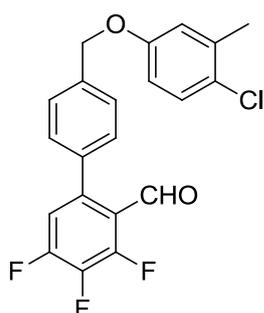
¹H NMR (400 MHz, CDCl₃) δ = 1.42 (t, *J* = 7.1 Hz, 3H), 3.83 (s, 6H), 4.43 (q, *J* = 7.1 Hz, 2H), 6.50 (d, *J* = 2.2 Hz, 2H), 6.56 (t, *J* = 2.2 Hz, 1H), 7.53 (d, *J* = 8.0 Hz, 1H), 8.27 (dd, *J* = 8.0, 1.8 Hz, 1H), 8.64 (d, *J* = 1.8 Hz, 1H), 10.02 (s, 1H) ppm.

¹³C NMR (101 MHz, CDCl₃) δ = 14.5, 55.7, 61.6, 100.6, 108.4, 129.0, 130.4, 130.9, 134.0, 134.1, 139.0, 149.7, 161.0, 165.7, 191.6 ppm.

HRMS calcd. for C₁₈H₁₈O₅Na₁: 337.104646; found 337.104791.

IR (neat) $\bar{\nu}$ = 694, 731, 764, 830, 856, 872, 920, 949, 991, 1021, 1035, 1059, 1101, 1114, 1157, 1199, 1220, 1242, 1257, 1292, 1328, 1336, 1366, 1422, 1461, 1472, 1562, 1593, 1692, 1717, 2882, 2986 cm⁻¹.

Compound 9f:



Prepared from 6-bromo-2,3,4-trifluorobenzaldehyde (200 mg, 0.84 mmol) and (4-((4-chloro-3-methylphenoxy)methyl)phenyl)boronic acid (252 mg, 0.92 mmol) following the general procedure and purified by flash chromatography (hexanes/EtOAc, 85/15). White solid (194 mg, 59%).

¹H NMR (400 MHz, CDCl₃) δ = 2.35 (s, 3H), 5.10 (s, 2H), 6.75 (dt, *J* = 8.1, 4.1 Hz, 1H), 6.88 (d, *J* = 2.9 Hz, 1H), 7.06 (ddd, *J* = 10.0, 6.6, 2.0

Hz, 1H), 7.23 (d, $J = 8.7$ Hz, 1H), 7.31 - 7.37 (m, 2H), 7.54 (d, $J = 8.3$ Hz, 2H), 9.84 (dd, $J = 1.6$, 0.9 Hz, 1H) ppm.

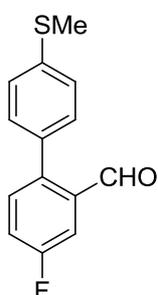
^{13}C NMR (101 MHz, CDCl_3) δ 20.4, 69.6, 113.4, 114.6 (dd, $J = 18.0$, 3.7 Hz), 117.5, 120.4 (t, $J = 3.6$ Hz), 126.5, 127.7, 129.8, 130.0, 135.4, 137.3, 138.1, 139.6 (dt, $J = 255.3$, 14.9 Hz), 141.5 (ddd, $J = 8.5$, 4.5, 1.4 Hz), 151.5 (ddd, $J = 267.2$, 10.4, 4.5 Hz), 153.2 (ddd, $J = 259.4$, 9.9, 4.4 Hz), 157.2, 187.3 ppm.

^{19}F NMR (376 MHz, CDCl_3) $\delta = -124.5$ (dd, $J = 20.7$, 13.8 Hz), -136.5 (dd, $J = 19.5$, 13.8 Hz), -159.5 (s, $J = 20.1$ Hz) ppm.

HRMS calcd. for $\text{C}_{21}\text{H}_{14}\text{O}_2\text{Cl}_1\text{F}_3\text{Na}_1$: 413.052661; found 413.052859.

IR (neat) $\bar{\nu} = 670$, 710, 732, 817, 845, 909, 1019, 1034, 1067, 1094, 1146, 1168, 1240, 1257, 1280, 1306, 1359, 1380, 1402, 1439, 1479, 1500, 1523, 1575, 1595, 1625, 1701, 2862, 3067 cm^{-1} .

Compound 9g:



Prepared from 2-bromo-5-fluorobenzaldehyde (250 mg, 1.23 mmol) and 4-(methylthio)phenylboronic acid (228 mg, 1.35 mmol) following the general procedure and purified by flash chromatography (hexanes/EtOAc, 95/5). Yellow oil (153 mg, 50%).

^1H NMR (400 MHz, CDCl_3) $\delta = 2.54$ (s, 3H), 7.26 - 7.29 (m, 2H), 7.31 - 7.37 (m, 3H), 7.42 (dd, $J = 8.5$, 5.2 Hz, 1H), 7.69 (dd, $J = 8.9$, 2.8 Hz, 1H), 9.93 (d, $J = 3.2$ Hz, 1H) ppm.

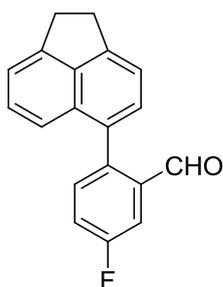
^{13}C NMR (101 MHz, CDCl_3) $\delta = 15.6$, 113.9 (d, $J = 22.4$ Hz), 120.9 (d, $J = 22.1$ Hz), 126.3, 130.5, 132.7 (d, $J = 7.2$ Hz), 133.3, 135.3 (d, $J = 6.3$ Hz), 139.5, 141.5 (d, $J = 3.0$ Hz), 162.3 (d, $J = 250.8$ Hz), 191.1 (d, $J = 1.6$ Hz) ppm.

^{19}F NMR (376 MHz, CDCl_3) $\delta = -113.1$ ppm.

HRMS calcd. for $\text{C}_{14}\text{H}_{11}\text{O}_1\text{F}_1\text{S}_1$: 246.051466; found 246.051497.

IR (neat) $\bar{\nu} = 654$, 718, 729, 739, 777, 814, 884, 967, 1003, 1096, 1147, 1206, 1260, 1295, 1392, 1417, 1438, 1476, 1579, 1596, 1684, 2752, 2852, 3066 cm^{-1} .

Compound 9h:



Prepared from 2-bromo-5-fluorobenzaldehyde (329 mg, 1.62 mmol) and acenaphthene-5-boronic acid (353 mg, 1.78 mmol) following the general procedure and purified by flash chromatography (hexanes/EtOAc, 95/5). White solid (293 mg, 65%).

^1H NMR (400 MHz, CDCl_3) $\delta = 3.46 - 3.51$ (m, 4H), 7.24 (d, $J = 8.3$ Hz, 1H), 7.32 - 7.37 (m, 3H), 7.38 - 7.45 (m, 2H), 7.49 (dd, $J = 8.4$, 5.2 Hz, 1H), 7.77 (dd, $J = 8.9$, 2.8 Hz, 1H), 9.65 (d, $J = 3.3$ Hz, 1H) ppm.

^{13}C NMR (101 MHz, CDCl_3) $\delta = 30.3$, 30.7, 113.5 (d, $J = 22.3$ Hz), 118.9, 120.27 (d, $J = 36.8$ Hz), 121.02 (d, $J = 21.9$ Hz), 129.1, 129.8, 130.6, 131.2, 133.9 (d, $J = 7.2$ Hz), 136.6 (d, $J = 6.3$

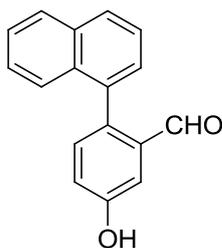
Hz), 139.4, 140.2 (d, $J = 3.3$ Hz), 146.6, 147.3, 162.5 (d, $J = 249.0$ Hz), 191.3 (d, $J = 1.9$ Hz) ppm.

^{19}F NMR (376 MHz, CDCl_3) $\delta = -113.1$ ppm.

HRMS calcd. for $\text{C}_{19}\text{H}_{13}\text{O}_1\text{F}_1$: 276.095042; found 276.094836.

IR (neat) $\bar{\nu} = 706, 747, 767, 775, 837, 882, 966, 1110, 1139, 1205, 1258, 1367, 1390, 1419, 1483, 1499, 1576, 1591, 1601, 1690, 2863, 3062$ cm^{-1} .

Compound 9i:



Prepared from 2-bromo-5-hydroxybenzaldehyde (404 mg, 2.01 mmol) and 1-naphthylboronic acid (380 mg, 2.21 mmol) following the general procedure and purified by flash chromatography (hexanes/EtOAc, 8/2). White solid (325 mg, 65%).

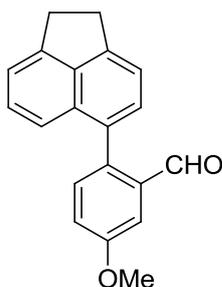
^1H NMR (400 MHz, CDCl_3) $\delta = 5.72$ (s, 1H), 7.23 (dd, $J = 8.3, 2.8$ Hz, 1H), 7.36 (d, $J = 8.3$ Hz, 1H), 7.38 - 7.46 (m, 2H), 7.48 - 7.57 (m, 3H), 7.63 (d, $J = 2.8$ Hz, 1H), 7.93 (d, $J = 8.2$ Hz, 2H), 9.57 (s, 1H) ppm.

^{13}C NMR (101 MHz, CDCl_3) $\delta = 112.9, 121.6, 125.2, 126.0, 126.3, 126.9, 128.5, 128.7, 128.7, 133.3, 133.5, 133.6, 135.2, 135.9, 137.3, 155.9, 192.4$ ppm.

HRMS calcd. for $\text{C}_{17}\text{H}_{12}\text{O}_2$: 248.083732; found 248.083686.

IR (neat) $\bar{\nu} = 695, 730, 759, 776, 802, 842, 886, 950, 966, 976, 1016, 1104, 1162, 1210, 1249, 1286, 1345, 1391, 1443, 1498, 1565, 1603, 1674, 3043, 3401$ cm^{-1} .

Compound 9j:



Prepared from 2-bromo-5-methoxybenzaldehyde (300 mg, 1.40 mmol) and acenaphthene-5-boronic acid (304 mg, 1.53 mmol) following the general procedure and purified by flash chromatography (hexanes/EtOAc, 95/5). Pale yellow solid (213 mg, 53%).

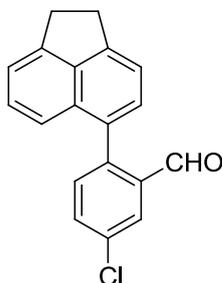
^1H NMR (400 MHz, CDCl_3) $\delta = 3.50$ (s, 4H), 3.97 (s, 3H), 7.29 (dd, $J = 5.8, 2.6$ Hz, 1H), 7.31 - 7.41 (m, 4H), 7.43 (t, $J = 3.5$ Hz, 1H), 7.45 (t, $J = 3.5$ Hz, 1H), 7.63 (d, $J = 2.8$ Hz, 1H), 9.72 (s, 1H) ppm.

^{13}C NMR (101 MHz, CDCl_3) $\delta = 30.3, 30.7, 55.8, 109.7, 118.9, 119.9, 120.8, 121.6, 128.8, 130.6, 130.6, 131.5, 133.2, 135.8, 137.1, 139.3, 146.4, 146.7, 159.4, 192.4$ ppm.

HRMS calcd. for $\text{C}_{20}\text{H}_{16}\text{O}_2$: 288.115029; found 288.115273.

IR (neat) $\bar{\nu} = 703, 750, 774, 824, 838, 864, 1001, 1015, 1032, 1091, 1112, 1156, 1191, 1222, 1268, 1310, 1367, 1387, 1420, 1464, 1489, 1502, 1598, 1681, 2850, 2922$ cm^{-1} .

Compound 9k:



Prepared from 2-bromo-5-chlorobenzaldehyde (278 mg, 1.28 mmol) and acenaphthene-5-boronic acid (251 mg, 1.28 mmol) following the general procedure and purified by flash chromatography (hexanes/EtOAc, 10/1). Pale yellow solid (291 mg, 79%).

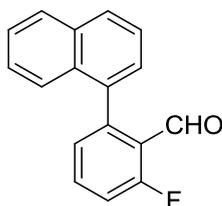
$^1\text{H NMR}$ (400 MHz, CDCl_3) δ = 3.48 (s, 4H), 7.25 (d, J = 7.7 Hz, 2H), 7.32 - 7.38 (m, 3H), 7.40 - 7.47 (m, 2H), 7.65 (dd, J = 8.2, 2.3 Hz, 1H), 8.07 (d, J = 2.3 Hz, 1H), 9.65 (s, 1H) ppm.

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ = 30.3, 30.7, 119.0, 120.2, 120.4, 127.3, 129.2, 129.7, 130.4, 131.0, 133.4, 133.7, 134.6, 136.1, 139.4, 142.4, 146.6, 147.5, 191.2 ppm.

HRMS calcd. for $\text{C}_{19}\text{H}_{13}\text{O}_1\text{Cl}_1$: 292.065495; found 292.065197.

IR (neat) $\bar{\nu}$ = 680, 728, 745, 772, 826, 845, 894, 1016, 1081, 1108, 1162, 1176, 1190, 1230, 1248, 1365, 1385, 1419, 1476, 1500, 1587, 1604, 1688, 2855, 2920 cm^{-1}

Compound 9l:



Prepared from 2-bromo-6-fluorobenzaldehyde (305 mg, 1.50 mmol) and 1-naphthylboronic acid (258 mg, 1.50 mmol) following the general procedure and purified by flash chromatography (hexanes/EtOAc, 6/1). White solid (271 mg, 73%).

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ = 7.24 (d, J = 7.6 Hz, 1H), 7.27 - 7.31 (m, 1H), 7.38 (dd, J = 7.0, 0.8 Hz, 1H), 7.41 - 7.46 (m, 1H), 7.47 - 7.57 (m, 3H), 7.65 (m, 1H), 7.94 (dd, J = 8.2, 3.5 Hz, 2H), 9.73 (s, 1H) ppm.

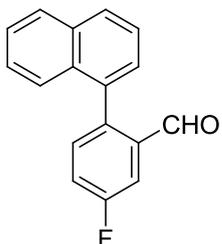
$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ = 116.4 (d, J = 21.3 Hz), 123.8 (d, J = 7.0 Hz), 125.2, 125.6, 126.4, 127.0, 127.7 (d, J = 3.7 Hz), 127.9, 128.6, 129.0, 132.4, 133.5, 134.7 (d, J = 10.2 Hz), 135.2 (d, J = 2.3 Hz), 145.5, 162.4 (d, J = 263.8 Hz), 189.1 ppm.

$^{19}\text{F NMR}$ (376 MHz, CDCl_3) δ = -115.7 ppm.

HRMS calcd. for $\text{C}_{17}\text{H}_{11}\text{O}_1\text{F}_1$: 250.079390; found 250.079520.

IR (neat) $\bar{\nu}$ = 682, 729, 776, 785, 802, 833, 867, 900, 1009, 105, 1061, 1129, 1155, 1182, 1204, 1236, 1290, 1393, 1410, 1440, 1457, 1474, 1506, 1566, 1590, 1608, 1698, 2886, 3054 cm^{-1} .

Compound 9m:



Prepared from 2-bromo-5-fluorobenzaldehyde (300 mg, 1.48 mmol) and 1-naphthylboronic acid (280 mg, 1.63 mmol) following the general procedure and purified by flash chromatography (hexanes/EtOAc, 95/5). Colorless oil (220 mg, 60%).

^1H NMR (400 MHz, CDCl_3) δ = 7.39 - 7.48 (m, 5H), 7.50 - 7.59 (m, 2H), 7.75 - 7.81 (m, 1H), 7.92 - 7.99 (m, 2H), 9.55 (d, J = 3.3 Hz, 1H) ppm.

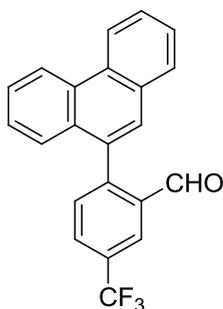
^{13}C NMR (101 MHz, CDCl_3) δ = 113.5 (d, J = 22.3 Hz), 121.0 (d, J = 22.1 Hz), 125.2, 125.7, 126.8 (d, J = 64.2 Hz), 128.6, 128.7, 129.1, 132.9, 133.6, 133.7, 133.8, 134.5, 136.7 (d, J = 6.4 Hz), 140.3 (d, J = 3.3 Hz), 162.6 (d, J = 249.4 Hz), 191.0 (d, J = 1.8 Hz) ppm.

^{19}F NMR (376 MHz, CDCl_3) δ = -112.5 ppm.

HRMS calcd. for $\text{C}_{17}\text{H}_{11}\text{O}_1\text{F}_1$: 250.079392; found 250.079194.

IR (neat) $\bar{\nu}$ = 678, 755, 776, 801, 838, 885, 970, 1145, 1210, 1260, 1294, 1389, 1412, 1490, 1509, 1578, 1604, 1688, 2849, 3061 cm^{-1} .

Compound 9o:



Prepared from 2-bromo-5-(trifluoromethyl)benzaldehyde (458 mg, 1.81 mmol) and 9-phenanthracenylboronic acid (442 mg, 1.99 mmol) following the general procedure and purified by flash chromatography (hexanes/EtOAc, 95/5). White solid (363 mg, 59%).

^1H NMR (400 MHz, CDCl_3) δ = 7.47 (dd, J = 8.2, 1.0 Hz, 1H), 7.56 (ddd, J = 8.1, 6.9, 1.2 Hz, 1H), 7.66 - 7.72 (m, 3H), 7.72 - 7.79 (m, 2H), 7.92 (dd, J = 7.9, 1.4 Hz, 1H), 7.98 (ddd, J = 7.9, 2.0, 0.5 Hz, 1H), 8.41 - 8.45 (m, 1H), 8.77 (dd, J = 8.3, 0.4 Hz, 1H), 8.80 - 8.85 (m, 1H), 9.74 (s, 1H) ppm.

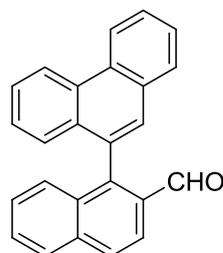
^{13}C NMR (101 MHz, CDCl_3) δ = 122.9, 123.4, 123.82 (q, J = 272.4 Hz), 124.6 (q, J = 3.8 Hz), 126.6, 127.4, 127.6, 127.6, 127.8, 129.0, 129.5, 130.1 (q, J = 3.5 Hz), 130.6, 130.6, 130.9, 131.1 (q, J = 32.8 Hz), 131.5, 132.7, 132.9, 135.5, 147.6 (d, J = 0.8 Hz), 190.6 ppm.

^{19}F NMR (376 MHz, CDCl_3) δ = -62.8 ppm.

HRMS calcd. for $\text{C}_{22}\text{H}_{13}\text{O}_1\text{F}_3$: 350.091851; found 350.091851.

IR (neat) $\bar{\nu}$ = 684, 727, 761, 834, 907, 1069, 1108, 1118, 1135, 1155, 1181, 1259, 1328, 1450, 1491, 1528, 1567, 1614, 1699, 2849, 3071 cm^{-1} .

Compound 9p:



In a first step, compound **9p**(H_2) was prepared from 1-chloro-3,4-dihydronaphthalene-2-carbaldehyde (480 mg, 2.49 mmol) and 9-phenanthracenylboronic acid (609 mg, 2.74 mmol) following the general procedure and purified by chromatography (hexanes/EtOAc, 95/5). Pale yellow solid (620 mg, 74%).

^1H NMR (400 MHz, CDCl_3) δ = 2.70 - 2.79 (m, 1H), 2.90 - 2.98 (m, 1H), 3.03 - 3.12 (m, 2H), 6.77 (dd, J = 7.8, 0.6 Hz, 1H), 6.97 (td, J = 7.8, 1.4 Hz, 1H), 7.24 - 7.28 (m, 1H), 7.32 (dd, J = 7.4, 0.7 Hz, 1H), 7.49 (ddd, J = 8.2, 6.9, 1.2 Hz, 1H), 7.64 - 7.69 (m, 3H), 7.71 - 7.78 (m, 2H), 7.90 (dd, J = 7.8, 1.3 Hz, 1H), 8.78 (t, J = 7.5 Hz, 2H), 9.57 (s, 1H) ppm.

^{13}C NMR (101 MHz, CDCl_3) δ = 20.4, 27.8, 122.8, 123.2, 127.0, 127.1, 127.1, 127.3, 127.3, 127.5, 128.1, 128.2, 128.9, 129.7, 130.4, 130.5, 130.6, 131.0, 131.6, 131.7, 135.0, 136.3, 138.3, 153.1, 193.2 ppm.

HRMS calcd. for $\text{C}_{25}\text{H}_{18}\text{O}_4$: 334.135763; found 334.139508.

IR (neat) $\bar{\nu}$ = 670, 708, 723, 737, 745, 753, 761, 777, 807, 890, 914, 1036, 1152, 1179, 1267, 1363, 1452, 1562, 1661, 2856, 3071 cm^{-1} .

Oxidation of **9p(H₂)** (398 mg, 1.19 mmol) was carried out by treatment with DDQ (1.25 eq.) in refluxing toluene overnight. After cooling to room temperature, the mixture was filtered over celite, the filtrate was washed with 1M NaOH solution and the aqueous phase was extracted with toluene. The combined organic phases were dried over Na_2SO_4 and evaporated, and the crude product was purified by flash chromatography (hexanes/EtOAc, 95/5) affording **9p** as a pale brown solid (210 mg, 53%).

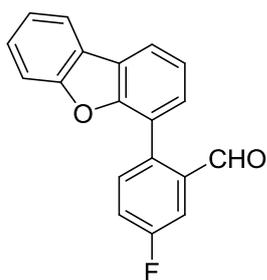
^1H NMR (400 MHz, CDCl_3) δ = 7.28 - 7.36 (m, 2H), 7.40 - 7.46 (m, 1H), 7.52 (d, J = 8.4 Hz, 1H), 7.61 (ddd, J = 8.1, 6.9, 1.1 Hz, 1H), 7.69 (ddd, J = 8.5, 3.0, 1.3 Hz, 2H), 7.78 (ddd, J = 8.4, 7.1, 1.4 Hz, 1H), 7.82 (s, 1H), 7.92 (dd, J = 7.9, 0.9 Hz, 1H), 8.00 (d, J = 8.2 Hz, 1H), 8.07 (d, J = 8.7 Hz, 1H), 8.22 (d, J = 8.7 Hz, 1H), 8.84 (t, J = 8.1 Hz, 2H), 9.86 (d, J = 0.6 Hz, 1H) ppm.

^{13}C NMR (101 MHz, CDCl_3) δ = 122.3, 122.9, 123.1, 127.2, 127.3, 127.4, 127.5, 127.6, 127.9, 128.4, 128.9, 129.0, 129.1, 130.3, 130.4, 130.6, 131.1, 131.8, 132.5, 132.6, 132.7, 133.2, 136.3, 144.9, 192.6 ppm.

HRMS calcd. for $\text{C}_{25}\text{H}_{16}\text{O}_4$: 332.120118; found 332.120126.

IR (neat) $\bar{\nu}$ = 715, 725, 751, 772, 821, 911, 1030, 1213, 1230, 1371, 1430, 1420, 1493, 1595, 1675, 2870, 3052 cm^{-1} .

Compound 9q:



Prepared from 2-bromo-5-fluorobenzaldehyde (400 mg, 1.97 mmol) and 4-(dibenzofuranyl)boronic acid (460 mg, 2.17 mmol) following the general procedure and purified by flash chromatography (hexanes/EtOAc, 95/5). White solid (376 mg, 66%).

^1H NMR (400 MHz, CDCl_3) δ = 7.36 - 7.43 (m, 2H), 7.43 - 7.47 (m, 2H), 7.47 - 7.53 (m, 2H), 7.62 (dd, J = 8.5, 5.1 Hz, 1H), 7.82 (dd, J = 8.8, 2.8 Hz, 1H), 7.99 - 8.02 (m, 1H), 8.05 (dd, J = 7.6, 1.4 Hz, 1H), 9.84 (d,

J = 3.2 Hz, 1H) ppm.

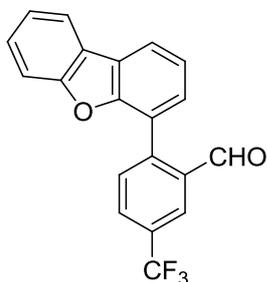
^{13}C NMR (101 MHz, CDCl_3) δ = 112.1, 113.9, 114.1, 121.0, 121.2, 121.2 (d, J = 22.0 Hz), 121.4, 123.3, 124.4 (d, J = 76.7 Hz), 127.8, 129.0, 133.5 (d, J = 7.4 Hz), 135.8, 135.9, 136.1 (d, J = 3.2 Hz), 153.8, 156.3, 162.8 (d, J = 250.1 Hz), 190.7 (d, J = 1.6 Hz) ppm.

^{19}F NMR (376 MHz, CDCl_3) δ = -112.1 ppm.

HRMS calcd. for $\text{C}_{19}\text{H}_{11}\text{O}_2\text{F}$: 290.074307; found 290.074048.

IR (neat) $\bar{\nu}$ = 653, 720, 740, 754, 799, 838, 883, 962, 1063, 1126, 1145, 1184, 1206, 1257, 1305, 1395, 1424, 1450, 1481, 1500, 1585, 1602, 1682, 2865, 3066 cm^{-1} .

Compound 9r:



Prepared from 2-bromo-5-(trifluoromethyl)benzaldehyde (385 mg, 1.52 mmol) and 4-(dibenzofuran-2-yl)boronic acid (355 mg, 1.67 mmol) following the general procedure and purified by flash chromatography (hexanes/EtOAc, 95/5). White solid (372 mg, 72%).

^1H NMR (400 MHz, CDCl_3) δ = 7.37 - 7.43 (m, 1H), 7.44 - 7.49 (m, 2H), 7.49 - 7.54 (m, 2H), 7.78 (d, J = 8.0 Hz, 1H), 7.96 - 8.00 (m, 1H), 8.00 - 8.04 (m, 1H), 8.09 (dd, J = 7.6, 1.4 Hz, 1H), 8.40 - 8.44 (m, 1H), 9.91 (s, 1H) ppm.

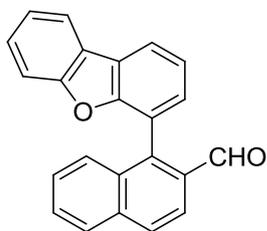
^{13}C NMR (101 MHz, CDCl_3) δ = 112.0, 120.9, 121.0, 121.7, 123.4, 123.7 (q, J = 272.6 Hz), 124.9, 124.9 (q, J = 4.1 Hz), 128.0, 128.6, 130.1 (q, J = 3.5 Hz), 131.0 (q, J = 33.4 Hz), 132.2, 134.3, 143.0, 153.5, 156.2, 190.4 ppm.

^{19}F NMR (376 MHz, CDCl_3) δ = -62.8 ppm.

HRMS calcd. for $\text{C}_{20}\text{H}_{11}\text{O}_2\text{F}_3$: 340.071119; found 340.070959.

IR (neat) $\bar{\nu}$ = 707, 731, 741, 749, 795, 841, 869, 909, 1013, 1071, 1108, 1171, 1247, 1330, 1400, 1426, 1449, 1473, 1568, 1614, 1693, 2903, 3058 cm^{-1} .

Compound 9s:



In a first step, **9s(H₂)** was prepared from 1-chloro-3,4-dihydro-naphthalene-2-carbaldehyde (297 mg, 1.54 mmol) and 4-(dibenzofuran-2-yl)boronic acid (360 mg, 1.70 mmol) following the general procedure and purified by flash chromatography (hexanes/EtOAc, 95/5). Pale yellow solid (356 mg, 71%).

^1H NMR (400 MHz, CDCl_3) δ = 2.79 - 2.90 (m, 2H), 2.96 - 3.14 (m, 2H), 6.82 (d, J = 7.8 Hz, 1H), 7.03 - 7.10 (m, 1H), 7.29 - 7.33 (m, 2H), 7.35 - 7.41 (m, 2H), 7.43 - 7.50 (m, 3H), 8.02 (d, J = 7.5 Hz, 1H), 8.08 (dd, J = 7.7, 1.2 Hz, 1H), 9.58 (s, 1H) ppm.

^{13}C NMR (101 MHz, CDCl_3) δ = 20.4, 27.7, 112.2, 119.6, 120.9, 121.3, 122.9, 123.2, 124.0, 124.7, 126.9, 127.8, 127.9, 128.1, 129.4, 130.4, 134.4, 135.7, 138.6, 149.0, 154.4, 156.4, 193.0 ppm.

HRMS calcd. for $\text{C}_{23}\text{H}_{16}\text{O}_2\text{Na}$: 347.104248; found 347.104347.

IR (neat) $\bar{\nu}$ = 714, 734, 751, 799, 829, 845, 1151, 1186, 1241, 1298, 1362, 1411, 1448, 1474, 1563, 1597, 1660, 2836, 2939, 3058 cm^{-1} .

Oxidation of **9s(H₂)** (273 mg, 0.84 mmol) was carried out by treatment with DDQ (1.25 eq.) in refluxing toluene overnight. After cooling to room temperature, the mixture was filtered over celite, the filtrate was washed with 1M NaOH solution and the aqueous phase was extracted with toluene. The combined organic phases were dried over Na_2SO_4 and evaporated, and the

crude product was purified by flash chromatography (hexanes/DCM, 1/1) affording **9s** as a white solid (140 mg, 52%).

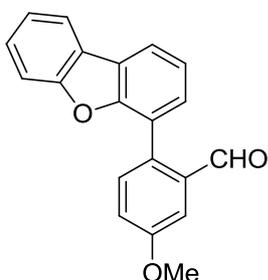
^1H NMR (400 MHz, CDCl_3) δ = 7.36 - 7.46 (m, 4H), 7.48 (dd, J = 7.4, 1.3 Hz, 1H), 7.55 (t, J = 7.5 Hz, 1H), 7.59 - 7.66 (m, 2H), 7.99 (d, J = 8.2 Hz, 1H), 8.02 - 8.09 (m, 2H), 8.15 (dd, J = 7.6, 1.3 Hz, 1H), 8.18 (d, J = 8.6 Hz, 1H), 9.88 (d, J = 0.7 Hz, 1H) ppm.

^{13}C NMR (101 MHz, CDCl_3) δ = 112.2, 119.5, 121.0, 121.4, 122.5, 123.0, 123.3, 124.1, 124.7, 127.2, 127.5, 127.8, 128.6, 129.1, 129.3, 130.2, 131.9, 132.5, 136.4, 140.8, 154.8, 156.5, 192.4 ppm.

HRMS calcd. for $\text{C}_{23}\text{H}_{14}\text{O}_2\text{Na}_1$: 345.088602; found 345.088961.

IR (neat) $\bar{\nu}$ = 671, 737, 742, 755, 814, 845, 1188, 1247, 1332, 1383, 1413, 1452, 1595, 1675, 2853, 3065 cm^{-1} .

Compound 9t:



Prepared from 2-bromo-5-methoxybenzaldehyde (350 mg, 1.63 mmol) and 4-(dibenzofuranyl)boronic acid (380 mg, 1.79 mmol) following the general procedure and purified by flash chromatography (hexanes/EtOAc, 95/5). White solid (318 mg, 65%).

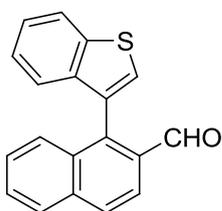
^1H NMR (400 MHz, CDCl_3) δ = 3.95 (s, 3H), 7.30 (dd, J = 8.5, 2.9 Hz, 1H), 7.37 (td, J = 7.6, 1.2 Hz, 1H), 7.42 (td, J = 6.4, 1.5 Hz, 1H), 7.44 - 7.48 (m, 2H), 7.51 (d, J = 8.0 Hz, 1H), 7.55 (d, J = 8.5 Hz, 1H), 7.64 (d, J = 2.8 Hz, 1H), 7.97 - 8.04 (m, 2H), 9.88 (s, 1H) ppm.

^{13}C NMR (101 MHz, CDCl_3) δ = 55.8, 110.3, 112.1, 120.7, 121.0, 121.7, 122.2, 123.2, 123.2, 124.2, 124.6, 127.7, 129.1, 132.8, 132.9, 135.0, 154.0, 156.3, 159.9, 191.9 ppm.

HRMS calcd. for $\text{C}_{20}\text{H}_{14}\text{O}_3\text{Na}_1$: 325.083516; found 325.083249.

IR (neat) $\bar{\nu}$ = 751, 794, 832, 877, 933, 1013, 1091, 1159, 1187, 1233, 1260, 1282, 1394, 1448, 1484, 1505, 1566, 1584, 1606, 1693, 2852, 2938 cm^{-1} .

Compound 9u:



Compound **9u(H₂)** was prepared from 1-chloro-3,4-dihydro-naphthalene-2-carbaldehyde (370 mg, 1.92 mmol) and benzo[b]thien-3-ylboronic acid (376 mg, 2.10 mmol) following the general procedure and purified by flash chromatography (hexanes/EtOAc, 9/1). Yellow solid (380 mg, 68%).

^1H NMR (400 MHz, CD_2Cl_2) δ = 2.56 - 2.68 (m, 1H), 2.82 - 2.91 (m, 1H), 2.95 - 3.05 (m, 2H), 6.83 (d, J = 7.7 Hz, 1H), 7.01 - 7.08 (m, 1H), 7.26 - 7.34 (m, 3H), 7.36 - 7.44 (m, 2H), 7.52 (s, 1H), 7.97 (d, J = 8.7 Hz, 1H), 9.59 (s, 1H) ppm.

^{13}C NMR (101 MHz, CD_2Cl_2) δ = 20.9, 28.0, 123.2, 123.5, 125.1, 125.4, 127.1, 128.0, 128.1, 128.4, 130.8, 131.2, 134.7, 137.7, 139.0, 140.0, 140.4, 148.4, 192.8 ppm.

HRMS calcd. for $\text{C}_{19}\text{H}_{14}\text{O}_1\text{S}_1$: 290.076537; found 290.076239.

IR (neat) $\bar{\nu}$ = 688, 712, 727, 734, 759, 797, 903, 1021, 1082, 1152, 1184, 1260, 1275, 1359, 1428, 1514, 1564, 1603, 1652, 2844, 3074 cm^{-1} .

Oxidation of **9u(H₂)** (380 mg, 1.31 mmol) was carried out by treatment with DDQ (1.25 eq.) in refluxing toluene overnight. After cooling to room temperature, the mixture was filtered over celite, the filtrate was washed with 1M NaOH solution and the aqueous phase was extracted with toluene. The combined organic phases were dried over Na₂SO₄ and evaporated, and the crude product was purified by flash chromatography (hexanes/EtOAc, 95/5) affording **9u** as a yellow solid (157 mg, 42%).

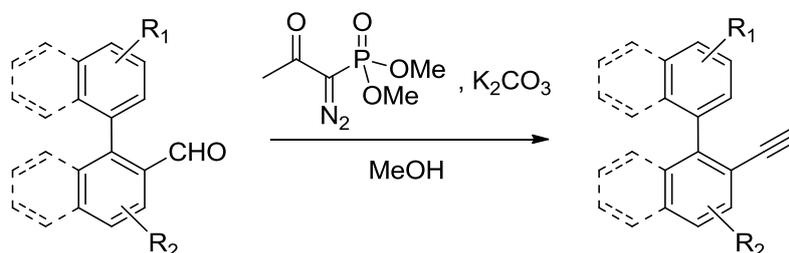
¹H NMR (400 MHz, CDCl₃) δ = 7.22 (d, *J* = 8.0 Hz, 1H), 7.26 - 7.33 (m, 1H), 7.37 - 7.47 (m, 2H), 7.55 (s, 1H), 7.59 - 7.66 (m, 2H), 7.97 (d, *J* = 8.1 Hz, 1H), 8.02 (dd, *J* = 8.4, 3.6 Hz, 2H), 8.14 (d, *J* = 8.6 Hz, 1H), 9.86 (d, *J* = 0.7 Hz, 1H) ppm.

¹³C NMR (101 MHz, CDCl₃) δ = 122.4, 123.0, 123.3, 125.1, 125.2, 127.3, 127.5, 127.7, 128.5, 129.2, 129.2, 130.9, 132.9, 133.1, 136.4, 139.8, 140.2, 140.6, 192.4 ppm.

HRMS calcd. for C₁₉H₁₄O₁S₁: 288.060890; found 288.060753.

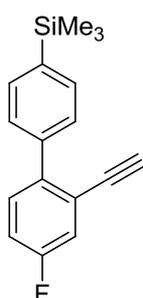
IR (neat) $\bar{\nu}$ = 662, 707, 737, 766, 816, 841, 906, 1026, 1078, 1224, 1260, 1322, 1428, 1454, 1591, 1616, 1677, 2855, 3059 cm^{-1} .

General Procedure for the Ohira-Bestmann reaction



Ohira-Bestmann reagent (1.5 eq.) and K₂CO₃ (2 eq.) were added to a solution of corresponding aldehyde in dry MeOH and the resulting mixture was stirred overnight. Afterwards, the solvent was evaporated and the crude partitioned between CH₂Cl₂ and brine. The combined organic layers were dried (Na₂SO₄), evaporated, and the residue was purified by flash chromatography.

Compound 10c:



Prepared from compound **9c** (418 mg, 1.54 mmol) following the general procedure and purified by flash chromatography (hexanes/EtOAc, 95/5). White solid (363 mg, 88%).

¹H NMR (400 MHz, CDCl₃) δ = 0.33 (s, 9H), 3.09 (s, 1H), 7.12 (td, *J* = 8.4, 2.8 Hz, 1H), 7.29 - 7.38 (m, 2H), 7.52 - 7.62 (m, 4H) ppm.

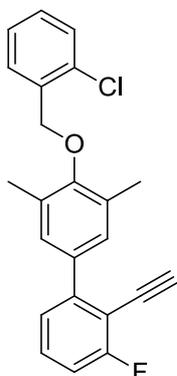
¹³C NMR (101 MHz, CDCl₃) δ = -0.94, 81.3, 82.2 (d, *J* = 2.9 Hz), 116.6 (d, *J* = 21.2 Hz), 120.3, 120.6, 122.2 (d, *J* = 9.5 Hz), 128.6, 131.4 (d, *J* = 8.5 Hz), 133.3, 139.8 (d, *J* = 17.7 Hz), 140.8 (d, *J* = 3.4 Hz), 161.5 (d, *J* = 247.1 Hz) ppm.

¹⁹F NMR (376 MHz, CDCl₃) δ = -115.7 ppm.

HRMS calcd. for $C_{17}H_{17}F_1Si_1$: 268.108358; found 268.108129.

IR (neat) $\bar{\nu}$ = 656, 722, 739, 757, 813, 832, 872, 938, 1002, 1093, 1114, 1146, 1210, 1247, 1276, 1387, 1406, 1471, 1485, 1507, 1575, 1600, 2957, 3291 cm^{-1} .

Compound 10d:



Prepared from 2-bromo-6-fluorobenzaldehyde (220 mg, 1.08 mmol) and 4-(2'-chlorobenzoyloxy)-3,5-dimethylphenylboronic acid (346 mg, 1.19 mmol) following the general procedure and purified by flash chromatography (hexanes/EtOAc, 9/1) a pale yellow solid (268 mg, 67%). As the purification of the aldehyde was not satisfactory, the mixture obtained containing mainly **9d** (130 mg, 0.35 mmol) was submitted to the general Ohira-Bestmann conditions and purified by flash chromatography (hexanes/EtOAc, 95/5). White solid (118 mg, 92%).

1H NMR (400 MHz, $CDCl_3$) δ = 2.38 (s, 6H), 3.34 (d, J = 0.4 Hz, 1H), 5.01 (s, 2H), 7.03 - 7.12 (m, 1H), 7.18 (d, J = 7.7 Hz, 1H), 7.30 (s, J = 4.4 Hz, 2H), 7.31 - 7.40 (m, 3H), 7.43 (dd, J = 7.8, 1.3 Hz, 1H), 7.79 (dd, J = 7.6, 1.4 Hz, 1H) ppm.

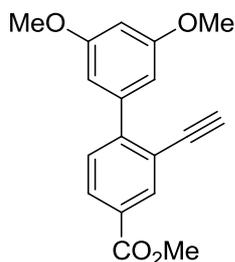
^{13}C NMR (101 MHz, $CDCl_3$) δ = 16.5, 70.9, 76.4 (d, J = 0.8 Hz), 85.8 (d, J = 4.4 Hz), 109.5 (d, J = 15.7 Hz), 113.8 (d, J = 21.7 Hz), 125.2 (d, J = 3.2 Hz), 127.1, 129.0 (d, J = 2.2 Hz), 129.4, 129.8, 129.9, 131.0, 132.6, 135.0 (d, J = 2.5 Hz), 135.7, 146.5, 155.7, 164.34 (d, J = 251.6 Hz) ppm.

^{19}F NMR (376 MHz, $CDCl_3$) δ = -108.8 ppm.

HRMS calcd. for $C_{23}H_{18}O_1Cl_1F_1$: 364.103025; found 364.103101.

IR (neat) $\bar{\nu}$ = 687, 721, 735, 748, 764, 824, 847, 874, 888, 898, 951, 958, 1023, 1042, 1054, 1107, 1123, 1186, 1203, 1252, 1368, 1461, 1491, 1567, 1607, 2919, 3301 cm^{-1} .

Compound 10e:



Prepared from compound **9e** (460 mg, 1.46 mmol) following the general procedure and purified by flash chromatography (hexanes/EtOAc, 15/5). White solid (398 mg, 92%).

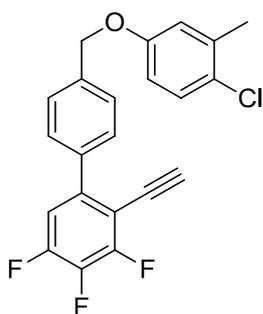
1H NMR (400 MHz, $CDCl_3$) δ = 3.13 (s, 1H), 3.83 (s, 6H), 3.94 (s, 3H), 6.52 (t, J = 2.3 Hz, 1H), 6.75 (d, J = 2.3 Hz, 2H), 7.46 (d, J = 8.1 Hz, 1H), 8.03 (dd, J = 8.1, 1.8 Hz, 1H), 8.28 (d, J = 1.7 Hz, 1H) ppm.

^{13}C NMR (101 MHz, $CDCl_3$) δ = 52.4, 55.6, 81.4, 82.3, 100.7, 107.5, 120.9, 129.3, 129.8, 129.9, 135.4, 141.2, 148.5, 160.6, 166.3 ppm.

HRMS calcd. for $C_{18}H_{16}O_4Na_1$: 319.094076; found 319.094351.

IR (neat) $\bar{\nu}$ = 674, 694, 764, 870, 927, 980, 991, 1033, 1063, 1077, 1102, 1122, 1153, 1185, 1203, 1240, 1276, 1291, 1347, 1387, 1424, 1456, 1500, 1559, 1593, 1709, 2839, 2953, 2997, 3252, 3291 cm^{-1} .

Compound 10f:



Prepared from compound **9f** (144 mg, 0.37 mmol) following the general procedure and purified by flash chromatography (hexanes/EtOAc, 95/5). White solid (132 mg, 93%).

^1H NMR (400 MHz, CDCl_3) δ = 2.36 (s, 3H), 3.31 (s, 1H), 5.08 (s, 2H), 6.77 (dd, J = 8.7, 3.0 Hz, 1H), 6.89 (d, J = 2.9 Hz, 1H), 7.01 (ddd, J = 10.4, 7.1, 2.0 Hz, 1H), 7.25 (d, J = 8.7 Hz, 1H), 7.49 (d, J = 8.2 Hz, 2H), 7.55 (d, J = 8.2 Hz, 2H) ppm.

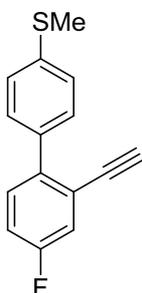
^{13}C NMR (101 MHz, CDCl_3) δ = 20.5, 69.9, 74.5 (t, J = 2.9 Hz), 86.8 (dd, J = 4.9, 2.2 Hz), 107.4 (dd, J = 13.2, 3.7 Hz), 113.3 (dd, J = 18.4, 3.5 Hz), 113.5, 117.6, 126.5, 127.4, 129.4, 129.8, 137.3, 137.3 - 137.4 (m), 137.4, 138.0 (dt, J = 252.9, 15.5 Hz), 140.7 (dd, J = 7.7, 4.0 Hz), 151.1 (ddd, J = 253.8, 10.1, 4.1 Hz), 153.4 (ddd, J = 254.8, 10.7, 4.2 Hz), 157.3 ppm.

^{19}F NMR (376 MHz, CDCl_3) δ = -128.4 (dd, J = 20.7, 8.6 Hz), -131.2 (dd, J = 21.3, 8.6 Hz), -160.7 (t, J = 20.9 Hz) ppm.

HRMS calcd. for $\text{C}_{22}\text{H}_{14}\text{O}_1\text{Cl}_1\text{F}_3$: 386.068531; found 386.068286.

IR (neat) $\bar{\nu}$ = 677, 726, 816, 840, 862, 972, 999, 1014, 1065, 1124, 1169, 1236, 1260, 1304, 1361, 1380, 1406, 1443, 1467, 1483, 1501, 1525, 1593, 2875, 2932 cm^{-1} .

Compound 10g:



Prepared from compound **9g** (123 mg, 0.50 mmol) following the general procedure and purified by flash chromatography (hexanes/EtOAc, 95/5). Pale brown solid (115 mg, 95%).

^1H NMR (400 MHz, CDCl_3) δ = 2.53 (s, 3H), 3.10 (s, 1H), 7.11 (td, J = 8.4, 2.7 Hz, 1H), 7.28 - 7.36 (m, 4H), 7.46 - 7.52 (m, 2H) ppm.

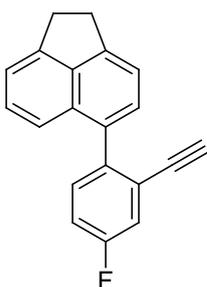
^{13}C NMR (101 MHz, CDCl_3) δ = 15.7, 81.3, 82.1 (d, J = 2.9 Hz), 116.6 (d, J = 21.2 Hz), 120.4 (d, J = 23.0 Hz), 122.1 (d, J = 9.5 Hz), 126.1, 129.7, 131.2 (d, J = 8.4 Hz), 136.1, 138.3, 140.2 (d, J = 3.3 Hz), 161.4 (d, J = 247.1 Hz) ppm.

^{19}F NMR (376 MHz, CDCl_3) δ = -115.6 ppm.

HRMS calcd. for $\text{C}_{14}\text{H}_{11}\text{O}_1\text{F}_1\text{S}_1$: 246.051466; found 246.051497.

IR (neat) $\bar{\nu}$ = 716, 751, 810, 835, 872, 939, 1003, 1021, 1091, 1100, 1145, 1190, 1211, 1262, 1279, 1391, 1409, 1437, 1473, 1551, 1575, 1598, 2920, 3065, 3288 cm^{-1} .

Compound 10h:



Prepared from compound **9h** (120 mg, 0.43 mmol) following the general procedure and purified flash chromatography (hexanes/EtOAc, 95/5). Brown solid (109 mg, 92%).

^1H NMR (400 MHz, CDCl_3) δ = 2.84 (s, 1H), 3.39 – 3.52 (m, 4H), 7.16 (td, J = 8.4, 2.7 Hz, 1H), 7.32 (dd, J = 13.2, 5.3 Hz, 2H), 7.36 - 7.39 (m, 3H), 7.40 - 7.45 (m, 2H) ppm.

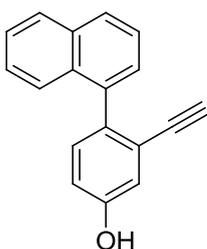
^{13}C NMR (101 MHz, CDCl_3) δ = 30.3, 30.7, 81.2, 82.0 (d, J = 3.0 Hz), 116.0, 116.2, 119.2 (d, J = 62.0 Hz), 119.8, 120.0, 121.1, 124.0 (d, J = 9.5 Hz), 128.1, 129.5, 130.3, 132.5, 132.6, 132.8, 139.3 (d, J = 3.3 Hz), 146.3 (d, J = 8.8 Hz), 161.6 (d, J = 246.6 Hz) ppm.

^{19}F NMR (376 MHz, CDCl_3) δ = -115.5 ppm.

HRMS calcd. for $\text{C}_{20}\text{H}_{13}\text{F}$: 272.100125; found 272.099874.

IR (neat) $\bar{\nu}$ = 674, 748, 778, 820, 835, 843, 872, 943, 1094, 1143, 1217, 1255, 1367, 1422, 1487, 1498, 1570, 1589, 1602, 3064, 3276 cm^{-1} .

Compound 10i:



Prepared from compound **9i** (232 mg, 0.93 mmol) following the general procedure and purified by flash chromatography (hexanes/EtOAc, 8/2). White solid (209 mg, 92%).

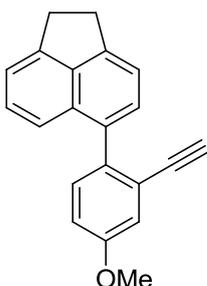
^1H NMR (400 MHz, CDCl_3) δ = 2.75 (s, 1H), 5.08 (s, 1H), 6.95 (dd, J = 8.3, 2.7 Hz, 1H), 7.15 (d, J = 2.7 Hz, 1H), 7.26 (d, J = 8.3 Hz, 1H), 7.39 - 7.46 (m, 2H), 7.46 - 7.51 (m, 1H), 7.51 - 7.51 (m, 1H), 7.64 (d, J = 8.3 Hz, 1H), 7.90 (t, J = 8.6 Hz, 2H) ppm.

^{13}C NMR (101 MHz, CDCl_3) δ = 80.5, 82.4, 116.3, 119.6, 123.6, 125.3, 125.8, 126.0, 126.3, 127.7, 128.0, 128.3, 132.2, 132.3, 133.7, 136.4, 138.2, 154.6 ppm.

HRMS calcd. for $\text{C}_{18}\text{H}_{12}\text{O}$: 244.088812; found 244.088598.

IR (neat) $\bar{\nu}$ = 682, 738, 779, 803, 868, 938, 963, 1017, 1091, 1153, 1222, 1278, 1347, 1393, 1449, 1493, 1507, 1570, 1602, 3045, 3301, 3357 cm^{-1} .

Compound 10j:



Prepared from compound **9j** (200 mg, 0.69 mmol) following the general procedure and purified by flash chromatography (hexanes/MTBE, 95/5). White solid (183 mg, 93%).

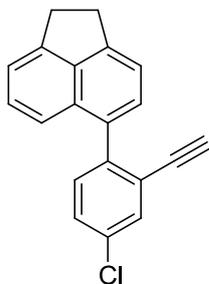
^1H NMR (400 MHz, CDCl_3) δ = 2.83 (s, 1H), 3.46 (s, 4H), 3.90 (s, 3H), 7.03 (dd, J = 8.5, 2.7 Hz, 1H), 7.23 (d, J = 2.6 Hz, 1H), 7.30 (d, J = 5.9 Hz, 1H), 7.35 (d, J = 8.4 Hz, 2H), 7.38 - 7.45 (m, 2H), 7.47 (d, J = 7.0 Hz, 1H) ppm.

^{13}C NMR (101 MHz, CDCl_3) δ = 30.3, 30.7, 55.6, 80.0, 83.1, 115.5, 117.9, 118.9, 119.3, 121.4, 123.1, 127.8, 129.4, 130.5, 132.1, 133.5, 135.7, 139.5, 145.8, 146.2, 158.5 ppm.

HRMS calcd. for C₂₁H₁₆O₁: 284.120117; found 284.120247.

IR (neat) $\bar{\nu}$ = 665, 708, 749, 773, 821, 840, 863, 912, 1015, 1037, 1058, 1111, 1156, 1188, 1223, 1238, 1283, 1367, 1395, 1423, 1452, 1466, 1488, 1504, 1558, 1599, 2834, 2931, 3278 cm⁻¹.

Compound 10k:



Prepared from compound **9k** (87 mg, 0.30 mmol) following the general procedure and purified by flash chromatography (hexanes/EtOAc, 99/1). Pale brown solid (79 mg, 92%).

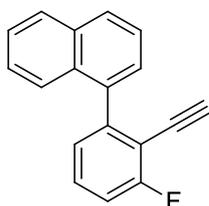
¹H NMR (400 MHz, CDCl₃) δ = 2.85 (s, 1H), 3.46 (s, 4H), 7.31 (d, *J* = 6.6 Hz, 1H), 7.33 - 7.39 (m, 3H), 7.38 - 7.47 (m, 3H), 7.67 (d, *J* = 1.7 Hz, 1H) ppm.

¹³C NMR (101 MHz, CDCl₃) δ = 30.3, 30.7, 81.4, 81.8, 118.9, 119.5, 121.0, 124.0, 128.1, 128.9, 129.4, 130.1, 132.3, 132.6, 133.0, 133.2, 139.4, 141.7, 146.3, 146.5 ppm.

HRMS calcd. for C₂₀H₁₃Cl₁: 288.070576; found 288.070293.

IR (neat) $\bar{\nu}$ = 669, 751, 781, 822, 835, 878, 1015, 1054, 1091, 1117, 1183, 1259, 1364, 1381, 1405, 1421, 1460, 1481, 1500, 1549, 1586, 1603, 2922, 3272 cm⁻¹.

Compound 10l:



Prepared from compound **9l** (150 mg, 0.60 mmol) following the general procedure and purified by flash chromatography (hexanes/EtOAc, 9/1). Yellow solid (136 mg, 92%).

¹H NMR (400 MHz, CDCl₃) δ = 3.00 (s, 1H), 7.16 - 7.23 (m, 2H), 7.40 - 7.48 (m, 3H), 7.51 (ddd, *J* = 8.2, 6.9, 1.3 Hz, 1H), 7.55 (dd, *J* = 8.1, 7.1 Hz, 1H), 7.61 (d, *J* = 8.5 Hz, 1H), 7.92 (d, *J* = 8.3 Hz, 2H) ppm.

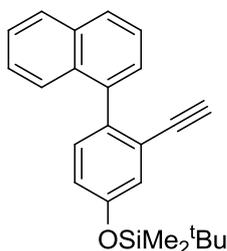
¹³C NMR (101 MHz, CDCl₃) δ = 75.9, 85.9 (d, *J* = 4.0 Hz), 111.6 (d, *J* = 15.4 Hz), 114.5 (d, *J* = 21.3 Hz), 125.2, 126.0, 126.0, 126.3, 126.6 (d, *J* = 3.3 Hz), 127.4, 128.4, 128.5, 129.7 (d, *J* = 8.9 Hz), 131.8, 133.6, 137.3 (d, *J* = 2.3 Hz), 145.9, 163.9 (d, *J* = 252.5 Hz) ppm.

¹⁹F NMR (376 MHz, CDCl₃) δ = -109.2 ppm.

HRMS calcd. for C₁₈H₁₁F₁: 246.084475; found 246.084200.

IR (neat) $\bar{\nu}$ = 662, 676, 735, 757, 779, 796, 895, 974, 1006, 1024, 1130, 1239, 1270, 1392, 1447, 1473, 1505, 1564, 1591, 1605, 3050, 3270 cm⁻¹.

Compound 10m:



Triethylamine (27 μ L, 0.20 mmol) and *tert*-butyldimethylsilane chloride (28 mg, 0.19 mmol) were added to a solution of the compound **10i** (43.8 mg, 0.18 mmol) in DCM (5 mL) and the mixture stirred overnight. Then, the solvent was evaporated and crude compound **10m** purified by flash chromatography (hexanes/EtOAc, 95/5). Colorless oil (63 mg, 97%).

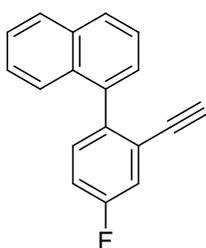
^1H NMR (400 MHz, CDCl_3) δ = 0.32 (s, J = 3.1 Hz, 6H), 1.07 (s, J = 3.0 Hz, 9H), 2.74 (s, 1H), 6.97 (dd, J = 8.3, 2.6 Hz, 1H), 7.18 (d, J = 2.6 Hz, 1H), 7.25 (d, J = 8.4 Hz, 1H), 7.43 (ddd, J = 8.2, 5.5, 1.4 Hz, 1H), 7.45 - 7.51 (m, 2H), 7.54 (dd, J = 8.1, 7.1 Hz, 1H), 7.65 (d, J = 8.4 Hz, 1H), 7.86 - 7.93 (m, 2H) ppm.

^{13}C NMR (101 MHz, CDCl_3) δ = -4.2, 18.4, 125.8, 80.1, 82.7, 120.9, 123.4, 124.3, 125.3, 125.8, 125.9, 126.4, 127.7, 127.9, 128.3, 132.0, 132.3, 133.7, 136.7, 138.4, 154.9 ppm.

HRMS calcd. for $\text{C}_{24}\text{H}_{26}\text{O}_1\text{Si}_1$: 358.175293; found 358.175011.

IR (neat) $\bar{\nu}$ = 678, 699, 774, 799, 812, 837, 970, 1093, 1158, 1226, 1253, 1288, 1389, 1461, 1471, 1488, 1553, 1599, 2857, 2929, 2955, 3060, 3291 cm^{-1} .

Compound 10n:



Prepared from compound **9n** (200 mg, 0.80 mmol) following the general procedure and purified by flash chromatography (hexanes/EtOAc, 95/5). Pale yellow solid (183 mg, 93%).

^1H NMR (400 MHz, CDCl_3) δ = 2.78 (s, 1H), 7.18 (td, J = 8.4, 2.7 Hz, 1H), 7.32 - 7.45 (m, 4H), 7.45 - 7.59 (m, 3H), 7.88 - 7.93 (m, 2H) ppm.

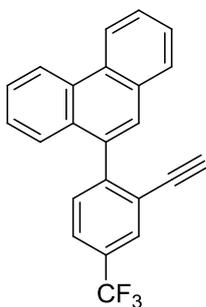
^{13}C NMR (101 MHz, CDCl_3) δ = 81.3, 81.6 (d, J = 3.0 Hz), 116.13 (d, J = 21.2 Hz), 119.6, 119.9, 124.3 (d, J = 9.6 Hz), 125.2, 125.9, 126.0, 126.2, 127.6, 128.4 (d, J = 2.2 Hz), 132.1, 132.5 (d, J = 8.5 Hz), 133.7, 137.5, 139.7 (d, J = 3.5 Hz), 161.7 (d, J = 247.0 Hz) ppm.

^{19}F NMR (376 MHz, CDCl_3) δ = -115.0 ppm.

HRMS calcd. for $\text{C}_{18}\text{H}_{11}\text{F}_1$: 246.084481; found 246.084549.

IR (neat) $\bar{\nu}$ = 666, 780, 793, 802, 833, 873, 933, 1090, 1143, 1219, 1256, 1276, 1390, 1458, 1478, 1490, 1574, 1600, 3043, 3276 cm^{-1} .

Compound 10o:



Prepared from compound **9o** (219 mg, 0.63 mmol) following the general procedure and purified by flash chromatography (hexanes/EtOAc, 95/5). White solid (207 mg, 96%).

^1H NMR (400 MHz, CDCl_3) δ = 2.81 (s, 1H), 7.53 - 7.61 (m, 3H), 7.62 - 7.71 (m, 3H), 7.72 - 7.78 (m, 2H), 7.92 (dd, J = 7.8, 1.4 Hz, 1H), 7.97 - 8.01 (m, 1H), 8.78 (dd, J = 14.7, 8.1 Hz, 2H) ppm.

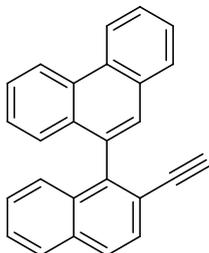
^{13}C NMR (101 MHz, CDCl_3) δ = 81.2, 82.4, 123.9 (q, J = 272.4 Hz), 122.8, 123.1, 123.8, 125.3 (q, J = 3.6 Hz), 126.7, 126.8, 127.1, 127.2, 128.2, 129.0, 130.1 (q, J = 3.8 Hz), 130.2 (q, J = 33.0 Hz), 130.5, 130.7, 131.3, 131.5, 135.9, 147.2 ppm.

^{19}F NMR (376 MHz, CDCl_3) δ = -62.7 ppm.

HRMS calcd. for $\text{C}_{23}\text{H}_{13}\text{F}_3$: 346.096937; found 346.0972041.

IR (neat) $\bar{\nu}$ = 658, 724, 745, 766, 838, 877, 898, 940, 1072, 1112, 1122, 1163, 1264, 1327, 1404, 1450, 1492, 1529, 1613, 3063, 3287 cm^{-1} .

Compound 10p.



Prepared from compound **9p** (123 mg, 0.37 mmol) following the general procedure and purified by flash chromatography (hexanes/EtOAc, 95/5). Brown solid (112 mg, 92%).

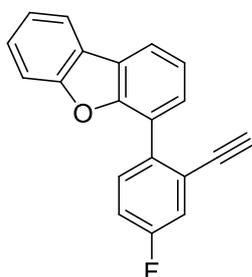
^1H NMR (400 MHz, CDCl_3) δ = 2.78 (s, 1H), 7.24 - 7.30 (m, 1H), 7.30 - 7.37 (m, 2H), 7.37 - 7.44 (m, 1H), 7.45 - 7.53 (m, 1H), 7.62 - 7.70 (m, 2H), 7.70 - 7.80 (m, 3H), 7.89 - 7.97 (m, 3H), 8.76 - 8.87 (m, 2H) ppm.

^{13}C NMR (101 MHz, CDCl_3) δ = 81.3, 83.2, 120.5, 122.9, 123.0, 126.7, 126.9, 127.0, 127.0, 127.0, 127.2, 128.0, 128.1, 128.9, 129.0, 129.1, 130.6, 131.8, 131.9, 133.1, 133.3, 135.3, 142.1 ppm.

HRMS calcd. for $\text{C}_{26}\text{H}_{16}$: 328.125198; found 328.125114.

IR (neat) $\bar{\nu}$ = 666, 726, 749, 755, 819, 894, 1026, 1264, 1332, 1369, 1422, 1447, 1489, 1559, 3055, 3267 cm^{-1} .

Compound 10q.



Prepared from compound **9q** (281 mg, 0.97 mmol) following the general procedure and purified by flash chromatography (hexanes/EtOAc, 95/5). White solid (270 mg, 97%).

^1H NMR (400 MHz, CDCl_3) δ = 2.94 (s, 1H), 7.22 (td, J = 8.4, 2.7 Hz, 1H), 7.37 (td, J = 7.5, 1.0 Hz, 1H), 7.39 - 7.48 (m, 3H), 7.64 - 7.62 (m, 3H), 7.96 - 8.03 (m, 2H) ppm.

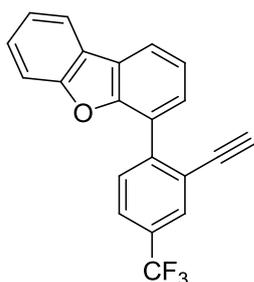
^{13}C NMR (101 MHz, CDCl_3) δ = 81.2, 81.7 (d, J = 3.0 Hz), 112.0, 116.3, 116.6, 120.3 (d, J = 23.1 Hz), 120.5, 120.8, 122.6, 123.0, 123.7 (d, J = 9.7 Hz), 124.0, 124.5 (d, J = 25.8 Hz), 127.4, 128.8, 132.3 (d, J = 8.6 Hz), 135.6 (d, J = 3.4 Hz), 153.7, 156.3, 161.92 (d, J = 247.7 Hz) ppm.

^{19}F NMR (376 MHz, CDCl_3) δ = -114.3 ppm.

HRMS calcd. for $\text{C}_{20}\text{H}_{11}\text{O}_1\text{F}_1$: 286.079390; found 286.079443.

IR (neat) $\bar{\nu}$ = 661, 746, 796, 824, 877, 944, 1016, 1058, 1094, 1153, 1193, 1262, 1284, 1419, 1452, 1484, 1505, 1573, 1605, 3062, 3277 cm^{-1} .

Compound 10r:



Prepared from compound **9r** (160 mg, 0.47 mmol) and purified by flash chromatography (hexanes/EtOAc, 95/5). White solid (143 mg, 90%).

^1H NMR (400 MHz, CDCl_3) δ = 3.00 (s, 1H), 7.39 (td, J = 7.6, 0.9 Hz, 1H), 7.43 - 7.52 (m, 2H), 7.58 (d, J = 8.2 Hz, 1H), 7.65 (dd, J = 7.6, 1.2 Hz, 1H), 7.73 - 7.82 (m, 2H), 7.98 - 8.06 (m, 3H) ppm.

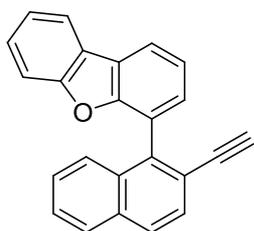
^{13}C NMR (101 MHz, CDCl_3) δ = 81.5, 81.9, 112.0, 120.9, 121.1, 122.7, 122.8, 123.1, 123.5, 123.9 (q, J = 272.3 Hz), 124.3, 124.9, 125.5 (q, J = 3.6 Hz), 127.6, 128.5, 130.3 (q, J = 33.0 Hz), 130.7 (q, J = 3.9 Hz), 131.2, 142.8 (q, J = 1.2 Hz), 153.5, 156.3 ppm.

^{19}F NMR (376 MHz, CDCl_3) δ = -62.7 ppm.

HRMS calcd. for $\text{C}_{21}\text{H}_{11}\text{O}_1\text{F}_3$: 336.076204; found 336.075869.

IR (neat) $\bar{\nu}$ = 659, 669, 734, 743, 753, 801, 836, 892, 903, 1014, 1059, 1075, 1109, 1163, 1177, 1184, 1294, 1331, 1397, 1417, 1450, 1472, 1585, 1612, 3069, 3275 cm^{-1} .

Compound 10s.



Prepared from compound **9s** (70 mg, 0.22 mmol) following the general procedure and purified by flash chromatography (hexanes/EtOAc, 95/5). White solid (64 mg, 93%).

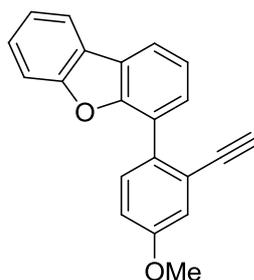
^1H NMR (400 MHz, CDCl_3) δ = 2.89 (s, 1H), 7.35 - 7.40 (m, 2H), 7.41 - 7.47 (m, 2H), 7.49 - 7.54 (m, 4H), 7.75 (d, J = 8.6 Hz, 1H), 7.93 (d, J = 8.2 Hz, 2H), 8.01 - 8.07 (m, 1H), 8.08 - 8.12 (m, 1H) ppm.

^{13}C NMR (101 MHz, CDCl_3) δ = 80.9, 83.2, 112.1, 120.2, 120.6, 120.8, 122.8, 122.8, 123.0, 124.4, 124.5, 126.7, 126.9, 127.0, 127.3, 128.3, 128.4, 129.2, 129.6, 132.2, 133.4, 138.3, 154.5, 156.4 ppm.

HRMS calcd. for $\text{C}_{24}\text{H}_{14}\text{O}_1$: 318.104469; found 318.104400.

IR (neat) $\bar{\nu}$ = 663, 745, 756, 825, 1008, 1188, 1255, 1334, 1410, 1449, 1504, 1583, 2923, 3054, 3283 cm^{-1} .

Compound 10t:



Prepared from compound **9t** (300 mg, 0.99 mmol) using the general procedure and purified by flash chromatography (hexanes/EtOAc, 9/1). Pale brown solid (283 mg, 96%).

^1H NMR (400 MHz, CDCl_3) δ = 2.92 (s, 1H), 3.90 (s, 3H), 7.08 (dd, J = 8.6, 2.7 Hz, 1H), 7.25 (d, J = 2.7 Hz, 1H), 7.36 (td, J = 7.5, 0.9 Hz, 1H), 7.42 (t, J = 7.6 Hz, 1H), 7.44 - 7.49 (m, 1H), 7.57 (d, J = 8.5 Hz, 2H), 7.62 (dd, J = 7.5, 1.2 Hz, 1H), 7.97 (dd, J = 7.7, 1.2 Hz, 1H), 8.00 (dd, J

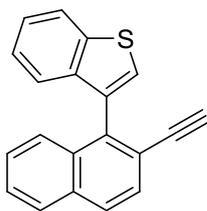
= 7.7, 0.7 Hz, 1H) ppm.

^{13}C NMR (101 MHz, CDCl_3) δ = 55.6, 80.1, 82.8, 112.0, 115.7, 118.3, 120.0, 120.8, 122.5, 122.8, 122.8, 124.5, 124.6, 127.2, 128.9, 131.8, 131.9, 153.9, 156.3, 159.0 ppm.

HRMS calcd. for $\text{C}_{21}\text{H}_{14}\text{O}_2$: 298.099381; found 298.099450.

IR (neat) $\bar{\nu}$ = 660, 728, 741, 796, 818, 841, 883, 916, 1013, 1047, 1098, 1119, 1128, 1162, 1172, 1191, 1232, 1258, 1273, 1294, 1400, 1416, 1451, 1485, 1505, 1567, 1604, 2827, 2921, 3277 cm^{-1} .

Compound 10u:



Prepared from compound **9u** (145 mg, 0.50 mmol) following the general procedure and purified by flash chromatography (hexanes/EtOAc, 95/5). Pale brown solid (128 mg, 90%).

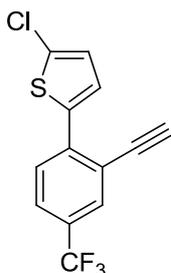
^1H NMR (400 MHz, CDCl_3) δ = 2.94 (s, 1H), 7.22 - 7.30 (m, 2H), 7.32 - 7.43 (m, 2H), 7.47 - 7.55 (m, 3H), 7.70 (d, J = 8.5 Hz, 1H), 7.86 - 7.93 (m, 2H), 7.98 (dt, J = 8.1, 0.7 Hz, 1H) ppm.

^{13}C NMR (101 MHz, CDCl_3) δ = 81.2, 83.2, 120.7, 122.8, 123.5, 124.3, 124.5, 126.4, 126.8, 126.9, 127.0, 128.2, 128.3, 129.2, 132.9, 133.4, 134.1, 137.4, 139.5, 139.9 ppm.

HRMS calcd. for $\text{C}_{20}\text{H}_{12}\text{S}_1$: 284.065976; found 284.065701.

IR (neat) $\bar{\nu}$ = 661, 684, 713, 741, 754, 765, 821, 840, 870, 946, 1026, 1083, 1256, 1307, 1427, 1454, 1498, 1567, 1593, 3055, 3270 cm^{-1} .

Compound 10v:



Prepared from 2-bromo-5-(trifluoromethyl)benzaldehyde (313 mg, 1.24 mmol) and 5-chlorothiophene-boronic acid (221 mg, 1.36 mmol) following the general procedure and purified by flash chromatography (hexanes/EtOAc, 98/2) a brown oil (212 mg, 60%). As the purification of the aldehyde was not satisfactory, the mixture obtained containing mainly **9v** (154 mg, 0.53 mmol) was submitted to the general Ohira-Bestmann conditions and purified by flash chromatography (hexanes). Brown oil (138 mg, 91%).

^1H NMR (400 MHz, CDCl_3) δ = 3.39 (s, 1H), 6.95 (d, J = 4.0 Hz, 1H), 7.46 (d, J = 4.0 Hz, 1H), 7.53 - 7.62 (m, 2H), 7.84 (s, 1H) ppm.

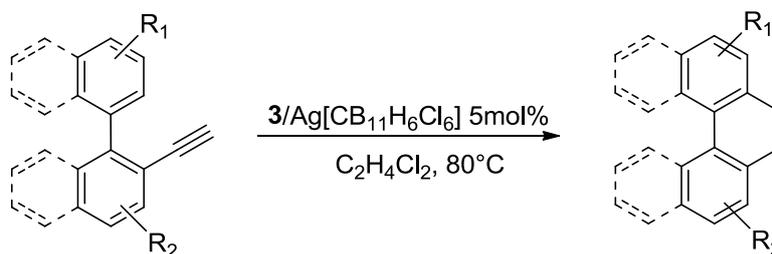
^{13}C NMR (101 MHz, CDCl_3) δ = 81.8, 84.1, 120.1, 123.6 (q, J = 272.2 Hz), 125.9 (q, J = 3.6 Hz), 126.8, 127.6, 129.0, 129.7 (q, J = 33.3 Hz), 131.8 (q, J = 3.9 Hz), 132.0, 138.7, 138.8 ppm.

^{19}F NMR (376 MHz, CDCl_3) δ = -62.9 ppm.

HRMS calcd. for $\text{C}_{13}\text{H}_6\text{Cl}_1\text{F}_3\text{S}_1$: 285.983087; found 285.982950.

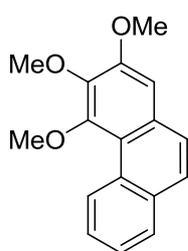
IR (neat) $\bar{\nu}$ = 685, 733, 794, 832, 863, 904, 952, 1006, 1078, 1121, 1166, 1265, 1327, 1404, 1438, 1490, 1565, 1611, 3303 cm^{-1} .

General Procedure for the Pt catalysed cycloisomerization



A suspension of alkyne (1 eq.), Ag[CB₁₁H₆Cl₆] (0.05 eq.) and compound **3** (0.05 eq.) in dry DCE (0.2 M) was stirred at 80°C under Ar. Reaction progress was followed by GC and once completed, the solvents were evaporated and the residue purified by flash chromatography.

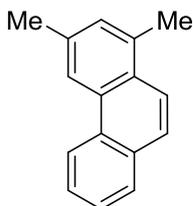
Compound 11a



Prepared from compound **10a** (53.6 mg, 0.2 mmol) following the general procedure and purified by flash chromatography (hexanes/EtOAc, 6/1). White solid (40 mg, 75%).

NMR spectra were identical to those already reported.

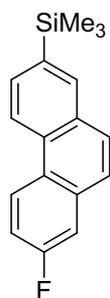
Compound 11b



Prepared from compound **10b** (41.2 mg, 0.2 mmol) following the general procedure and purified by flash chromatography (hexanes/EtOAc, 15/1). An isomeric mixture of **11b/12b** 82/18 (40 mg, 97%) was obtained.

NMR spectra were identical to those already reported.

Compound 11c:



Prepared from compound **10c** (80.4 mg, 0.3 mmol) following the general procedure and purified by flash chromatography (hexanes/EtOAc, 95/5). White solid (53 mg, 75%).

¹H NMR (400 MHz, CDCl₃) δ = 0.38 (s, 9H), 7.35 - 7.43 (m, 1H), 7.52 (dd, *J* = 9.5, 2.7 Hz, 1H), 7.67 (d, *J* = 8.9 Hz, 1H), 7.75 - 7.83 (m, 2H), 8.04 (s, 1H), 8.58 (d, *J* = 8.3 Hz, 1H), 8.67 (dd, *J* = 9.1, 5.4 Hz, 1H) ppm.

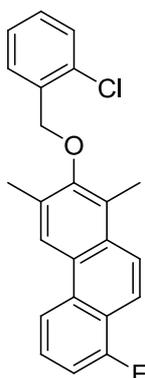
¹³C NMR (101 MHz, CDCl₃) δ = -0.90, 112.6, 112.7 (d, *J* = 20.4 Hz), 115.6 (d, *J* = 23.7 Hz), 121.7, 125.2 (d, *J* = 8.8 Hz), 126.21 (d, *J* = 3.7 Hz), 127.0 (d, *J* = 1.8 Hz), 128.6, 130.6, 131.0 (d, *J* = 1.2 Hz), 131.6, 133.8 (d, *J* = 8.7 Hz), 134.5, 138.7, 161.5 (d, *J* = 246.3 Hz) ppm.

^{19}F NMR (376 MHz, CDCl_3) $\delta = -115.0$ ppm.

HRMS calcd. for $\text{C}_{17}\text{H}_{17}\text{F}_1\text{Si}_1$: 268.108355; found 268.108080.

IR (neat) $\bar{\nu} = 694, 708, 753, 772, 808, 836, 868, 900, 949, 1090, 1140, 1146, 1186, 1233, 1250, 1263, 1302, 1366, 1429, 1468, 1525, 1567, 1618, 2957$ cm^{-1} .

Compound 11d:



Prepared from compound **10d** (40.7 mg, 0.11 mmol) following the general procedure. An isomeric mixture of **11d/12d**, 90/10 (35.3 mg, 87%) was obtained and compound **11d** purified by flash chromatography (hexanes/EtOAc, 95/5). White solid.

^1H NMR (400 MHz, CDCl_3) $\delta = 2.58$ (s, 3H), 2.69 (s, 3H), 5.03 (s, 2H), 7.25 (ddd, $J = 10.0, 7.8, 0.6$ Hz, 1H), 7.32 (td, $J = 7.6, 1.8$ Hz, 1H), 7.38 (td, $J = 7.5, 1.5$ Hz, 1H), 7.45 (dd, $J = 7.7, 1.4$ Hz, 1H), 7.55 (td, $J = 8.1, 5.9$ Hz, 1H), 7.78 (dd, $J = 7.5, 1.6$ Hz, 1H), 7.96 (d, $J = 9.4$ Hz, 1H), 8.02 (d, $J = 9.4$ Hz, 1H), 8.41 (d, $J = 10.6$ Hz, 2H) ppm.

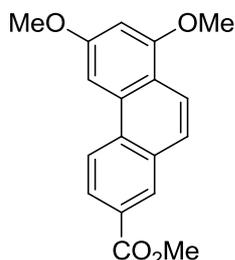
^{13}C NMR (101 MHz, CDCl_3) $\delta = 12.3, 17.8, 71.9, 110.5$ (d, $J = 20.3$ Hz), 118.1 (d, $J = 6.8$ Hz), 118.6 (d, $J = 3.8$ Hz), 121.1 (d, $J = 15.7$ Hz), 123.3, 123.5 (d, $J = 1.9$ Hz), 126.5 (d, $J = 8.8$ Hz), 126.8, 126.8, 127.2, 129.2, 129.3, 129.5, 131.1, 131.5, 132.3 (d, $J = 4.4$ Hz), 132.9, 135.5, 154.9, 159.5 (d, $J = 249.9$ Hz) ppm.

^{19}F NMR (376 MHz, CDCl_3) $\delta = -122.6$ ppm.

HRMS calcd. for $\text{C}_{23}\text{H}_{18}\text{O}_1\text{Cl}_1\text{F}_1$: 364.103020; found 364.103188.

IR (neat) $\bar{\nu} = 672, 688, 745, 805, 840, 867, 939, 973, 1057, 1076, 1188, 1235, 1259, 1379, 1447, 1475, 1510, 1603, 2920, 3061$ cm^{-1} .

Compound 11e:



Prepared from compound **10e** (59.4 mg, 0.20 mmol) following the general procedure. An isomeric mixture of **11e/12e**, 93/7 (51.6 mg, 87%) was obtained and compound **11e** purified by flash chromatography (hexanes/EtOAc, 10/1). White solid.

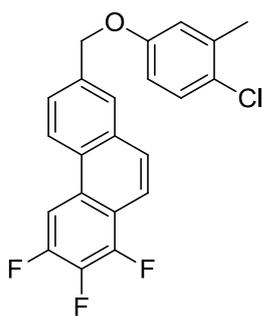
^1H NMR (400 MHz, CDCl_3) $\delta = 3.99$ (s, 3H), 4.00 (s, 3H), 4.00 (s, 3H), 6.68 (d, $J = 2.1$ Hz, 1H), 7.56 (d, $J = 1.9$ Hz, 1H), 7.64 (t, $J = 6.8$ Hz, 1H), 8.15 (d, $J = 8.9$ Hz, 2H), 8.54 (d, $J = 8.8$ Hz, 1H), 8.56 (d, $J = 1.7$ Hz, 1H) ppm.

^{13}C NMR (101 MHz, CDCl_3) $\delta = 52.3, 55.6, 55.9, 95.8, 98.7, 119.6, 121.3, 123.4, 124.0, 125.7, 128.0, 131.1, 131.8, 132.2, 132.5, 157.2, 159.4, 167.3$ ppm.

HRMS calcd. for $\text{C}_{18}\text{H}_{16}\text{O}_4\text{Na}_1$: 319.094080; found 319.094080.

IR (neat) $\bar{\nu} = 669, 730, 756, 776, 808, 833, 917, 943, 992, 1029, 1058, 1088, 1151, 1172, 1203, 1255, 1279, 1367, 1390, 1408, 1433, 1454, 1498, 1524, 1603, 1619, 1716, 2953, 3008$ cm^{-1} .

Compound 11f:



Prepared from compound **10f** (46.5 mg, 0.12 mmol) following the general procedure. An isomeric mixture of **11f/12f**, 99/1 (41.3 mg, 89%) was obtained and compound **11f** purified by flash chromatography (hexanes/EtOAc, 95/5). White solid.

^1H NMR (400 MHz, CDCl_3) δ = 2.36 (s, 3H), 5.08 (s, 2H), 6.77 (dd, J = 8.7, 3.0 Hz, 1H), 6.89 (d, J = 2.9 Hz, 1H), 7.01 (ddd, J = 10.6, 7.1, 2.1 Hz, 1H), 7.24 (d, J = 8.7 Hz, 1H), 7.49 (d, J = 8.5 Hz, 2H), 7.55 (d, J = 8.3 Hz, 2H) ppm.

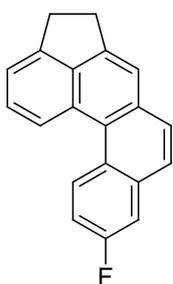
^{13}C NMR (101 MHz, CDCl_3) δ = 20.5, 69.9, 86.8 (dd, J = 4.9, 2.2 Hz), 107.4 (dd, J = 13.2, 3.7 Hz), 113.3 (dd, J = 18.4, 3.5 Hz), 113.5, 113.6, 117.5, 126.5, 126.7, 127.4, 129.4, 129.8, 137.3, 137.3-137.4 (m), 137.4, 139.3 (dt, J = 252.8, 15.5 Hz), 140.7 (dd, J = 7.6, 4.1 Hz), 151.1 (ddd, J = 253.9, 10.1, 4.1 Hz), 153.4 (ddd, J = 254.9, 10.7, 4.2 Hz), 157.3 ppm.

^{19}F NMR (376 MHz, CDCl_3) δ = -128.4 (dd, J = 20.7, 8.6 Hz), -131.2 (dd, J = 21.2, 8.6 Hz), -160.7 (t, J = 20.9 Hz) ppm.

HRMS calcd. for $\text{C}_{22}\text{H}_{14}\text{OCIF}_3$: 386.068532; found 386.068280.

IR (neat) $\bar{\nu}$ = 677, 726, 816, 840, 862, 873, 957, 972, 999, 1014, 1065, 1124, 1169, 1236, 1260, 1304, 1361, 1380, 1406, 1443, 1467, 1483, 1501, 1525, 1593, 2875, 2932 cm^{-1} .

Compound 11h:



Prepared from compound **10h** (41.9 mg, 0.15 mmol) following the general procedure. An isomeric mixture of **11h/12h/13h**, 88/2/10 (38.3 mg, 91%) was obtained and the major compound purified by semi-preparative HPLC (YMC, 2 cm x 15 cm, MeOH/ H_2O 90/10, 15 mL/min; 32.0 mg in 1.5 mL of CH_3CN). Yellow solid.

^1H NMR (400 MHz, CDCl_3) δ = 3.44 - 3.54 (m, 4H), 7.45 (ddd, J = 9.4, 8.1, 2.8 Hz, 1H), 7.49 (d, J = 6.9 Hz, 1H), 7.60 (s, 1H), 7.62 (dd, J = 9.0, 2.3 Hz, 1H), 7.68 (dd, J = 8.4, 7.0 Hz, 1H), 7.81 (q, J = 8.6 Hz, 2H), 8.81 (d, J = 8.5 Hz, 1H), 9.24 (dd, J = 9.4, 5.5 Hz, 1H) ppm.

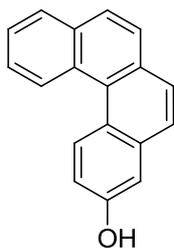
^{13}C NMR (101 MHz, CDCl_3) δ = 29.5, 30.8, 112.3 (d, J = 20.1 Hz), 115.4 (d, J = 23.4 Hz), 120.3, 120.9, 123.3, 124.9, 126.62 (d, J = 4.0 Hz), 128.2, 128.5, 128.8, 129.0, 129.3 (d, J = 8.3 Hz), 133.2, 134.2 (d, J = 8.5 Hz), 139.5, 145.1, 146.3, 160.3 (d, J = 246.2 Hz) ppm.

^{19}F NMR (376 MHz, CDCl_3) δ = -116.5 ppm.

HRMS calcd. for $\text{C}_{20}\text{H}_{13}\text{F}$: 272.100129; found 272.100053.

IR (neat) $\bar{\nu}$ = 669, 740, 753, 838, 858, 883, 898, 951, 1077, 118, 1138, 1181, 1204, 1251, 1343, 1362, 1390, 1423, 1435, 1486, 1529, 1574, 1695, 1615, 2915, 3042 cm^{-1} .

Compound 11i:



Prepared from compound **10i** (22.1 mg, 0.09 mmol) following the general procedure. An isomeric mixture of **11i/12i/13i**, 95/3/2 (19.1 mg, 86%) was obtained and compound **11i** isolated after flash chromatography (hexanes/EtOAc, 4/1).

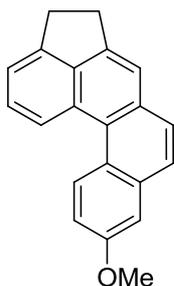
^1H NMR (400 MHz, CDCl_3) δ = 5.01 (s, 1H), 7.27 (dd, J = 9.1, 2.9 Hz, 1H), 7.36 (d, J = 2.7 Hz, 1H), 7.59 - 7.64 (m, 1H), 7.67 (ddd, J = 8.5, 6.9, 1.6 Hz, 1H), 7.76 (d, J = 8.6 Hz, 1H), 7.80 (dd, J = 8.5, 2.5 Hz, 2H), 7.85 (d, J = 8.5 Hz, 1H), 8.01 (dd, J = 7.8, 1.4 Hz, 1H), 9.00 - 9.10 (m, 2H) ppm.

^{13}C NMR (101 MHz, CDCl_3) δ = 111.4, 116.7, 125.4, 126.0, 126.1, 126.5, 126.7, 127.0, 127.8, 128.0, 128.7, 129.9, 130.0, 130.2, 133.8, 135.3, 153.5 ppm.

HRMS calcd. for $\text{C}_{18}\text{H}_{12}\text{O}$: 244.088818; found 244.088765.

IR (neat) $\bar{\nu}$ = 669, 741, 790, 800, 831, 859, 930, 966, 984, 1043, 1108, 1155, 1195, 1222, 1254, 1373, 1421, 1456, 1500, 1536, 1570, 1613, 2920, 3050, 3264 cm^{-1} .

Compound 11j:



Prepared from compound **10j** (25.1 mg, 0.09 mmol) following the general procedure. An isomeric mixture of **11j/12j/13j**, 93/5/2 (22 mg, 88%) was obtained and compound **11j** isolated after flash chromatography (hexanes/EtOAc, 95/5). Pale brown solid

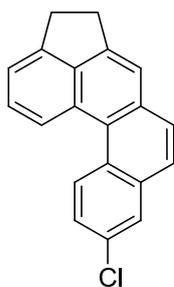
^1H NMR (400 MHz, CDCl_3) δ = 3.44 - 3.55 (m, 4H), 4.01 (s, 3H), 7.34 - 7.36 (m, 1H), 7.37 (s, 1H), 7.48 (d, J = 6.7 Hz, 1H), 7.61 (s, J = 1.4 Hz, 1H), 7.67 (dd, J = 8.4, 7.0 Hz, 1H), 7.80 (s, J = 9.2 Hz, 2H), 8.86 (d, J = 8.5 Hz, 1H), 9.15 - 9.23 (m, 1H) ppm.

^{13}C NMR (101 MHz, CDCl_3) δ = 29.5, 30.9, 55.5, 108.2, 117.3, 120.4, 120.7, 123.7, 125.2, 126.2, 126.8, 128.2, 128.4, 128.6, 128.9, 132.5, 134.5, 139.5, 144.2, 146.2, 157.2 ppm.

HRMS calcd. for $\text{C}_{21}\text{H}_{16}\text{O}$: 284.120118; found 284.120148.

IR (neat) $\bar{\nu}$ = 673, 694, 719, 739, 755, 782, 805, 832, 842, 865, 942, 981, 1036, 1119, 1155, 1214, 1257, 1294, 1355, 1392, 1422, 1430, 1486, 1523, 1603, 1624, 2832, 2915 cm^{-1} .

Compound 11k:



Prepared from compound **10k** (57.7 mg, 0.2 mmol) following the general procedure. An isomeric mixture of **11k/12k/13k**, 91/7/2 (53 mg, 92%) was obtained and compound **11k** isolated after flash chromatography (hexanes/EtOAc, 8/1). White solid

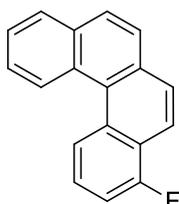
^1H NMR (400 MHz, CDCl_3) δ = 3.46 - 3.58 (m, 4H), 7.50 (d, J = 6.9 Hz, 1H), 7.59 - 7.65 (m, J = 11.4 Hz, 2H), 7.69 (dd, J = 8.4, 7.0 Hz, 1H), 7.78 (d, J = 8.6 Hz, 1H), 7.85 (d, J = 8.6 Hz, 1H), 7.97 (d, J = 2.3 Hz, 1H), 8.81 (d, J = 8.5 Hz, 1H), 9.19 (d, J = 9.1 Hz, 1H) ppm.

^{13}C NMR (101 MHz, CDCl_3) δ = 29.6, 30.9, 120.3, 121.0, 123.4, 124.8, 126.4, 126.7, 127.5, 128.7, 128.9, 129.1, 129.7, 131.1, 133.8, 134.0, 139.5, 145.7, 146.4 ppm.

HRMS calcd. for $\text{C}_{20}\text{H}_{13}\text{Cl}$: 288.070582; found 288.070414.

IR (neat) $\bar{\nu}$ = 670, 737, 756, 789, 820, 836, 875, 888, 903, 1073, 1099, 1174, 1194, 1224, 1338, 1365, 1420, 1432, 1484, 1515, 1599, 1609, 1634, 2918, 3033 cm^{-1} .

Compound 11l:



Prepared from compound **10l** (49.2 mg, 0.2 mmol) following the general procedure. Compound **11l** was isolated after flash chromatography (hexanes/EtOAc, 8/1) as a pale yellow solid (46.2 mg, 94%).

^1H NMR (400 MHz, CDCl_3) δ = 7.32 (ddd, J = 10.0, 7.8, 0.8 Hz, 1H), 7.8 - 7.63 (m, 1H), 7.65 (ddd, J = 7.0, 6.6, 1.3 Hz, 1H), 7.70 (ddd, J = 8.5, 6.9, 1.6 Hz, 1H), 7.84 (d, J = 8.5 Hz, 1H), 7.89 (dd, J = 10.5, 6.1 Hz, 1H), 7.93 (d, J = 8.5 Hz, 1H), 8.04 (dd, J = 7.8, 1.5 Hz, 1H), 8.22 (d, J = 8.8 Hz, 1H), 8.92 (d, J = 8.6 Hz, 1H), 9.10 (dd, J = 8.4, 0.5 Hz, 1H) ppm.

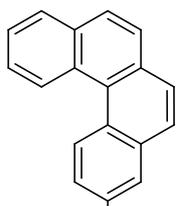
^{13}C NMR (101 MHz, CDCl_3) δ = 110.2 (d, J = 20.2 Hz), 119.4 (d, J = 7.7 Hz), 123.4 (d, J = 15.5 Hz), 123.9 (d, J = 3.9 Hz), 126.1 (d, J = 8.7 Hz), 126.3, 126.5, 126.9, 127.1 (d, J = 2.7 Hz), 127.5 (d, J = 1.9 Hz), 128.1, 128.2, 128.8, 130.4, 131.5, 132.1 (d, J = 3.9 Hz), 133.8, 159.3 (d, J = 249.7 Hz) ppm.

^{19}F NMR (376 MHz, CDCl_3) δ = -121.7 ppm.

HRMS calcd. for $\text{C}_{18}\text{H}_{11}\text{F}$: 246.084476; found 246.084598.

IR (neat) $\bar{\nu}$ = 653, 671, 738, 750, 794, 818, 834, 880, 1025, 1077, 1126, 1159, 1208, 1231, 1239, 1365, 1421, 1454, 1492, 1561, 1601, 1615, 3050 cm^{-1} .

Compound 11m:



Prepared from compound **10m** (46.5 mg, 0.13 mmol) following the general procedure. An isomeric mixture of **11m/12m/13m**, 95/4/1 (40.1 mg, 86%) was obtained and compound **11m** purified by semi-preparative HPLC (Dupont, 2.1 cm x 25 cm, iso-Hexane, 20 mL/min; 34.5 mg in 2.0 mL of iso-Hexane) as a colorless oil.

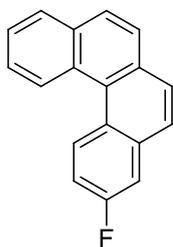
^1H NMR (400 MHz, CDCl_3) δ = 0.33 (s, 6H), 1.07 (s, 9H), 7.26 (dd, J = 9.1, 2.7 Hz, 1H), 7.40 (d, J = 2.6 Hz, 1H), 7.58 - 7.64 (m, 1H), 7.64 - 7.70 (m, 1H), 7.75 - 7.82 (m, 3H), 7.85 (d, J = 8.5 Hz, 1H), 8.01 (dd, J = 7.9, 0.9 Hz, 1H), 9.02 (d, J = 9.2 Hz, 1H), 9.09 (d, J = 8.4 Hz, 1H) ppm.

^{13}C NMR (101 MHz, CDCl_3) δ = -4.1, 18.5, 25.9, 116.6, 121.1, 125.7, 125.9, 126.1, 126.7, 126.9, 127.0, 127.4, 127.7, 128.0, 128.7, 129.5, 130.0, 130.3, 133.7, 135.3, 153.7 ppm.

HRMS calcd. for $\text{C}_{24}\text{H}_{26}\text{O}_1\text{Si}_1$: 358.175294; found 358.175393.

IR (neat) $\bar{\nu}$ = 671, 700, 742, 778, 803, 830, 855, 948, 974, 989, 1109, 1158, 1168, 1199, 1236, 1267, 1343, 1423, 1452, 1471, 1489, 1503, 1516, 1560, 1607, 2856, 2928, 2953, 3048 cm^{-1} .

Compound 11n.



Prepared from compound **10n** (22.6 mg, 0.09 mmol) following the general procedure. An isomeric mixture of **11n/12n/13n**, 97/2/1 (21.5 mg, 95%) was obtained and compound **11n** purified by semi-preparative HPLC (Dupont, 2.1 cm x 25 cm, iso-Hexane, 15 mL/min; 51.2 mg in 1.0 mL of MTBE). White solid.

^1H NMR (400 MHz, CDCl_3) δ = 7.44 (ddd, J = 9.3, 8.1, 2.8 Hz, 1H), 7.61 - 7.67 (m, 2H), 7.67 - 7.73 (m, 1H), 7.79 - 7.87 (m, 3H), 7.90 (d, J = 8.5 Hz, 1H), 8.03 (d, J = 7.7 Hz, 1H), 9.04 (d, J = 8.4 Hz, 1H), 9.11 (dd, J = 9.3, 5.6 Hz, 1H) ppm.

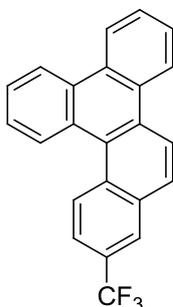
^{13}C NMR (101 MHz, CDCl_3) δ = 112.3 (d, J = 20.2 Hz), 115.4 (d, J = 23.5 Hz), 126.3 (d, J = 20.3 Hz), 126.8 (d, J = 4.1 Hz), 126.9, 127.2 (d, J = 1.8 Hz), 127.5, 127.6, 127.8, 128.2, 128.8, 130.1, 130.4 (d, J = 8.5 Hz), 130.5 (d, J = 1.6 Hz), 133.8, 135.0 (d, J = 8.6 Hz), 160.6 (d, J = 247.2 Hz) ppm.

^{19}F NMR (376 MHz, CDCl_3) δ = -115.6 ppm.

HRMS calcd. for $\text{C}_{18}\text{H}_{11}\text{F}$: 246.084480; found 246.084640.

IR (neat) $\bar{\nu}$ = 661, 743, 775, 789, 801, 824, 856, 928, 970, 1103, 1133, 1148, 1194, 1227, 1251, 1349, 1359, 1419, 1452, 1500, 1523, 1565, 1617, 2921, 3052 cm^{-1} .

Compound 11o:



Prepared from compound **10o** (39.4 mg, 0.11 mmol) following the general procedure. An isomeric mixture of **11o/12o/13o**, 94/5/1 (37.2 mg, 94%) was obtained and compound **11o** isolated after flash chromatography (hexanes/MTBE, 95/5). Light yellow solid

^1H NMR (400 MHz, CDCl_3) δ = 7.61 (ddd, J = 8.3, 7.1, 1.3 Hz, 1H), 7.65 - 7.72 (m, 3H), 7.74 (, J = 9.1, 1.9 Hz, 1H), 7.95 (d, J = 8.9 Hz, 1H), 8.24 (s, 1H), 8.54 - 8.60 (m, 2H), 8.64 - 8.75 (m, 3H), 8.92 (d, J = 8.9 Hz, 1H) ppm.

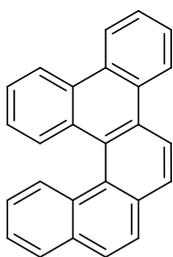
^{13}C NMR (101 MHz, CDCl_3) δ = 121.6 (q, J = 3.2 Hz), 122.2, 123.3, 123.7, 124.0, 124.6 (d, J = 271.9 Hz), 125.7 (q, J = 4.4 Hz), 126.5, 127.1, 127.2, 127.6 (q, J = 32.6 Hz), 127.7, 127.9, 127.9, 129.1, 129.3, 129.4, 129.5, 130.4, 131.1, 131.8, 132.6 ppm.

^{19}F NMR (376 MHz, CDCl_3) δ = -62.1 ppm.

HRMS calcd. for $\text{C}_{23}\text{H}_{13}\text{F}_3$: 346.096935; found 346.096996.

IR (neat) $\bar{\nu}$ = 681, 720, 753, 781, 792, 812, 832, 892, 904, 950, 963, 1077, 1112, 1153, 1186, 1243, 1296, 1308, 1326, 1362, 1447, 1479, 1496, 1576, 1626, 2923, 3071 cm^{-1} .

Compound 11p:



Prepared from compound **10p** (41.8 mg, 0.13 mmol) following the general procedure. An isomeric mixture of **11p/12p**, 90/10 (39.6 mg, 95%) was obtained and compound **11p** purified by semi-preparative HPLC (Dupont, 2.1 cm x 25 cm, iso-Hexane/MTBE 90/10, 15 mL/min; 23.6 mg in 5.0 mL of MTBE/2.0 mL of n-Heptan). White solid.

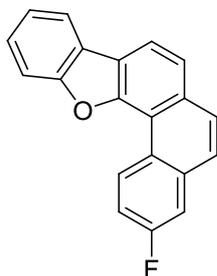
^1H NMR (400 MHz, CDCl_3) δ = 7.23 (t, J = 7.7 Hz, 2H), 7.53 (dt, J = 26.6, 7.5 Hz, 2H), 7.65 - 7.84 (m, 2H), 7.88 (q, J = 8.7 Hz, 2H), 7.94 (dd, J = 14.2, 8.3 Hz, 2H), 8.41 (dd, J = 35.1, 8.4 Hz, 2H), 8.54 - 8.62 (m, 3H), 8.62 - 8.82 (m, 1H) ppm.

^{13}C NMR (101 MHz, CDCl_3) δ = 121.6, 123.3, 123.7, 124.1, 124.6, 125.3, 126.3, 126.4, 127.0, 127.3, 127.4, 127.5, 127.6, 127.7, 127.8, 128.1, 129.6, 129.9, 130.0, 130.3, 130.5, 130.5, 130.9, 131.2, 132.5, 132.9 ppm.

HRMS calcd. for $\text{C}_{26}\text{H}_{16}$: 328.125202; found 328.124882.

IR (neat) $\bar{\nu}$ = 719, 744, 757, 764, 795, 835, 1434, 1481, 1605, 3064 cm^{-1} .

Compound 11q:



Prepared from compound **10q** (36.3 mg, 0.13 mmol) following the general procedure. An isomeric mixture of **11q/12q**, 93/7 (33.0 mg, 91%) was obtained and compound **11q** purified by semi-preparative HPLC (Dupont, 2.1 cm x 25 cm, iso-Hexane, 15 mL/min; 28.7 mg in 1.6 mL of MTBE). White solid.

^1H NMR (400 MHz, CDCl_3) δ = 7.44 (t, J = 7.2 Hz, 1H), 7.50 - 7.60 (m, 3H), 7.71 (d, J = 8.8 Hz, 1H), 7.79 (d, J = 8.2 Hz, 1H), 7.82 (d, J = 8.2 Hz, 1H), 7.87 (d, J = 8.8 Hz, 1H), 8.05 (d, J = 7.6 Hz, 1H), 8.09 (d, J = 8.2 Hz, 1H), 9.74 (dd, J = 9.1, 5.7 Hz, 1H) ppm.

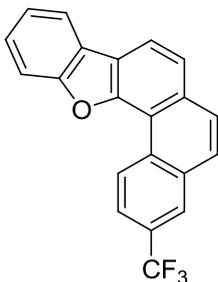
^{13}C NMR (101 MHz, CDCl_3) δ = 112.0, 112.4 (d, J = 20.5 Hz), 115.9 (d, J = 23.0 Hz), 117.8, 118.7, 120.5, 122.5, 123.3, 124.2, 124.3, 125.4 (d, J = 1.7 Hz), 126.5 (d, J = 3.8 Hz), 127.0, 128.5, 130.3 (d, J = 8.5 Hz), 132.0 (d, J = 1.4 Hz), 134.2 (d, J = 9.0 Hz), 153.0, 156.2, 161.2 (d, J = 246.8 Hz) ppm.

^{19}F NMR (376 MHz, CDCl_3) δ = -114.4 ppm.

HRMS calcd. for $\text{C}_{20}\text{H}_{11}\text{O}_1\text{F}_1$: 286.079390; found 286.079443.

IR (neat) $\bar{\nu}$ = 661, 746, 796, 824, 877, 944, 1016, 1058, 1094, 1153, 1193, 1262, 1284, 1419, 1452, 1484, 1505, 1573, 1605, 3062, 3277 cm^{-1} .

Compound 11r:



Prepared from compound **10r** (48.1 mg, 0.14 mmol) following the general procedure. An isomeric mixture of **11r/12r**, 97/3 (42.0 mg, 87%) was obtained and compound **11r** isolated after flash chromatography (hexanes/DCM, 9/1). White solid.

^1H NMR (400 MHz, CDCl_3) δ = 7.44 (td, J = 7.6, 0.9 Hz, 1H), 7.54 (ddd, J = 8.3, 7.4, 1.3 Hz, 1H), 7.73 - 7.81 (m, 3H), 7.86 (d, J = 8.8 Hz, 1H), 7.92 (dd, J = 8.8, 1.8 Hz, 1H), 8.01 (dd, J = 7.7, 0.6 Hz, 1H), 8.09 (d, J = 8.2 Hz, 1H), 8.16 (s, 1H), 9.73 (d, J = 8.8 Hz, 1H) ppm.

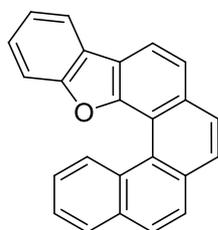
^{13}C NMR (101 MHz, CDCl_3) δ = 112.0, 117.2, 119.9, 120.6, 122.6, 122.8 (q, J = 3.3 Hz), 123.4, 124.0, 124.1, 124.6 (q, J = 272.1 Hz), 125.4 (q, J = 4.2 Hz), 126.9, 127.1, 128.3 (q, J = 32.4 Hz), 128.7, 130.6, 130.6, 131.7, 133.0, 153.3, 156.2 ppm.

^{19}F NMR (376 MHz, CDCl_3) δ = -61.9 ppm.

HRMS calcd. for $\text{C}_{21}\text{H}_{11}\text{O}_1\text{F}_3$: 336.076200; found 336.076284.

IR (neat) $\bar{\nu}$ = 672, 712, 724, 742, 750, 793, 805, 824, 835, 862, 900, 909, 1014, 1074, 1103, 1145, 1170, 1191, 1204, 1221, 1296, 1311, 1326, 1355, 1405, 1453, 1467, 1537, 1571, 1626, 2921, 3057 cm^{-1} .

Compound 11s:



Prepared from compound **10s** (26.4 mg, 0.08 mmol) following the general procedure. An isomeric mixture of **11s/12s**, 99/1 (21.9 mg, 83%) was obtained and compound **11s** isolated after flash chromatography (hexanes/toluene, 9/1). Pale yellow solid

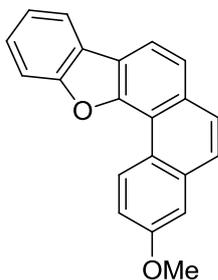
^1H NMR (400 MHz, CDCl_3) δ = 7.43 (td, J = 7.4, 1.1 Hz, 1H), 7.46 - 7.53 (m, 1H), 7.584 - 7.64 (m, 2H), 7.69 (ddd, J = 8.0, 7.0, 1.2 Hz, 1H), 7.88 (dd, J = 8.5, 3.3 Hz, 2H), 8.01 (d, J = 8.5 Hz, 1H), 8.04 (t, J = 8.9 Hz, 3H), 8.09 (dd, J = 7.2, 1.1 Hz, 1H), 8.23 (d, J = 8.2 Hz, 1H), 8.64 (d, J = 8.5 Hz, 1H) ppm.

^{13}C NMR (101 MHz, CDCl_3) δ = 112.0, 117.3, 119.1, 120.3, 121.7, 123.1, 124.1, 124.4, 124.9, 125.3, 126.3, 126.5, 126.9, 127.6, 128.0, 125.6, 130.1, 130.1, 132.2, 133.2, 133.9, 152.6, 154.8 ppm.

HRMS calcd. for $\text{C}_{24}\text{H}_{14}\text{O}_1$: 318.104462; found 318.104317.

IR (neat) $\bar{\nu}$ = 692, 729, 742, 757, 782, 798, 830, 861, 923, 1011, 1062, 1110, 1170, 1188, 1212, 1266, 1334, 1353, 1397, 1456, 1494, 1531, 1599, 2918, 3045 cm^{-1} .

Compound 11t:



Prepared from compound **10t** (29.7 mg, 0.10 mmol) following the general procedure. An isomeric mixture of **11t/12t**, 88/12 (22.9 mg, 77%) was obtained and compound **11t** isolated after flash chromatography (hexanes/EtOAc, 95/5). White solid.

^1H NMR (400 MHz, CDCl_3) δ = 4.01 (s, 3H), 7.34 (d, J = 2.8 Hz, 1H), 7.41 - 7.45 (m, 1H), 7.46 (dd, J = 8.4, 2.0 Hz, 1H), 7.53 (ddd, J = 8.3, 7.3, 1.3 Hz, 1H), 7.75 (d, J = 8.8 Hz, 1H), 7.82 (dd, J = 8.2, 0.7 Hz, 1H), 7.84 (d, J = 8.2 Hz, 1H), 7.88 (d, J = 8.8 Hz, 1H), 8.03 - 8.12 (m, 2H), 9.71 (d, J = 9.2 Hz,

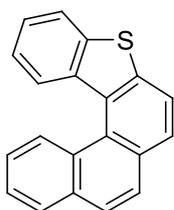
1H) ppm.

^{13}C NMR (101 MHz, CDCl_3) δ = 55.5, 108.6, 112.0, 117.5, 117.9, 118.2, 120.5, 122.2, 123.1, 123.2, 124.2, 124.5, 126.7, 126.8, 127.9, 129.5, 131.6, 134.3, 153.1, 156.3, 158.3 ppm.

HRMS calcd. for $\text{C}_{21}\text{H}_{14}\text{O}_2$: 298.099378; found 298.099577.

IR (neat) $\bar{\nu}$ = 657, 721, 740, 939, 1015, 1038, 1098, 1129, 1162, 1203, 1232, 1269, 1321, 1352, 1404, 1453, 1499, 1532, 1599, 1613, 1621, 2831, 2956 cm^{-1} .

Compound 11u:



Prepared from compound **10u** (20.9 mg, 0.07 mmol) following the general procedure. An isomeric mixture of **11u/12u**, 80/20 (17.0 mg, 81%) was obtained and compound **11u** isolated after flash chromatography (hexanes/EtOAc, 95/5). Orange solid.

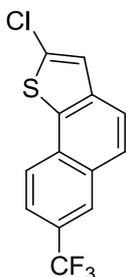
^1H NMR (400 MHz, CDCl_3) δ = 7.36 (ddd, J = 8.3, 7.2, 1.2 Hz, 1H), 7.43 - 7.48 (m, 1H), 7.51 (ddd, J = 8.3, 7.0, 1.4 Hz, 1H), 7.61 - 7.66 (m, 1H), 7.83 (s, 2H), 7.85 (d, J = 8.4 Hz, 1H), 7.97 (dd, J = 8.5, 2.4 Hz, 3H), 8.72 (d, J = 8.3 Hz, 1H), 9.05 (d, J = 8.3 Hz, 1H) ppm.

^{13}C NMR (101 MHz, CDCl_3) δ = 121.7, 123.1, 123.1, 124.3, 125.6, 126.1, 126.4, 127.0, 127.2, 127.3, 128.0, 128.3, 128.3, 129.0, 130.6, 130.9, 133.2, 137.0, 139.8, 140.2 ppm.

HRMS calcd. for $\text{C}_{20}\text{H}_{12}\text{S}_1$: 284.065969; found 284.065718.

IR (neat) $\bar{\nu}$ = 727, 752, 797, 822, 867, 905, 1019, 1135, 1158, 1192, 1219, 1254, 1316, 1332, 1435, 1456, 1491, 1581, 1712, 2850, 2921, 3049 cm^{-1} .

Compound 11v:



Prepared from compound **10v** (39.0 mg, 0.14 mmol) following the general procedure. An isomeric mixture of **11v/12v**, 98/2 (33.6 mg, 86%) was obtained and compound **11v** isolated after flash chromatography (hexanes). Brown oil.

^1H NMR (400 MHz, CDCl_3) δ = 7.32 (s, 1H), 7.72 (dd, J = 8.3, 2.0 Hz, 1H), 7.74 (d, J = 8.5 Hz, 1H), 7.78 (d, J = 8.7 Hz, 1H), 8.02 (d, J = 8.6 Hz, 1H), 8.18 (s, 1H) ppm.

^{13}C NMR (101 MHz, CDCl_3) δ = 120.1, 122.7, 122.8 (q, J = 3.2 Hz), 123.6 (q, J = 272.0 Hz), 124.3, 126.4, 126.8, 127.6, 126.7 (q, J = 4.4 Hz), 129.1, 129.8, 132.6, 138.0 ppm.

^{19}F NMR (376 MHz, CDCl_3) δ = -62.1 ppm.

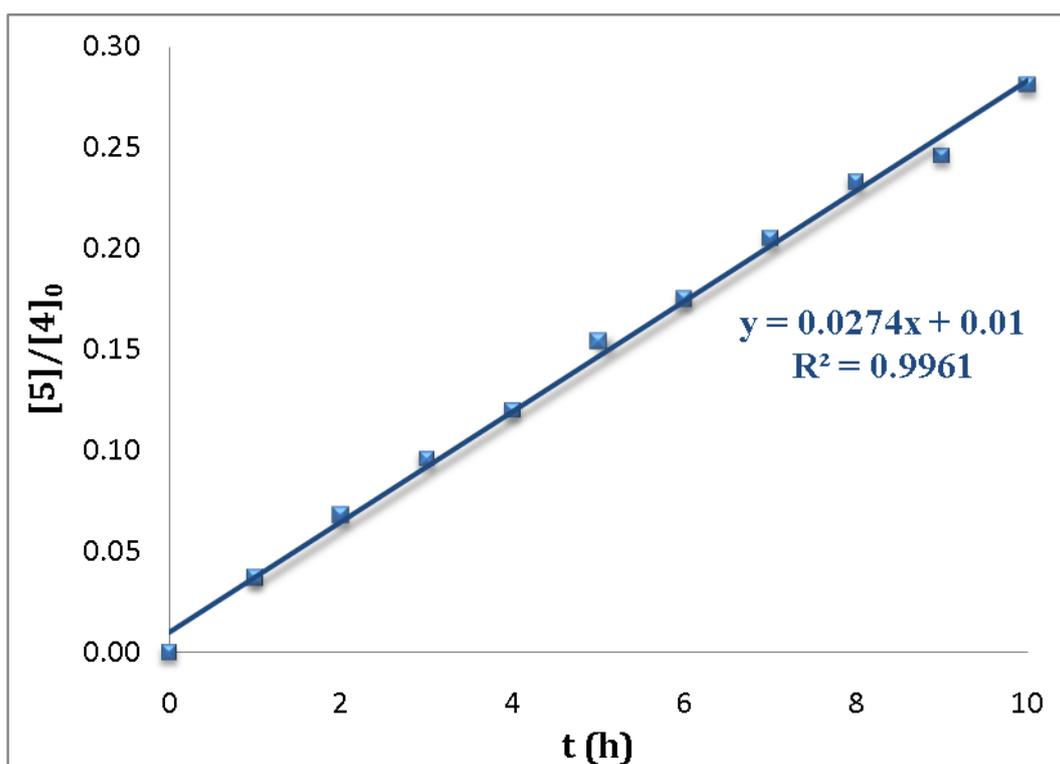
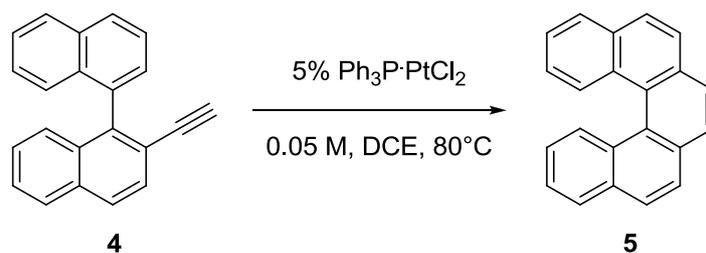
HRMS calcd. for $\text{C}_{13}\text{H}_6\text{ClF}_3\text{S}$: 285.983083; found 285.983251.

IR (neat) $\bar{\nu}$ = 653, 685, 726, 733, 795, 832, 863, 903, 982, 1006, 1069, 1079, 1120, 1166, 1260, 1316, 1328, 1404, 1438, 1466, 1487, 1565, 1611, 2854, 2927 cm^{-1} .

Kinetic Experiments:

All kinetic experiments were performed monitoring the conversion of **4** into helicene **5** by GC-MS (Agilent 19091S-433 column (30 m × 0.25 mm); T = 70 → 280 °C. T_{detector} = 250 °C T_{inlet} = 250 °C).

Figure S1. Plot of $[5]_t/[4]_0$ versus time (h) at 5 mol% catalyst loading.



The order in compound **4** was determined by monitoring $[5]_t/[4]_0$ vs. time at 5 mol% catalyst loading. The plot is linear providing a $k_{\text{obs}} = 0,0274 \text{ h}^{-1}$, $R^2 = 0.9961$.

Figure S2. Plot of $[5]_t/[4]_0$ versus time (h) at 2 to 5 mol% catalyst loading.

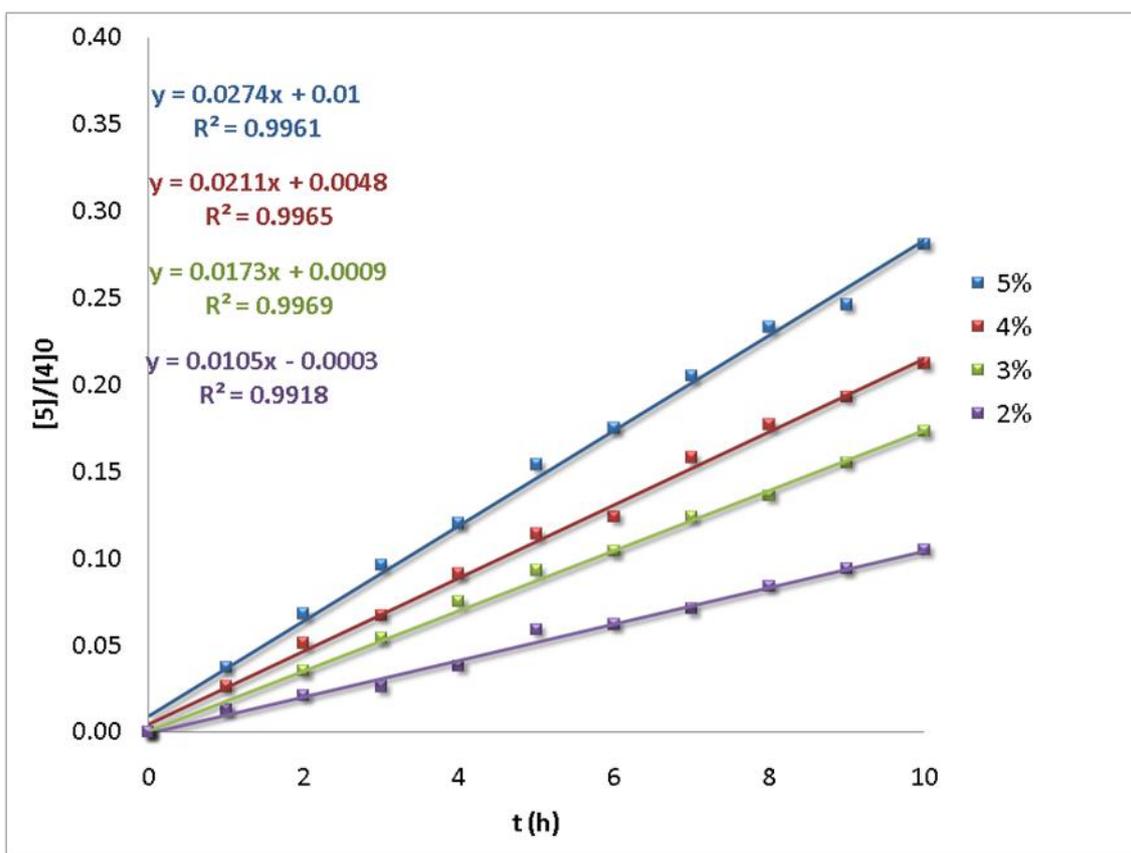
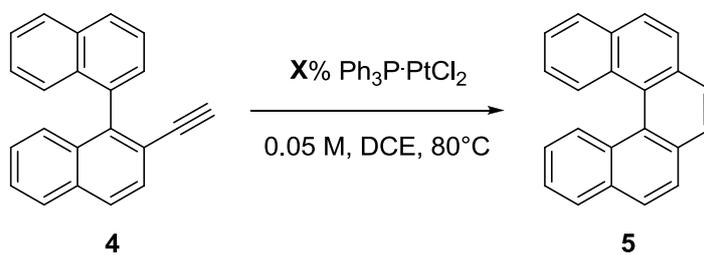
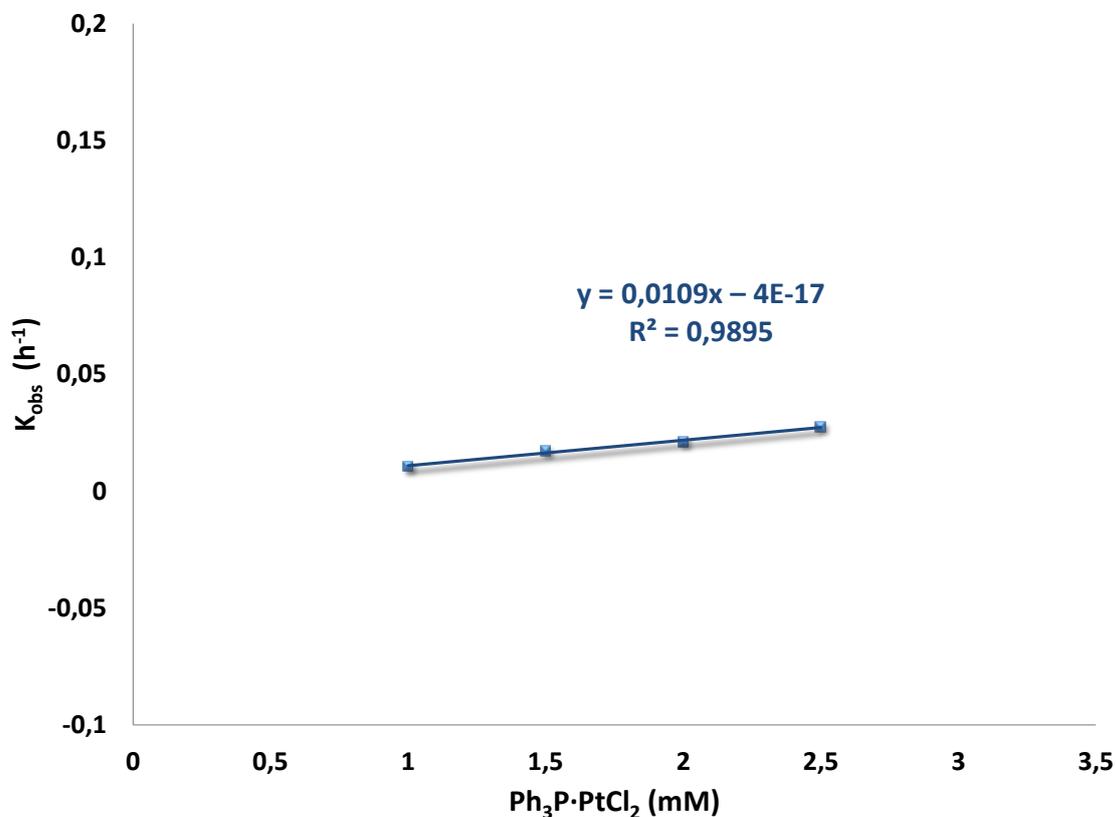


Figure S3. Plot of k_{obs} versus $[\text{Ph}_3\text{P}\cdot\text{PtCl}_2]$ at different catalysts loadings (1-2.5 mM).

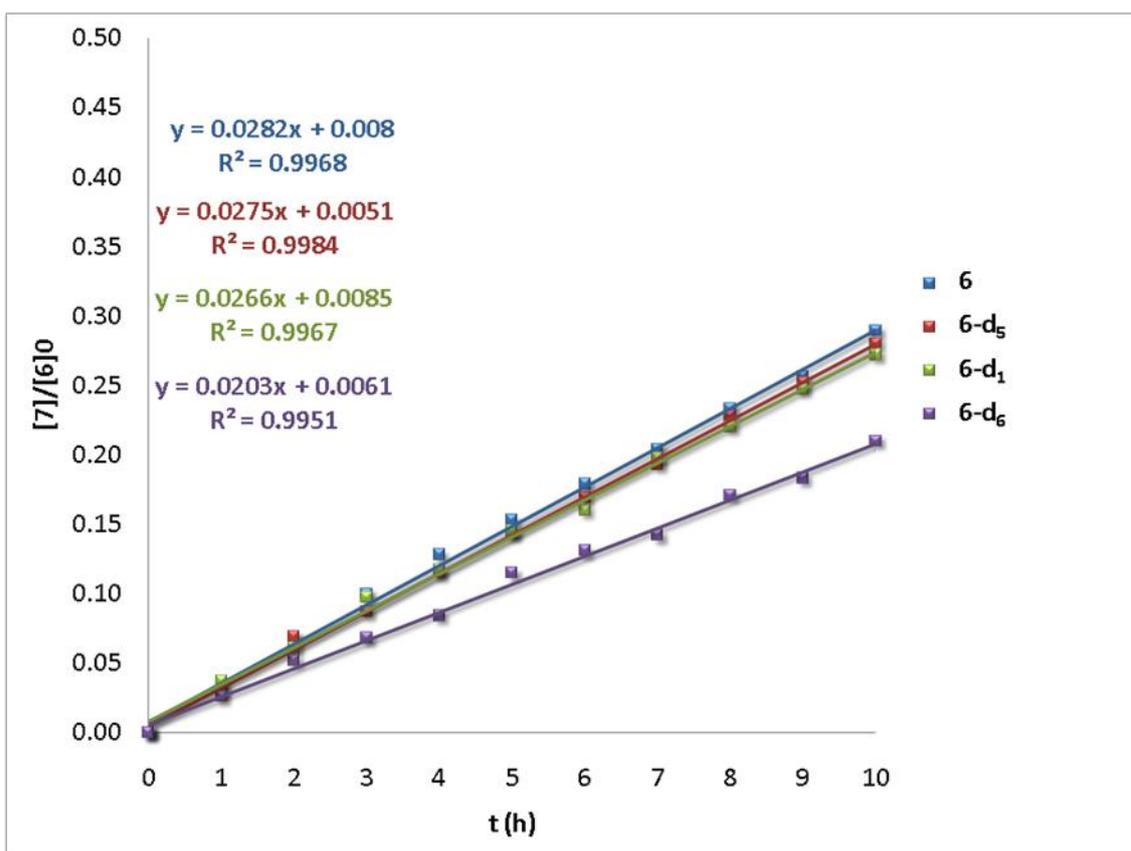
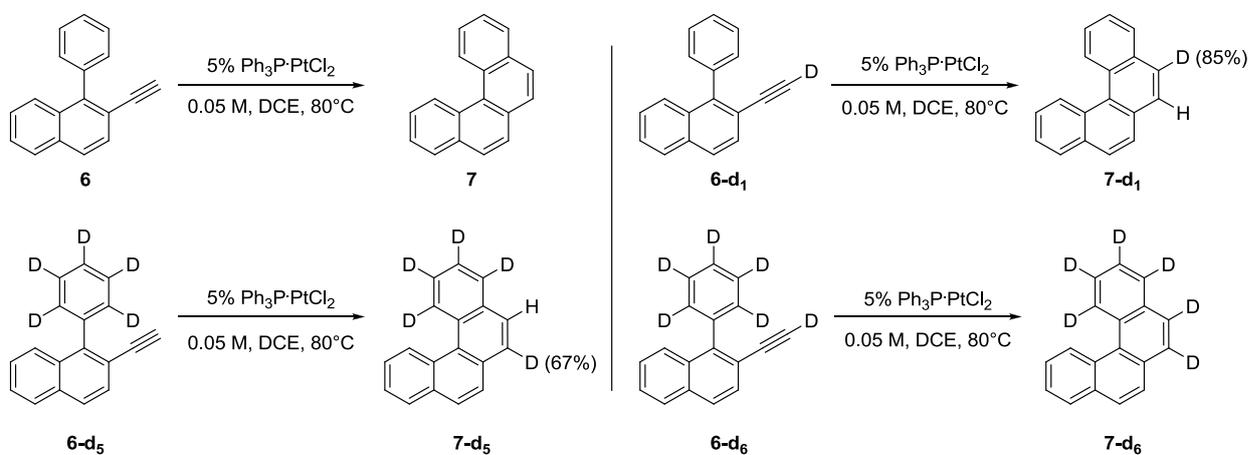


Order in Pt. Each rate constant (k_{obs}) is obtained from the slope of the $[\mathbf{5}]_t/[\mathbf{4}]_0$ versus time plot at 2, 4, 5 and 5 mol% catalyst loading. The results are tabulated in Table 1. A plot of average k_{obs} versus $[\text{Ph}_3\text{P}\cdot\text{PtCl}_2]$ provided a straight line with slope = 0.01, $R^2 = 0.9895$, suggesting a 1st order dependence on $\text{Ph}_3\text{P}\cdot\text{PtCl}_2$.

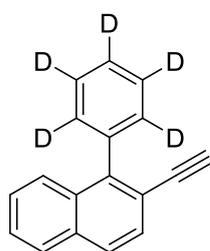
Table S1.

$[\text{Ph}_3\text{P}\cdot\text{PtCl}_2]$	k_{obs}
2,5	0,0274
2	0,0211
1,5	0,0173
1	0,0105

Figure S4. Deuterium labeling experiments



Compound 6-d₅



Pale brown solid

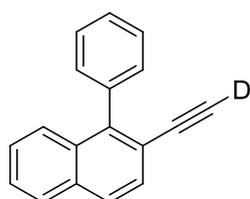
¹H NMR (400 MHz, CDCl₃) δ = 3.09 (s, 1H), 7.48 (t, *J* = 7.6 Hz, 1H), 7.56 (t, *J* = 7.4 Hz, 1H), 7.71 (d, *J* = 8.5 Hz, 1H), 7.75 (d, *J* = 8.5 Hz, 1H), 7.88 (d, *J* = 8.5 Hz, 1H), 7.92 (t, *J* = 7.3 Hz, 1H) ppm.

¹³C NMR (101 MHz, CDCl₃) δ = 80.9, 83.6, 119.0, 126.7, 126.7, 126.9, 127.0 (t, *J* = 24.5 Hz), 127.6, 127.7 (t, *J* = 24.2 Hz), 128.1, 129.1, 130.1 (t, *J* = 24.4 Hz), 132.2, 133.4, 138.5, 143.7 ppm.

HRMS calcd. for C₁₈H₇D₅: 233.125288; found 233.125166.

IR (neat) $\bar{\nu}$ = 666, 679, 700, 744, 791, 818, 841, 865, 914, 971, 1026, 1144, 1213, 1262, 1315, 1327, 1347, 1372, 1426, 1503, 1557, 1592, 1618, 3061, 3286 cm⁻¹.

Compound 6-d₁



Pale brown solid.

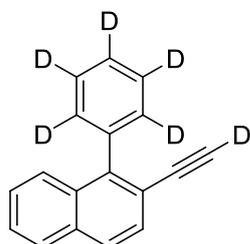
¹H NMR (400 MHz, CDCl₃) δ = 7.42 (ddd, *J* = 8.3, 6.8, 1.3 Hz, 1H), 7.45 - 7.50 (m, 2H), 7.50 - 7.58 (m, 4H), 7.62 (d, *J* = 8.6 Hz, 1H), 7.67 (d, *J* = 8.5 Hz, 1H), 7.83 (d, *J* = 8.5 Hz, 1H), 7.89 (d, *J* = 8.1 Hz, 1H) ppm.

¹³C NMR (101 MHz, CDCl₃) δ = 80.6 (t, *J* = 38.7 Hz), 83.2 (t, *J* = 7.2 Hz), 119.0, 126.7, 126.7, 126.9, 127.6, 127.8, 128.1, 128.2, 129.2, 130.5, 132.3, 133.4, 138.7, 143.8 ppm.

HRMS calcd. for C₁₈H₁₁D₁: 229.100176; found 229.100252.

IR (neat) $\bar{\nu}$ = 670, 681, 696, 707, 747, 760, 823, 871, 901, 978, 1024, 1073, 1150, 1179, 1193, 1270, 1332, 1380, 1442, 1491, 1503, 1558, 1590, 1969, 2572, 2923, 3054 cm⁻¹.

Compound 6-d₆



White solid.

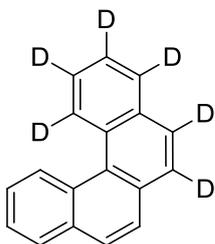
¹H NMR (400 MHz, CDCl₃) δ = 7.43 (ddd, *J* = 8.3, 6.8, 1.3 Hz, 1H), 7.52 (ddd, *J* = 8.1, 6.8, 1.2 Hz, 1H), 7.64 (d, *J* = 8.8 Hz, 1H), 7.68 (d, *J* = 8.5 Hz, 1H), 7.84 (d, *J* = 8.5 Hz, 1H), 7.89 (d, *J* = 8.1 Hz, 1H) ppm.

¹³C NMR (101 MHz, CDCl₃) δ = 80.6 (t, *J* = 38.1 Hz), 83.2 (t, *J* = 7.3 Hz), 119.0, 126.7, 126.7, 126.9, 127.2 (t, *J* = 24.6 Hz), 127.6, 127.7 (t, *J* = 24.5 Hz), 128.1, 129.2, 130.1 (t, *J* = 24.5 Hz), 132.3, 133.4, 138.5, 143.8 ppm.

HRMS calcd. for C₁₈H₆D₆: 234.131560; found 234.131683.

IR (neat) $\bar{\nu}$ = 681, 700, 748, 791, 804, 823, 841, 867, 954, 968, 981, 1024, 1150, 1189, 1202, 1314, 1326, 1347, 1500, 1556, 1589, 1969, 1572, 2922, 3055 cm⁻¹.

Compound 7-d₆



Pale yellow oil.

¹H NMR (400 MHz, CDCl₃) δ = 7.62 - 7.67 (m, 1H), 7.70 (ddd, *J* = 8.5, 6.9, 1.5 Hz, 1H), 7.84 (d, *J* = 8.6 Hz, 1H), 7.92 (d, *J* = 8.5 Hz, 1H), 8.04 (dd, *J* = 7.9, 1.4 Hz, 1H), 9.16 (d, *J* = 8.4 Hz, 1H) ppm.

¹³C NMR (101 MHz, CDCl₃) δ = 125.5 (t, *J* = 24.6 Hz), 125.5 (t, *J* = 24.6 Hz), 126.0, 126.3, 126.9, 127.4 (t, *J* = 25.4 Hz), 127.6, 127.7 (t, *J* = 24.7 Hz), 128.0, 128.7, 130.4 (t, *J* = 25.2 Hz), 130.5, 131.1, 133.6 (t, *J* = 21.2 Hz), 133.6 ppm.

MS calcd. for C₁₈H₆D₆: 234.32; found 234.33.

IR (neat) $\bar{\nu}$ = 663, 695, 728, 743, 754, 788, 815, 832, 853, 869, 882, 904, 960, 1035, 1050, 1108, 1196, 1211, 1259, 1332, 1431, 1453, 1507, 1601, 2258, 3047 cm⁻¹.

Computational methods and results

Geometries were optimized at the DFT level using the B3LYP hybrid functional.^{2,3} Platinum was described by the combination of LANL2DZ effective core potential (ECP) and the associated double- ζ basis set⁴ while the 6-31G* basis set was employed for all other atoms (B3LYP-I level). The optimized stationary points were characterized as local minima or transition structures by harmonic force constant analysis, and intrinsic reaction coordinate (IRC) calculations were performed to verify the transition state structures.⁵ For single-point calculations, the 6-31G* basis was replaced by the larger 6-31+G** basis for C, H, Li, O, P, and Cl, whereas LANL2DZ was replaced by LANL2TZ(f)⁶ for Pt (B3LYP-II level). Solvent single-point energy calculations employed the polarized continuum model (PCM).⁷ Dichloromethane was used as a solvent. Empirical dispersion corrections for the B3LYP functional were also included.⁸ The Gibbs free energies were in all cases computed by adding to the single-point energies both zero-point vibrational energies and thermal corrections (298K) obtained at the level of theory employed in the geometry optimization. Molecular orbital (MO) analyses were done at the B3LYP-II level. All calculations were performed using the Gaussian09 suite of quantum chemical program.⁹

The optimized geometries are depicted in Figure S4 for ligand **1** (trication PR_3^{3+}). Representative structural parameters are listed in Tables S2-S10 for all stationary points and for all ligands studied (PPh_3 , PR_3^{3+} , PPh_2R^+ , PPhR_2^{2+}). Selected natural charges are given in Tables S11-S13. All optimized Cartesian coordinates and the associated energies are documented in Table S15.

To determine the distance $d(\text{CO})$ and vibrational wavenumber $\nu(\text{CO})$ in $\text{Ni}(\text{CO})\text{L}$ complexes, structures were optimized at the mPW1PW91 level¹⁰ using the 6-311+G(2d) basis set for Ni and 6-311+G(d,p) for the C, H, O, N and P atoms. The DFT functional and basis set for these Ni

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⁷ (a) Cossi, M.; Barone, V.; Cammi, R.; Tomasi, J. *Chem. Phys. Lett.* **1996**, *255*, 327. (b) Cancès, E.; Mennucci, B.; Tomasi, J. *Chem. Phys.* **1997**, *107*, 3032 (c) Cossi, M.; Scalmani, G.; Rega, N.; Barone, V. *J. Chem. Phys.* **2002**, *117*, 43.

⁸ Grimme S. *J. Comput. Chem.* **2006**, *27*, 1787.

⁹ Gaussian 09, Revision **B.01**, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2009.

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complexes were chosen on the basis of a recent paper with a similar type of analysis.¹¹ The results are summarized in Table S14.

Concerning the interpretation of the computed free energy profiles (Scheme 4 of the main paper), we note that **TS1** is the highest-energy transition state for both ligands and would thus be rate-determining if the reactions were carried out in the gas phase. In a solvent environment, the reaction energy of each individual step is dissipated quickly, however, and other steps may therefore become rate-determining. The simplest interpretation for reactions in solution would focus on the individual step with the highest free energy barrier, which involves **TS1_a** in the case of the triphenyl phosphine ligand (16.2 kcal/mol, see Scheme 4) and **TS4_b** in the case of the tricationic phosphorus ligand **1** (14.5 kcal/mol, see Scheme 4). This is still qualitatively consistent with the kinetic data, but the difference between the two ligands is rather small from this point of view. A more detailed analysis will consider the kinetics of the whole catalytic cycle in solution and the corresponding turnover number, which determines the overall speed. This can be done using the energetic span model.¹² The energetic span δE of the catalytic cycle is defined as the difference of the free energies of the transition state (TDTS) and the intermediate (TDI) that maximize δE , plus the reaction free energy if TDTS appears before TDI.¹² An evaluation of δE from the data given in Scheme 4 of the main paper yields 14.8 kcal/mol in the case of the triphenyl phosphine ligand and 6.8 kcal/mol in the case of the tricationic phosphorus ligand **1**. Since δE serves as apparent activation energy of the whole cycle,¹² the reaction is predicted to be much faster when using ligand **1** (as observed experimentally). The difference in the computed δE values for the two ligands arises mainly from the different stability of the highest-energy transition states **TS1_a** and **TS1_b**, which are thus rate-determining in the framework of the energetic span model.

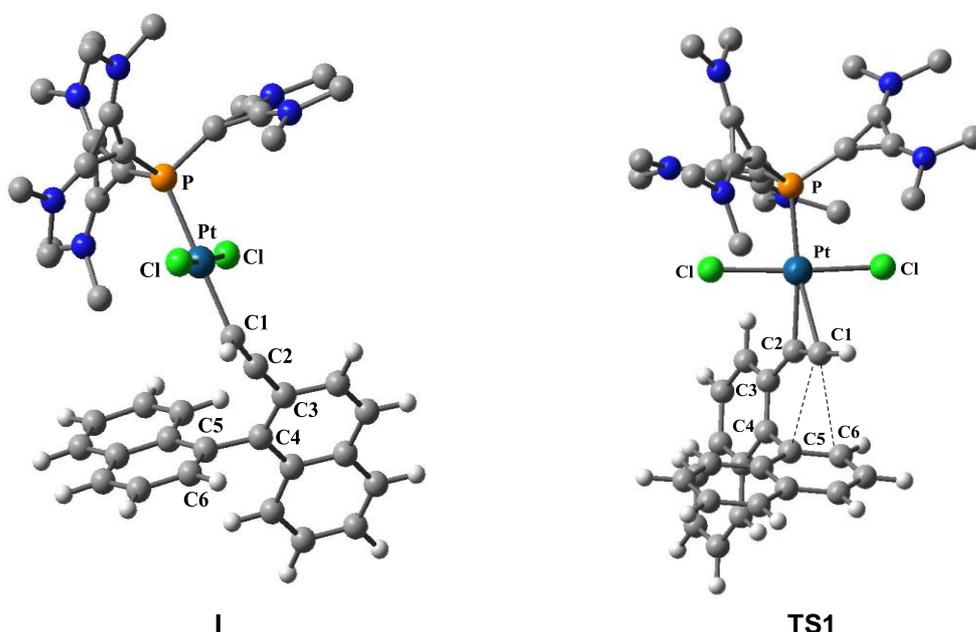
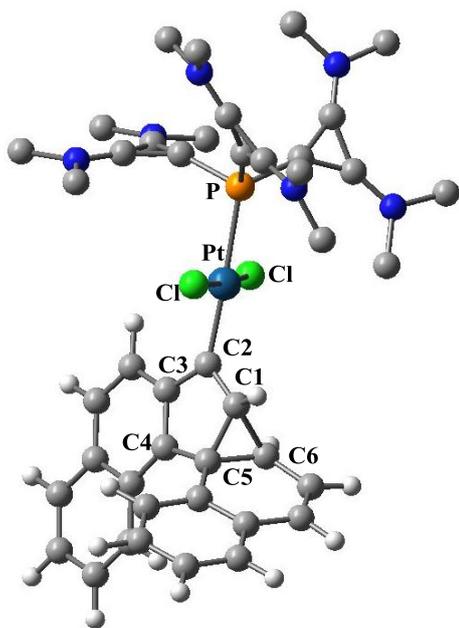


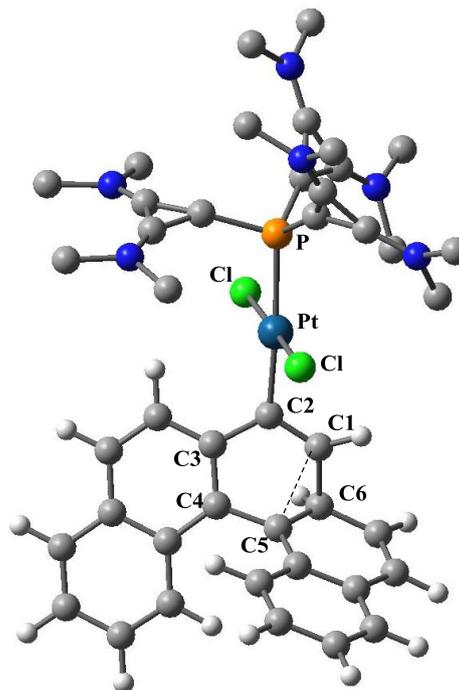
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¹¹ Gusev, D. G. *Organometallics*, **2009**, *28*, 763.

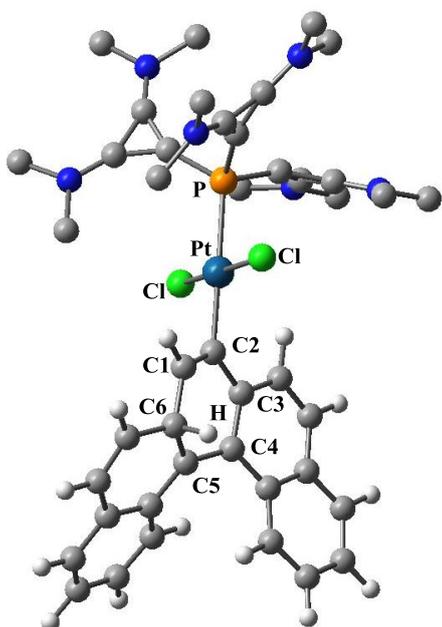
¹² Kozuch, S.; Shaik, S. *Acc. Chem. Res.* **2011**, *44*, 101-110.



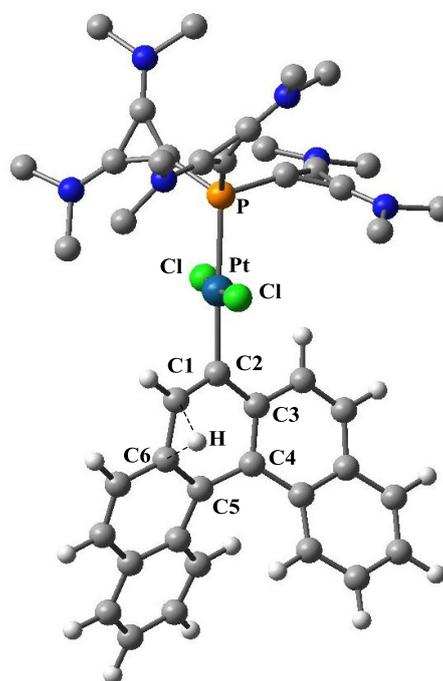
II



TS2



III



TS3

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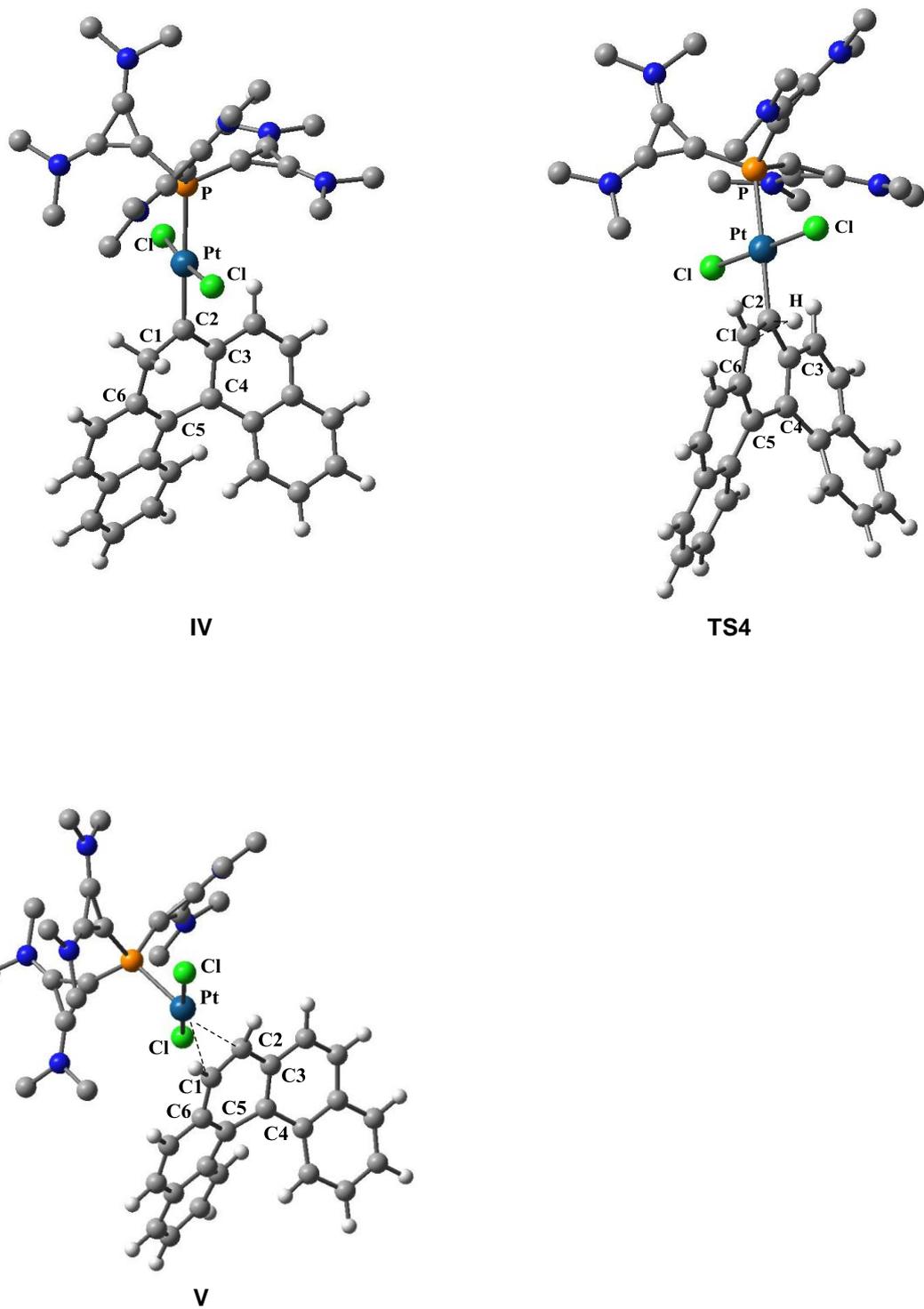
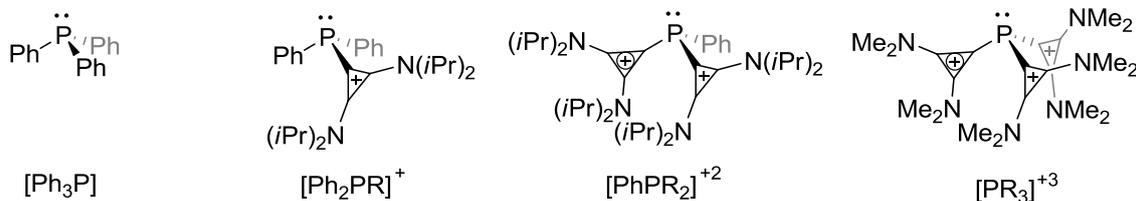


Figure S5. The B3LYP optimized reactant complex, transition states and intermediates. For sake of brevity, hydrogen atoms on the ligand are not shown.

Table S2. Representative structural parameters of reactant complex (**I**) computed at the B3LYP-I level; distances in Å.



Ligand (L)	Pt–C1	Pt–C2	C1–C2	C1–C5	C1–C6	C5–C6
PPh_3	2.24	2.51	1.24	3.67	3.88	1.38
PR_3^{3+}	2.07	3.02	1.28	3.73	3.74	1.39
PPh_2R^+	2.15	2.70	1.25	3.72	3.97	1.38
$PPhR_2^{2+}$	2.08	2.99	1.27	3.72	3.76	1.39

Table S3. Representative structural parameters of transition states **TS1** computed at the B3LYP-I level; distances in Å.

Ligand	Pt–C1	Pt–C2	C1–C2	C1–C5	C1–C6	C5–C6
PPh_3	2.84	2.07	1.30	2.07	2.30	1.41
PR_3^{3+}	2.46	2.18	1.26	2.81	2.86	1.40
PPh_2R^+	2.78	2.10	1.28	2.29	2.43	1.40
$PPhR_2^{2+}$	2.60	2.13	1.26	2.60	2.61	1.40

Table S4. Representative structural parameters of cyclopropane intermediate **II** computed at the B3LYP-I level; distances in Å.

Ligand	Pt–C1	Pt–C2	C1–C2	C1–C5	C1–C6	C5–C6
PPh_3	3.02	1.96	1.45	1.53	1.57	1.53
PR_3^{3+}	3.02	2.00	1.43	1.54	1.64	1.51
PPh_2R^+	3.04	1.97	1.45	1.53	1.59	1.52
$PPhR_2^{2+}$	3.00	1.99	1.44	1.54	1.62	1.52

Table S5. Representative structural parameters of transition state **TS2** computed at the B3LYP-I level; distances in Å.

Ligand	Pt–C1	Pt–C2	C1–C2	C1–C5	C1–C6	C5–C6
PPh ₃	2.92	2.05	1.33	2.36	1.64	1.46
PR ₃ ³⁺	2.94	2.03	1.36	2.08	1.61	1.46
PPh ₂ R ⁺	2.95	2.03	1.34	2.31	1.61	1.46
PPhR ₂ ²⁺	2.92	2.03	1.35	2.22	1.61	1.46

Table S6. Representative structural parameters of intermediate **III** computed at the B3LYP-I level; distances in Å.

Ligand	Pt–C2	C1–C2	C1–C6	C5–C6	C1–H	C6–H
PPh ₃	2.04	1.36	1.51	1.49	1.12	1.97
PR ₃ ³⁺	2.05	1.35	1.52	1.50	1.12	2.06
PPh ₂ R ⁺	2.04	1.35	1.51	1.49	1.12	2.00
PPhR ₂ ²⁺	2.05	1.35	1.51	1.49	1.12	2.04

Table S7. Representative structural parameters of transition state **TS3** computed at the B3LYP-I level; distances in Å.

Ligand	Pt–C2	C1–C2	C1–C6	C5–C6	C1–H	C6–H
PPh ₃	2.03	1.38	1.50	1.45	1.45	1.20
PR ₃ ³⁺	2.04	1.39	1.49	1.44	1.37	1.25
PPh ₂ R ⁺	2.03	1.38	1.50	1.44	1.41	1.22
PPhR ₂ ²⁺	2.04	1.39	1.49	1.44	1.39	1.24

Table S8. Representative structural parameters of intermediate **IV** computed at the B3LYP-I level; distances in Å.

Ligand	Pt–C2	C1–C2	C1–C6	C5–C6	C1–H	C6–H
PPh ₃	1.98	1.49	1.50	1.40	1.11	2.17
PR ₃ ³⁺	2.01	1.49	1.50	1.40	1.11	2.15
PPh ₂ R ⁺	1.99	1.49	1.50	1.40	1.11	2.16
PPhR ₂ ²⁺	2.00	1.49	1.50	1.40	1.11	2.15

Table S9. Representative structural parameters of transition state **TS4** computed at the B3LYP-I level; distances in Å.

Ligand	Pt–C2	C1–C2	C1–C6	C5–C6	C1–H	C2–H
PPh ₃	2.07	1.41	1.44	1.41	1.41	1.27
PR ₃ ³⁺	2.05	1.43	1.43	1.42	1.35	1.30
PPh ₂ R ⁺	2.06	1.42	1.43	1.41	1.38	1.27
PPhR ₂ ²⁺	2.06	1.43	1.43	1.42	1.37	1.28

Table S10. Representative structural parameters of product complex **V** computed at the B3LYP-I level; distances in Å.

Ligand	Pt–C1	Pt–C2	C1–C2	C1–C6	C5–C6	C2–H
PPh ₃	2.55	2.50	1.29	1.43	1.42	1.08
PR ₃ ³⁺	2.62	2.29	1.42	1.41	1.43	1.08
PPh ₂ R ⁺	2.43	2.52	1.40	1.43	1.42	1.08
PPhR ₂ ²⁺	2.57	2.36	1.41	1.42	1.43	1.08

Table S11 Natural charge of selected atoms of reactant complex (**I**) computed at the B3LYP-II level.

Ligand (L)	Pt	C1	C2	C5	C6	Ligand
PPh ₃	0.02	-0.26	0.10	-0.06	-0.19	0.56
PR ₃ ³⁺	-0.02	-0.45	0.26	-0.07	-0.19	3.23
PPh ₂ R ⁺	0.03	-0.36	0.18	-0.06	-0.20	1.41
PPhR ₂ ²⁺	-0.02	-0.44	0.26	-0.06	-0.19	2.32

Table S12. Natural charge of selected atoms of transition structure **TS1** computed at the B3LYP-II level.

Ligand	Pt	C1	C2	C5	C6	Ligand
PPh ₃	0.00	-0.07	-0.16	-0.04	-0.14	0.45
PR ₃ ³⁺	0.02	-0.06	-0.08	-0.04	-0.21	3.27
PPh ₂ R ⁺	0.02	-0.02	-0.16	-0.02	-0.17	1.38
PPhR ₂ ²⁺	0.03	-0.01	-0.14	-0.03	-0.21	2.33

Table S13. Natural charge of selected atoms of cyclopropane intermediate **II** computed at the B3LYP-II level.

Ligand	Pt	C1	C2	C5	C6	Ligand
PPh ₃	0.04	-0.26	0.08	-0.06	-0.18	0.39
PR ₃ ³⁺	0.01	-0.26	0.02	-0.05	-0.15	3.16
PPh ₂ R ⁺	0.04	-0.26	0.07	-0.06	-0.17	1.30
PPhR ₂ ²⁺	0.02	-0.29	0.05	-0.06	-0.16	2.24

Table S14. Distance $d(\text{CO})$ and wavenumber $\nu(\text{CO})$ (A_1) of Ni(CO)₃L from mPW1PW91^a.

Ligand (L)	$d(\text{CO})$	$\nu(\text{CO})$	$\nu(\text{CO})^b$
PPh ₃	1.14	2167	2067
PR ₃ ³⁺	1.13	2213	2111
PPh ₂ R ⁺	1.14	2187	2086
PPhR ₂ ²⁺	1.14	2203	2101

^a Basis set: 6-311+G(d,p) for C, H, O, P, Cl and N; 6-311+G(2d) for Ni. ^b Scaled frequency (scaling factor = 0.954105).

Table S15. Optimized geometries (B3LYP-I, Cartesian coordinates in Å) and single-point energies of reactants, intermediates and transition states (B3LYP-II, in a.u.). Notation: E = total electronic energy Tc = thermal correction at 298K to obtain the Gibbs free energy, Nimag = number of imaginary frequencies). Subscripts (a,b,c,d) refer to the four ligands studied computationally (PPh₃, PR₃³⁺, PPh₂R⁺, PPhR₂²⁺).

PPh ₃ (a)				4			
E = -2076.105029 Nimag = 0				E = -846.8195015 Nimag = 0			
Tc = 0.223695				Tc = 0.239452			
15	-0.394403	0.134947	-0.000297	6	-0.759624	3.858960	-0.359952
78	1.690632	-0.612843	0.042237	1	-1.479933	4.643417	-0.406039
17	2.676468	1.520989	0.130357	6	0.037896	2.950713	-0.300789
17	1.392723	-2.924894	-0.048159	6	1.023000	1.914712	-0.256436
6	-1.618358	-1.145662	-0.455574	6	0.712781	0.632416	0.202652
6	-1.830299	-2.231830	0.410814	6	2.345746	2.219031	-0.701497
6	-2.347518	-1.059237	-1.650070	6	1.731730	-0.374241	0.222550
6	-2.771327	-3.205905	0.089824	6	-0.668522	0.320498	0.689784
1	-1.248459	-2.323116	1.321864	6	3.327808	1.263606	-0.687699
6	-3.284525	-2.044586	-1.968791	1	2.553311	3.225193	-1.051504
1	-2.187967	-0.230570	-2.331035	6	3.055139	-0.053144	-0.229145
6	-3.498828	-3.114851	-1.100855	6	-1.004506	0.594159	2.002786
1	-2.926684	-4.044153	0.762654	6	-1.647323	-0.259442	-0.183029
1	-3.844001	-1.971764	-2.897061	1	4.331744	1.503988	-1.029076
1	-4.226765	-3.881376	-1.352062	6	-2.296408	0.313732	2.506308
6	-0.595300	1.484500	-1.219692	1	-0.259436	1.035523	2.658920
6	-1.528200	2.508877	-0.999852	6	-2.955922	-0.544738	0.332442
6	0.151114	1.464597	-2.407718	6	-3.251141	-0.244634	1.689091
6	-1.714220	3.499417	-1.964967	1	-2.526537	0.542936	3.543246

1	-2.101130	2.540817	-0.078700	1	-4.246077	-0.464288	2.069373
6	-0.044577	2.454768	-3.369544	6	4.059919	-1.056076	-0.205661
1	0.893229	0.688057	-2.564811	6	3.780833	-2.327399	0.243098
6	-0.975492	3.472693	-3.149183	1	4.558747	-3.085951	0.255683
1	-2.432285	4.294828	-1.786356	1	5.058840	-0.799159	-0.550402
1	0.540506	2.437113	-4.284398	6	2.477175	-2.648274	0.691322
1	-1.119284	4.248303	-3.896381	1	2.262559	-3.652743	1.045925
6	-0.928724	0.782344	1.629727	6	1.480202	-1.698062	0.682803
6	-0.016484	1.466709	2.449984	1	0.484682	-1.951474	1.030761
6	-2.265950	0.646801	2.042986	6	-1.375227	-0.563729	-1.545712
6	-0.441702	2.006613	3.663652	1	-0.390297	-0.345680	-1.945900
1	1.016611	1.576128	2.137697	6	-2.339913	-1.122881	-2.354179
6	-2.681253	1.192903	3.257988	6	-3.629400	-1.406774	-1.843185
1	-2.980545	0.114465	1.424605	1	-4.381876	-1.848100	-2.491226
6	-1.770584	1.870859	4.070375	1	-2.111753	-1.347190	-3.392724
1	0.271956	2.530352	4.293041	6	-3.927232	-1.122052	-0.530057
1	-3.716092	1.081953	3.569606	1	-4.916057	-1.334771	-0.130008
1	-2.095246	2.288853	5.019329				

I_a E = -2922.9506534 Nimag = 0 Tc = -2922.6736082				TS-I_a E = -2922.9251088 Nimag = 1 (-316.92 cm-1) Tc = 0.485864			
15	-2.940262	-0.024590	0.145015	15	-2.968338	-0.005626	0.083188
78	-0.809188	-0.509625	-0.651404	78	-0.606558	0.047876	-0.183375
17	-0.300267	-1.592694	1.418358	17	-0.872420	0.251182	-2.561336
17	-1.180533	0.513943	-2.769292	17	-0.147296	-0.153230	2.149808
6	1.041780	-1.407054	-1.527924	6	1.940044	1.122355	-0.840846
1	0.898555	-2.347532	-2.019756	1	1.763645	2.146031	-1.113284
6	1.648834	-0.395626	-1.163807	6	1.447270	-0.020171	-0.464009
6	2.359902	0.780849	-0.778405	6	2.367060	-1.130941	-0.223656
6	3.515111	0.687704	0.006770	6	3.710936	-0.770911	-0.330568
6	1.885801	2.045540	-1.249084	6	1.998841	-2.460648	0.091472
6	4.211614	1.890446	0.354802	6	4.742630	-1.734873	-0.159338
6	4.017472	-0.642004	0.474858	6	3.953657	0.664347	-0.681915
6	2.553238	3.194786	-0.920740	6	2.977102	-3.408687	0.275097
1	0.991062	2.063851	-1.862751	1	0.947524	-2.702742	0.197397
6	3.722946	3.156037	-0.113262	6	4.356504	-3.083615	0.154737
6	3.400310	-1.264314	1.543998	6	3.903346	1.028186	-2.044756
6	5.129837	-1.276958	-0.173086	6	4.469223	1.620851	0.282400
1	2.192936	4.156210	-1.277966	1	2.705701	-4.431759	0.523172
6	3.854057	-2.515391	2.023956	6	4.282686	2.321023	-2.477876
1	2.539670	-0.796999	2.011271	1	3.588736	0.282762	-2.768096
6	5.587733	-2.543556	0.322955	6	4.838807	2.925713	-0.172921
6	4.926973	-3.138094	1.431182	6	4.729565	3.242254	-1.560532
1	3.341088	-2.978364	2.861861	1	4.220247	2.571575	-3.532023
1	5.281281	-4.099083	1.796905	1	5.023250	4.237440	-1.886163
6	4.417498	4.341434	0.243093	6	5.370664	-4.060861	0.339746
6	5.544915	4.291035	1.032270	6	6.702693	-3.734785	0.218100
1	6.066742	5.206489	1.297604	1	7.466306	-4.494215	0.361567
1	4.039357	5.294215	-0.119543	1	5.072611	-5.078757	0.579360
6	6.025467	3.045949	1.503239	6	7.082907	-2.407088	-0.095970
1	6.911885	3.013527	2.130610	1	8.136226	-2.158239	-0.192602
6	5.376758	1.876899	1.173456	6	6.128598	-1.431659	-0.278862
1	5.747672	0.926699	1.540979	1	6.429315	-0.416110	-0.518241
6	5.794637	-0.712120	-1.297197	6	4.597176	1.311630	1.654919
1	5.452360	0.239940	-1.690052	1	4.308714	0.326189	2.004206
6	6.857572	-1.355718	-1.891952	6	5.070081	2.258043	2.544592
6	7.313893	-2.599974	-1.394793	6	5.435806	3.546676	2.099020
1	8.154025	-3.097305	-1.871964	1	5.805030	4.279623	2.810488

1	7.349014	-0.906417	-2.750764	1	5.157666	2.008051	3.597878
6	6.689565	-3.177683	-0.312850	6	5.321598	3.873677	0.763686
1	7.029056	-4.136439	0.072513	1	5.598159	4.864288	0.411550
6	-3.907420	1.211819	-0.811147	6	-3.606076	-0.538343	1.726856
6	-4.363082	0.879496	-2.098271	6	-3.333557	0.257699	2.852552
6	-4.187776	2.483400	-0.292303	6	-4.330853	-1.726759	1.892572
6	-5.100766	1.798628	-2.840786	6	-3.798038	-0.119563	4.110994
1	-4.135171	-0.092821	-2.521205	1	-2.751336	1.166412	2.745652
6	-4.920016	3.404479	-1.045085	6	-4.785249	-2.106446	3.157985
1	-3.841259	2.758447	0.697818	1	-4.545620	-2.358376	1.037375
6	-5.379586	3.063705	-2.316883	6	-4.523932	-1.303055	4.267533
1	-5.447564	1.529861	-3.834579	1	-3.580730	0.506149	4.972315
1	-5.132263	4.386490	-0.631167	1	-5.346855	-3.030040	3.271026
1	-5.950641	3.780827	-2.900541	1	-4.879853	-1.598222	5.251201
6	-2.888610	0.649825	1.852817	6	-3.787459	-1.149047	-1.103845
6	-3.908842	0.388370	2.777671	6	-5.102623	-0.942957	-1.545268
6	-1.823957	1.487535	2.218895	6	-3.087767	-2.283099	-1.541677
6	-3.866102	0.962663	4.049327	6	-5.708767	-1.860570	-2.404534
1	-4.731067	-0.268678	2.513275	1	-5.652705	-0.063442	-1.225257
6	-1.790729	2.066452	3.487109	6	-3.699400	-3.202956	-2.393874
1	-1.016068	1.669522	1.516421	1	-2.058624	-2.429449	-1.228779
6	-2.810411	1.803590	4.404748	6	-5.009782	-2.992845	-2.827666
1	-4.657022	0.747206	4.762590	1	-6.726021	-1.687426	-2.745688
1	-0.960374	2.710855	3.761961	1	-3.145778	-4.075457	-2.729901
1	-2.778114	2.247161	5.396273	1	-5.482429	-3.705054	-3.499019
6	-4.027574	-1.508593	0.193196	6	-3.775027	1.633933	-0.185679
6	-3.466385	-2.786408	0.344852	6	-3.212775	2.531946	-1.107409
6	-5.424700	-1.378905	0.105767	6	-4.950836	1.997719	0.491596
6	-4.290867	-3.910743	0.408719	6	-3.820682	3.765191	-1.346778
1	-2.390681	-2.895637	0.425750	1	-2.309414	2.256231	-1.641487
6	-6.242613	-2.507413	0.172595	6	-5.553009	3.233659	0.248972
1	-5.875081	-0.400342	-0.024434	1	-5.392519	1.321476	1.216081
6	-5.677279	-3.775336	0.322043	6	-4.989031	4.120211	-0.669963
1	-3.843995	-4.894228	0.524534	1	-3.375557	4.450224	-2.063490
1	-7.320990	-2.393805	0.102067	1	-6.461088	3.502612	0.782268
1	-6.315451	-4.653774	0.368027	1	-5.456840	5.083672	-0.855409

Π_a				TS_2a			
E = -2922.9504923 Nimag = 0				E = -2922.929256 Nimag = 1 (-213.24)			
Tc = 0.491325				Tc = 0.488474			
15	3.036291	0.035756	-0.063988	15	-2.984050	0.014154	0.164417
78	0.567265	-0.059649	-0.011444	78	-0.625782	0.045241	-0.330483
17	0.604819	1.003041	2.149298	17	0.049579	0.030623	1.970366
17	0.442875	-1.139827	-2.136988	17	-1.101926	0.059429	-2.682670
6	-2.206301	1.113150	0.265941	6	1.858201	1.225043	-1.320198
1	-1.868528	2.080797	-0.082912	1	1.300030	2.114549	-1.580189
6	-1.392063	-0.078621	0.083087	6	1.378797	0.122437	-0.745729
6	-2.286256	-1.208190	0.023227	6	2.312855	-0.983709	-0.442905
6	-3.626583	-0.790840	0.129276	6	3.696680	-0.721528	-0.431886
6	-1.950386	-2.588992	-0.053689	6	1.865839	-2.291776	-0.145310
6	-4.676913	-1.736840	0.239587	6	4.649680	-1.767066	-0.221971
6	-3.679094	0.703963	0.248482	6	4.055226	0.687450	-0.657459
6	-2.957088	-3.517669	-0.011013	6	2.760386	-3.310575	0.094440
1	-0.910811	-2.873309	-0.166577	1	0.797159	-2.463536	-0.095373
6	-4.323474	-3.130007	0.141803	6	4.159395	-3.090758	0.046208
6	-3.075889	1.167458	1.575624	6	3.423865	1.285343	-1.824679
6	-4.664877	1.590633	-0.424964	6	4.780799	1.493207	0.257151
1	-2.729551	-4.577818	-0.085253	1	2.397275	-4.309335	0.323673
6	-3.491508	2.474811	2.090012	6	3.805597	2.667978	-2.160657

1	-2.812400	0.409116	2.306461	1	3.431759	0.623662	-2.699170
6	-4.926963	2.873662	0.121827	6	5.073182	2.857576	-0.097111
6	-4.326630	3.271057	1.388939	6	4.584695	3.404253	-1.337315
1	-3.123716	2.774894	3.066832	1	3.405247	3.090163	-3.078498
1	-4.614700	4.239548	1.791446	1	4.844697	4.430488	-1.582639
6	-5.356902	-4.097833	0.215610	6	5.087098	-4.148350	0.246498
6	-6.670517	-3.721603	0.399649	6	6.442775	-3.929746	0.164343
1	-7.448241	-4.478149	0.458384	1	7.141198	-4.747968	0.314702
1	-5.093318	-5.149100	0.132527	1	4.699423	-5.142185	0.456365
6	-7.014391	-2.354116	0.522279	6	6.928933	-2.633260	-0.132635
1	-8.051086	-2.071670	0.681443	1	7.999510	-2.466708	-0.216350
6	-6.041191	-1.383345	0.442695	6	6.059259	-1.582919	-0.324281
1	-6.307297	-0.336590	0.537568	1	6.452847	-0.601232	-0.567428
6	-5.291140	1.212333	-1.618576	6	5.206113	1.000929	1.524336
1	-5.087076	0.232995	-2.040644	1	4.940859	-0.010020	1.808656
6	-6.159385	2.083908	-2.275134	6	5.923401	1.803933	2.385017
6	-6.418124	3.350896	-1.742860	6	6.240027	3.128012	2.014541
1	-7.092171	4.032139	-2.254306	1	6.808077	3.754401	2.696802
1	-6.628256	1.775533	-3.205273	1	6.234122	1.423464	3.352901
6	-5.807643	3.736265	-0.554161	6	5.818636	3.645109	0.799603
1	-6.007037	4.718444	-0.132116	1	6.047348	4.673458	0.533979
6	3.891734	-0.964736	-1.354524	6	-3.803794	1.647981	-0.113748
6	3.670126	-0.656269	-2.707741	6	-4.877368	2.093164	0.674168
6	4.734473	-2.037274	-1.031477	6	-3.347861	2.459703	-1.165810
6	4.295611	-1.394273	-3.710875	6	-5.483304	3.324368	0.415038
1	3.002960	0.155417	-2.977320	1	-5.236439	1.483727	1.497027
6	5.351295	-2.781262	-2.040570	6	-3.959902	3.687307	-1.422544
1	4.915366	-2.294133	0.006729	1	-2.522714	2.120392	-1.784259
6	5.136849	-2.459733	-3.380510	6	-5.025946	4.124148	-0.633345
1	4.115151	-1.143218	-4.752558	1	-6.311452	3.656911	1.035723
1	6.002571	-3.609538	-1.773910	1	-3.598360	4.304451	-2.240984
1	5.618761	-3.037586	-4.164868	1	-5.496661	5.083536	-0.832760
6	3.787855	-0.541325	1.515020	6	-3.942784	-1.163558	-0.880872
6	5.003688	-0.036049	1.997546	6	-3.310638	-2.333832	-1.326163
6	3.130791	-1.548672	2.237807	6	-5.288797	-0.947117	-1.210838
6	5.556114	-0.537219	3.177319	6	-4.017267	-3.278884	-2.070762
1	5.517220	0.753521	1.457845	1	-2.259430	-2.488956	-1.104320
6	3.689793	-2.054059	3.411870	6	-5.991176	-1.889934	-1.963005
1	2.173240	-1.922057	1.887301	1	-5.789308	-0.039668	-0.887185
6	4.902689	-1.548594	3.884176	6	-5.358176	-3.058566	-2.391244
1	6.496000	-0.133876	3.544984	1	-3.514610	-4.179509	-2.413044
1	3.169855	-2.832302	3.963907	1	-7.032331	-1.708313	-2.216975
1	5.333618	-1.935965	4.803735	1	-5.905851	-3.790616	-2.979232
6	3.705604	1.736690	-0.327077	6	-3.483947	-0.430326	1.883511
6	2.980097	2.837124	0.158175	6	-4.232503	-1.580876	2.169199
6	4.927421	1.961393	-0.983013	6	-3.076433	0.395822	2.945185
6	3.472597	4.132498	-0.007787	6	-4.574858	-1.894964	3.486882
1	2.039667	2.675330	0.674761	1	-4.554439	-2.234197	1.365459
6	5.413746	3.259523	-1.147925	6	-3.429835	0.085123	4.257178
1	5.496273	1.124393	-1.374833	1	-2.474590	1.275659	2.746517
6	4.687203	4.347801	-0.661393	6	-4.178636	-1.061711	4.532590
1	2.901063	4.974636	0.373287	1	-5.155970	-2.790698	3.690675
1	6.359244	3.417968	-1.660062	1	-3.107478	0.734588	5.066634
1	5.065163	5.358332	-0.793395	1	-4.447579	-1.305069	5.557335

III_a E = -2922.939401 Tc = 0.490187	Nimag = 0	TS3_a E = -2922.9309656 Tc = 0.488353	Nimag = 1 (-862.48)
15	3.117117 -0.034510 0.102607	15	-3.140933 0.040302 0.072779

78	0.718832	-0.163640	-0.142721	78	-0.727746	0.162512	-0.055672
17	0.286315	-0.006729	2.204581	17	-0.420352	-0.204556	2.283786
17	0.951325	-0.382366	-2.525386	17	-0.869716	0.624336	-2.415252
6	-1.789242	-1.452058	-0.954059	6	1.788275	1.503237	-0.698111
1	-1.140468	-2.172543	-1.441733	1	1.146304	2.273481	-1.109555
6	-1.303749	-0.306201	-0.415052	6	1.292229	0.291644	-0.248776
6	-2.255969	0.744208	-0.124949	6	2.241259	-0.756994	-0.011228
6	-3.681597	0.574990	-0.292681	6	3.658856	-0.560792	-0.171182
6	-1.784292	2.012778	0.334595	6	1.766882	-2.059185	0.361618
6	-4.533028	1.761047	-0.315913	6	4.504183	-1.744063	-0.300201
6	-4.166100	-0.762259	-0.368705	6	4.162990	0.783405	-0.214183
6	-2.619198	3.082555	0.483235	6	2.604637	-3.128468	0.447932
1	-0.728508	2.093148	0.560108	1	0.710562	-2.154699	0.578804
6	-3.994241	3.014036	0.098572	6	3.974480	-3.021892	0.050959
6	-3.270300	-1.720521	-1.075036	6	3.256899	1.793041	-0.715743
6	-5.383836	-1.268948	0.235140	6	5.455309	1.241091	0.276711
1	-2.227911	4.030939	0.843333	1	2.224454	-4.100365	0.751893
6	-3.695013	-3.143742	-1.150995	6	3.722409	3.150064	-0.966001
1	-3.365361	-1.367761	-2.136152	1	2.788592	1.359616	-1.736989
6	-5.758658	-2.637056	0.031603	6	5.876924	2.581493	0.005165
6	-4.894158	-3.541524	-0.696427	6	4.993700	3.497523	-0.667946
1	-3.011201	-3.837436	-1.632328	1	3.021412	3.861217	-1.393260
1	-5.212083	-4.575878	-0.798988	1	5.348088	4.506324	-0.862561
6	-4.799824	4.176568	0.056273	6	4.785232	-4.176054	-0.071922
6	-6.087499	4.128954	-0.440394	6	6.058783	-4.096715	-0.597286
1	-6.693997	5.029159	-0.480903	1	6.666144	-4.991464	-0.701124
1	-4.373420	5.117038	0.395908	1	4.369707	-5.135444	0.225617
6	-6.597570	2.910144	-0.928702	6	6.552422	-2.852158	-1.037384
1	-7.592006	2.874870	-1.364817	1	7.531420	-2.791226	-1.504371
6	-5.836160	1.756631	-0.870428	6	5.792680	-1.707175	-0.891728
1	-6.242784	0.833614	-1.268808	1	6.185251	-0.765080	-1.255265
6	-6.159917	-0.506571	1.147241	6	6.274303	0.459498	1.130834
1	-5.847006	0.497036	1.400505	1	5.939562	-0.523800	1.433639
6	-7.298523	-1.023331	1.737443	6	7.482220	0.935094	1.606294
6	-7.711243	-2.335660	1.450814	6	7.933820	2.219808	1.252133
1	-8.612925	-2.736475	1.904998	1	8.890701	2.582823	1.615958
1	-7.866690	-0.412987	2.433007	1	8.079180	0.312632	2.266527
6	-6.938298	-3.130350	0.619592	6	7.130931	3.030963	0.472309
1	-7.219392	-4.163717	0.434547	1	7.441268	4.045025	0.233490
6	3.913598	1.095060	-1.117967	6	-3.885255	-0.930608	-1.305782
6	5.241717	0.924543	-1.536273	6	-5.170975	-0.664671	-1.798943
6	3.176894	2.181929	-1.611231	6	-3.152122	-1.996053	-1.849625
6	5.823903	1.829921	-2.424498	6	-5.715745	-1.456004	-2.811381
1	5.821269	0.080781	-1.174182	1	-5.746394	0.164614	-1.399282
6	3.763795	3.090436	-2.493157	6	-3.702741	-2.791233	-2.855307
1	2.138302	2.299427	-1.317974	1	-2.143255	-2.186481	-1.496435
6	5.087153	2.915912	-2.901980	6	-4.984582	-2.522165	-3.338872
1	6.851977	1.683774	-2.745664	1	-6.710620	-1.235918	-3.189739
1	3.180771	3.925736	-2.871740	1	-3.122919	-3.611087	-3.270623
1	5.540829	3.618840	-3.596012	1	-5.409315	-3.135791	-4.129138
6	3.765212	0.558542	1.724994	6	-3.865318	-0.729501	1.584243
6	4.467414	1.765410	1.852386	6	-4.572548	-1.939126	1.537561
6	3.512785	-0.205739	2.877325	6	-3.674682	-0.100703	2.826785
6	4.918071	2.194255	3.103431	6	-5.086839	-2.504528	2.707066
1	4.668379	2.373649	0.977051	1	-4.728249	-2.442575	0.589520
6	3.974291	0.219721	4.121793	6	-4.198910	-0.662529	3.989671
1	2.947326	-1.128058	2.802014	1	-3.110076	0.823232	2.885706
6	4.676929	1.421571	4.239073	6	-4.905024	-1.866705	3.933888
1	5.461885	3.131913	3.184828	1	-5.633686	-3.442351	2.653340
1	3.772349	-0.383334	5.002928	1	-4.044008	-0.163581	4.942476

1	5.030296	1.754471	5.211664	1	-5.307700	-2.305787	4.843035
6	3.976668	-1.653281	-0.140180	6	-3.969792	1.689315	-0.014123
6	3.453172	-2.559516	-1.077118	6	-3.382834	2.699144	-0.794276
6	5.142786	-1.997779	0.562023	6	-5.175065	1.958772	0.654135
6	4.088631	-3.780716	-1.305804	6	-3.993458	3.949290	-0.902526
1	2.556510	-2.298746	-1.630587	1	-2.457048	2.496751	-1.323299
6	5.772269	-3.222892	0.332066	6	-5.780037	3.212465	0.544920
1	5.555849	-1.314340	1.296574	1	-5.637741	1.193459	1.268589
6	5.246617	-4.117164	-0.601738	6	-5.190406	4.210476	-0.232599
1	3.673371	-4.471699	-2.034844	1	-3.529187	4.721220	-1.510687
1	6.672291	-3.476881	0.886216	1	-6.710985	3.407473	1.071010
1	5.735854	-5.071762	-0.778015	1	-5.660666	5.187076	-0.314254

IV_a E = -2922.9832651 Nimag = 0 Tc = 0.491704				TS4_a E = -2922.9569383 Nimag = 1 (-912.29) Tc = 0.488870			
15	3.149056	-0.056062	0.061669	15	-3.129417	-0.039410	-0.097010
78	0.691127	-0.129827	-0.049599	78	-0.764575	-0.156940	0.209641
17	0.463455	-0.140385	2.330901	17	-0.412916	-0.086671	-2.158346
17	0.811889	-0.135371	-2.451836	17	-0.841342	-0.315760	2.606991
6	-1.814810	-1.478886	-0.863127	6	1.856252	-1.506844	0.856551
1	-1.203886	-2.354816	-0.612056	1	1.185182	-2.297834	1.182419
6	-1.282049	-0.273728	-0.176714	6	1.290879	-0.285870	0.420767
6	-2.217092	0.738357	0.173538	6	2.246157	0.783657	0.110074
6	-3.612968	0.546010	-0.072803	6	3.645228	0.566603	0.186970
6	-1.747286	2.020607	0.617301	6	1.740983	2.077034	-0.205238
6	-4.426990	1.723318	-0.241542	6	4.506692	1.735732	0.267715
6	-4.139006	-0.823339	-0.184263	6	4.133135	-0.811932	0.250737
6	-2.579573	3.098340	0.669620	6	2.577917	3.146917	-0.348314
1	-0.703271	2.097930	0.895738	1	0.668909	2.180068	-0.326584
6	-3.911186	2.999379	0.167948	6	3.965521	3.021988	-0.053008
6	-3.267835	-1.793510	-0.684851	6	3.259637	-1.792465	0.772495
6	-5.456940	-1.238520	0.260260	6	5.421829	-1.272317	-0.235636
1	-2.219550	4.062592	1.017590	1	2.183714	4.125031	-0.611303
6	-3.732075	-3.094405	-0.995379	6	3.720399	-3.100563	1.102999
1	-1.557543	-1.295595	-1.927248	1	1.338329	-0.482967	1.677525
6	-5.908008	-2.559313	-0.069461	6	5.865518	-2.592453	0.106889
6	-5.031893	-3.451625	-0.745277	6	5.006498	-3.468908	0.835320
1	-3.038656	-3.807884	-1.433289	1	3.023114	-3.795784	1.562556
1	-5.390849	-4.445470	-1.000830	1	5.369942	-4.457526	1.102370
6	-4.719828	4.153655	0.021195	6	4.797007	4.170362	0.006350
6	-5.959494	4.079962	-0.576972	6	6.098460	4.082374	0.447627
1	-6.560361	4.977072	-0.698566	1	6.720676	4.971129	0.505023
1	-4.327543	5.108311	0.361629	1	4.370796	5.131388	-0.270389
6	-6.436395	2.842270	-1.064908	6	6.606789	2.834041	0.867718
1	-7.389440	2.795978	-1.583633	1	7.611463	2.768537	1.276004
6	-5.693400	1.695130	-0.893751	6	5.833441	1.695266	0.777124
1	-6.064186	0.756709	-1.286116	1	6.240987	0.755276	1.126527
6	-6.292888	-0.455967	1.103581	6	6.220825	-0.527487	-1.145216
1	-5.946739	0.509557	1.449638	1	5.865376	0.431079	-1.500173
6	-7.526220	-0.912745	1.518986	6	7.425243	-1.013112	-1.609810
6	-8.001762	-2.179286	1.112850	6	7.903905	-2.270755	-1.183376
1	-8.981451	-2.521963	1.433560	1	8.862805	-2.637216	-1.538995
1	-8.132326	-0.293505	2.174496	1	8.003608	-0.425181	-2.316717
6	-7.198401	-2.987382	0.341397	6	7.129744	-3.046275	-0.348573
1	-7.526517	-3.984565	0.058136	1	7.460539	-4.038869	-0.053449
6	3.879613	1.147219	-1.125870	6	-4.157694	-0.422941	1.383953
6	5.148736	0.961418	-1.693086	6	-5.003234	-1.539909	1.433005
6	3.153469	2.305830	-1.439896	6	-4.068276	0.413705	2.509589

6	5.683774	1.921522	-2.553125	6	-5.752068	-1.810130	2.581126
1	5.718274	0.064359	-1.470525	1	-5.083155	-2.200507	0.576424
6	3.694664	3.268378	-2.292747	6	-4.825385	0.146948	3.648840
1	2.157232	2.441406	-1.030119	1	-3.402505	1.270255	2.497541
6	4.959623	3.077415	-2.851951	6	-5.668332	-0.966541	3.688455
1	6.665475	1.763392	-2.991836	1	-6.403338	-2.679933	2.603936
1	3.120506	4.159539	-2.531250	1	-4.746586	0.803800	4.510789
1	5.376695	3.822891	-3.523966	1	-6.253243	-1.176134	4.580232
6	3.904938	0.406222	1.677595	6	-3.728568	1.626203	-0.625394
6	4.619624	1.600363	1.848519	6	-4.976094	2.130301	-0.223198
6	3.728294	-0.445576	2.781595	6	-2.923169	2.399211	-1.478157
6	5.154495	1.932425	3.095662	6	-5.408354	3.382649	-0.664175
1	4.764391	2.273694	1.010529	1	-5.608245	1.550700	0.441417
6	4.273134	-0.115622	4.021293	6	-3.361963	3.648939	-1.917732
1	3.159312	-1.362632	2.674012	1	-1.963141	2.012507	-1.805101
6	4.986147	1.074926	4.182525	6	-4.602217	4.144944	-1.511031
1	5.706802	2.861259	3.211799	1	-6.374994	3.761221	-0.342245
1	4.129016	-0.784815	4.865119	1	-2.729791	4.235640	-2.579015
1	5.404746	1.332928	5.151827	1	-4.938811	5.120822	-1.851321
6	3.942095	-1.672068	-0.349758	6	-3.755513	-1.195761	-1.385656
6	3.323781	-2.506150	-1.295954	6	-3.062567	-2.394517	-1.610166
6	5.151346	-2.084297	0.234168	6	-4.921786	-0.931540	-2.118614
6	3.906974	-3.723784	-1.649116	6	-3.537548	-3.319347	-2.540842
1	2.394598	-2.193606	-1.761298	1	-2.142957	-2.589584	-1.067249
6	5.728440	-3.305163	-0.120746	6	-5.390242	-1.855023	-3.054045
1	5.640058	-1.459099	0.974385	1	-5.461692	-0.002208	-1.965360
6	5.107575	-4.127803	-1.062065	6	-4.700685	-3.050909	-3.264900
1	3.417913	-4.358300	-2.383487	1	-2.989892	-4.242604	-2.709241
1	6.662494	-3.612259	0.342457	1	-6.291731	-1.637190	-3.620649
1	5.556422	-5.079295	-1.335120	1	-5.065081	-3.767743	-3.996132

V_a			
E = -2923.0231613 Nimag = 0			
Tc = 0.493820			
15	-2.657663	0.002823	0.331773
78	-0.678532	-0.357905	-0.771729
17	0.487544	0.196936	1.228051
17	-1.721009	-0.992621	-2.822893
6	1.355658	-0.061556	-2.289977
1	0.711531	0.171621	-3.130915
6	1.385134	-1.348733	-1.769080
6	2.450829	-1.738846	-0.887165
6	3.454062	-0.806851	-0.526626
6	2.528375	-3.098594	-0.462183
6	4.701751	-1.350063	-0.006033
6	3.204490	0.606936	-0.795490
6	3.608544	-3.557163	0.231707
1	1.699313	-3.758888	-0.703026
6	4.746349	-2.716782	0.421895
6	2.252397	0.938489	-1.792478
6	3.810335	1.714998	-0.072964
1	3.653678	-4.587016	0.576700
6	2.152975	2.271864	-2.293428
1	0.771717	-2.127743	-2.211184
6	3.698332	3.041774	-0.600451
6	2.903224	3.278821	-1.762496
1	1.462537	2.462255	-3.111122

1	2.846783	4.287818	-2.163142
6	5.949120	-3.251328	0.949793
6	7.106256	-2.504081	0.983841
1	8.025208	-2.930352	1.376833
1	5.947727	-4.282205	1.295978
6	7.098455	-1.193712	0.461696
1	8.020129	-0.619367	0.425345
6	5.930188	-0.635781	-0.016994
1	5.958038	0.363665	-0.430739
6	4.401507	1.573099	1.210608
1	4.398435	0.602030	1.688313
6	4.947343	2.650404	1.878410
6	4.934419	3.935774	1.296696
1	5.382968	4.776067	1.819673
1	5.377888	2.506824	2.865575
6	4.308335	4.123864	0.083570
1	4.237492	5.117414	-0.352860
6	-4.152114	0.132593	-0.730011
6	-4.805741	1.358203	-0.918875
6	-4.645830	-1.014967	-1.373754
6	-5.939704	1.433345	-1.730894
1	-4.437806	2.254719	-0.432210
6	-5.782584	-0.935886	-2.174758
1	-4.139142	-1.966476	-1.255112
6	-6.431566	0.288255	-2.356403
1	-6.437695	2.389254	-1.868232
1	-6.154580	-1.830057	-2.666924
1	-7.315161	0.347738	-2.986246
6	-3.063811	-1.338108	1.525033
6	-4.398918	-1.601427	1.878960
6	-2.036756	-2.091829	2.114766
6	-4.697484	-2.596451	2.810510
1	-5.206669	-1.039103	1.422032
6	-2.343839	-3.086766	3.044122
1	-1.003741	-1.888262	1.855463
6	-3.670883	-3.341799	3.393556
1	-5.733410	-2.791201	3.074532
1	-1.540064	-3.663677	3.492970
1	-3.905573	-4.120031	4.114892
6	-2.632255	1.574830	1.281253
6	-1.909490	2.666189	0.776116
6	-3.366519	1.723505	2.466092
6	-1.936216	3.892194	1.440167
1	-1.311797	2.545782	-0.122156
6	-3.382120	2.950149	3.132018
1	-3.917322	0.884110	2.877997
6	-2.671020	4.036089	2.619142
1	-1.369107	4.729631	1.043637
1	-3.947006	3.053026	4.054525
1	-2.682361	4.989410	3.140654

I_b	$TS1_b$
E = -3377.7610606 Nimag = 0 Tc = 0.743641	E = -3377.7491082 Nimag = 1 (-184.45) Tc = 0.741659
6 3.690372 -0.699124 -0.783341	6 3.550042 -0.360383 -1.241820
6 4.979982 -0.669155 -1.295663	6 4.568212 0.027394 -2.104359
6 4.006833 -1.545057 -1.845367	6 3.836034 -1.166041 -2.343765

6	4.588964	-3.041189	-3.685012	6	4.376532	-2.586344	-4.256882
1	5.620856	-2.850506	-3.393832	1	5.319846	-2.042866	-4.275391
6	2.267027	-2.950011	-2.770774	6	2.482143	-3.134507	-2.724624
1	2.254902	-4.039667	-2.676721	1	2.856221	-4.157380	-2.625170
6	7.224537	-0.557842	-2.272736	6	6.296161	0.743101	-3.688436
1	7.659699	0.343103	-2.714009	1	6.267987	1.684398	-4.244159
6	6.596659	0.836425	-0.302783	6	5.789779	2.065778	-1.635609
1	5.780881	1.011600	0.399945	1	5.189503	2.041977	-0.725081
6	2.103324	-1.284140	1.495021	6	2.932369	-1.156676	1.415936
6	1.249653	-2.267814	1.992745	6	2.641258	-2.264877	2.210870
6	2.532840	-2.044611	2.574213	6	3.900828	-1.600920	2.308040
6	4.718894	-1.584760	3.502587	6	5.992209	-0.391371	2.420505
1	5.551902	-2.266229	3.303388	1	6.888384	-0.815616	1.957120
6	3.305007	-3.400686	4.466290	6	5.628566	-2.396109	3.859933
1	2.406171	-3.980781	4.267037	1	4.963077	-3.247276	3.987220
6	-0.867490	-2.673876	0.874561	6	0.531961	-3.432227	1.918263
1	-1.129416	-3.629693	0.412564	1	0.455618	-4.486047	1.635227
6	-0.236533	-3.972373	2.910895	6	2.152468	-4.163661	3.668168
1	0.381253	-3.895263	3.804473	1	3.014942	-3.816496	4.234112
6	2.951861	1.445499	0.974986	6	2.625685	1.618788	0.623518
6	3.207196	2.786412	0.682957	6	2.342348	2.935918	0.257817
6	2.803907	2.395397	1.983283	6	2.439398	2.570418	1.625105
6	2.438707	4.084971	3.713668	6	1.967548	4.219659	3.368457
1	3.012899	4.128191	4.643404	1	2.748843	4.589358	4.038420
6	1.880070	1.689221	4.105190	6	2.402879	1.827625	3.925695
1	1.975805	0.702467	3.654463	1	2.885972	0.941193	3.515558
6	3.561463	3.402800	-1.638264	6	1.868389	3.411114	-2.076412
1	2.885133	4.075059	-2.173906	1	0.909651	3.810038	-2.419803
6	3.668318	5.129859	0.163913	6	1.886958	5.249994	-0.382915
1	3.873932	5.227705	1.229045	1	2.322522	5.501512	0.583235
7	3.662233	-2.482177	-2.684140	7	3.611960	-2.243164	-3.043126
7	6.189473	-0.162679	-1.300284	7	5.489659	0.887825	-2.461764
7	3.450681	-2.328766	3.465135	7	5.090856	-1.476044	2.839803
7	0.128842	-2.928355	1.936893	7	1.838720	-3.223734	2.575271
7	2.443166	2.703693	3.201923	7	2.326638	2.871689	2.890952
7	3.491920	3.710917	-0.196520	7	2.073031	3.814844	-0.671156
15	2.295277	-0.047666	0.180363	15	2.337041	-0.085480	0.079108
1	4.520658	5.528265	-0.392268	1	2.398038	5.829877	-1.155636
1	2.772156	5.699728	-0.100365	1	0.822023	5.501326	-0.395295
1	3.239509	2.379082	-1.831257	1	1.832256	2.324857	-2.165524
1	4.581719	3.565845	-1.999613	1	2.667113	3.827538	-2.698353
1	2.884308	4.758794	2.984879	1	1.856686	4.900682	2.527224
1	1.408600	4.397054	3.911060	1	1.019868	4.166801	3.912568
1	2.414283	1.721162	5.059326	1	2.986053	2.208799	4.767914
1	0.819424	1.898366	4.274108	1	1.395100	1.565791	4.261840
1	-1.282016	-3.826211	3.192843	1	1.291626	-4.215172	4.339883
1	-0.124612	-4.963530	2.460258	1	2.347801	-5.159448	3.259052
1	-0.457095	-1.990359	0.132132	1	0.448908	-2.794915	1.039482
1	-1.761957	-2.224187	1.312597	1	-0.271689	-3.175759	2.613001
1	4.172940	-4.063801	4.409374	1	6.606149	-2.759661	3.531091
1	3.250563	-2.967878	5.469860	1	5.743442	-1.869674	4.812193
1	4.705027	-0.793832	2.751358	1	5.481753	0.257746	1.707533
1	4.855437	-1.142979	4.494526	1	6.291589	0.193440	3.295689
1	7.474423	0.472592	0.240681	1	6.852299	2.064862	-1.372909
1	6.859211	1.774035	-0.803144	1	5.569813	2.978459	-2.198595
1	6.784055	-1.155418	-3.068300	1	5.885729	-0.043716	-4.318002
1	8.012933	-1.127835	-1.771309	1	7.333689	0.510814	-3.429056
1	1.671514	-2.489857	-1.983798	1	2.004067	-2.811242	-1.800849
1	1.844209	-2.654223	-3.734427	1	1.744717	-3.085912	-3.530357
1	4.387121	-2.602764	-4.667326	1	3.787478	-2.350832	-5.148651

1	4.436791	-4.121939	-3.737333	1	4.592323	-3.657404	-4.242729
78	0.368423	0.517164	-0.953202	78	0.094876	-0.230108	-0.441294
17	-0.605603	0.817307	1.231483	17	-0.237809	-0.043979	1.935153
17	1.465665	0.396234	-3.067952	17	0.553767	-0.196662	-2.781019
6	-1.359887	1.032726	-1.961601	6	-2.034669	-1.206151	-1.194447
1	-1.221834	1.023376	-3.043937	1	-1.917394	-2.103084	-1.765381
6	-2.494601	1.321311	-1.447735	6	-2.060989	-0.043738	-0.720586
6	-3.681958	1.732536	-0.900688	6	-2.958595	1.017181	-0.337160
6	-4.755936	0.802505	-0.685894	6	-4.328128	0.723878	-0.441999
6	-3.835530	3.129485	-0.559457	6	-2.507880	2.294285	0.090791
6	-5.975369	1.288345	-0.150722	6	-5.279321	1.746564	-0.136329
6	-4.590781	-0.621706	-1.084803	6	-4.769529	-0.629732	-0.899612
6	-4.998075	3.575675	-0.013917	6	-3.415459	3.272065	0.404959
1	-3.003845	3.799105	-0.748252	1	-1.440844	2.474030	0.172705
6	-6.097936	2.685546	0.198349	6	-4.813037	3.036052	0.297415
6	-4.510320	-0.924168	-2.435960	6	-4.680814	-0.947740	-2.256229
6	-4.558093	-1.680934	-0.112623	6	-5.324382	-1.586196	0.016769
1	-5.118925	4.622485	0.248874	1	-3.079271	4.250413	0.738260
6	-4.437555	-2.261791	-2.886260	6	-5.141429	-2.187738	-2.754040
1	-4.556121	-0.122218	-3.167095	1	-4.297332	-0.203290	-2.948996
6	-4.487023	-3.036570	-0.581035	6	-5.790914	-2.842729	-0.499298
6	-4.433763	-3.295204	-1.978247	6	-5.687921	-3.112070	-1.892299
1	-4.411135	-2.464290	-3.952452	1	-5.085506	-2.391510	-3.819013
1	-4.404235	-4.326898	-2.318995	1	-6.062700	-4.060138	-2.269190
6	-7.319665	3.158733	0.718435	6	-5.758212	4.048862	0.600668
6	-8.396841	2.305049	0.878759	6	-7.109158	3.811381	0.474703
1	-9.333792	2.687066	1.273113	1	-7.824280	4.594771	0.706400
1	-7.410398	4.208744	0.980318	1	-5.399102	5.020227	0.929915
6	-8.296787	0.940607	0.515783	6	-7.572322	2.547548	0.035882
1	-9.158702	0.290562	0.626409	1	-8.638961	2.374661	-0.068992
6	-7.118487	0.443457	0.010720	6	-6.682885	1.540012	-0.262884
1	-7.052733	-0.597002	-0.283544	1	-7.050148	0.578706	-0.603592
6	-4.580248	-1.452026	1.292071	6	-5.438146	-1.341154	1.411864
1	-4.616430	-0.433991	1.666044	1	-5.093662	-0.394445	1.815135
6	-4.577294	-2.505181	2.183879	6	-5.995502	-2.283942	2.251573
6	-4.538136	-3.842692	1.719008	6	-6.462309	-3.516707	1.740735
1	-4.570826	-4.664011	2.429379	1	-6.909249	-4.244385	2.411330
1	-4.628076	-2.306893	3.251045	1	-6.086886	-2.074291	3.313315
6	-4.484733	-4.097904	0.366153	6	-6.358166	-3.789417	0.393057
1	-4.463005	-5.121027	-0.000839	1	-6.719335	-4.733217	-0.006638

II_b E = -3377.7733122 Nimag = 0 Tc = 0.747474				TS2_b E = -3377.7586231 Nimag = 1(-164.92) TC = 0.746283			
6	-3.318027	-0.074501	1.526394	6	-3.433849	0.063800	1.359364
6	-4.474455	0.138905	2.265189	6	-4.626507	0.434399	1.965143
6	-3.288103	-0.336120	2.895012	6	-3.567883	-0.127031	2.733261
6	-3.267493	-0.811168	5.292805	6	-3.841128	-0.476782	5.135683
1	-4.340314	-0.640270	5.227958	1	-4.890033	-0.257538	4.944187
6	-1.235693	-1.158965	3.887938	6	-1.717114	-1.081648	3.974604
1	-1.147439	-2.185801	4.255384	1	-1.762358	-2.084213	4.410360
6	-6.508624	0.568055	3.570293	6	-6.712015	1.145967	3.043652
1	-7.006229	1.538857	3.644613	1	-7.126700	2.157207	3.014814
6	-6.452368	0.896139	1.098958	6	-6.389815	1.338341	0.577941
1	-5.789588	0.811885	0.236628	1	-5.655997	1.156425	-0.208455
6	-3.111080	-1.470621	-0.935387	6	-3.005409	-1.521113	-0.952400
6	-3.021623	-2.838980	-1.185954	6	-2.926892	-2.903703	-1.107256
6	-3.902250	-2.016300	-1.937290	6	-3.757336	-2.121468	-1.952966
6	-5.405932	-0.564650	-3.160812	6	-5.184099	-0.733672	-3.331580

1	-6.492960	-0.656345	-3.069074	1	-6.274397	-0.797490	-3.254939
6	-5.226446	-2.978615	-3.761485	6	-5.019618	-3.184147	-3.765644
1	-4.575199	-3.840654	-3.630950	1	-4.385210	-4.043194	-3.555963
6	-1.453960	-4.158739	0.102404	6	-1.453776	-4.157239	0.348394
1	-1.776841	-4.875927	0.862889	1	-1.846045	-4.784583	1.154638
6	-2.918083	-5.243240	-1.604199	6	-2.851890	-5.333183	-1.352414
1	-3.861511	-5.096521	-2.127799	1	-3.751121	-5.201488	-1.952078
6	-2.798783	1.377071	-0.909636	6	-2.610611	1.309388	-1.099777
6	-2.900684	2.766721	-0.897377	6	-2.639086	2.699487	-1.198669
6	-2.516625	2.084376	-2.077952	6	-2.224410	1.909495	-2.297900
6	-2.032305	3.308567	-4.139040	6	-1.553142	2.940768	-4.412060
1	-2.421422	3.081527	-5.135100	1	-1.917397	2.663244	-5.404888
6	-1.565023	0.862409	-3.945652	6	-1.236859	0.496228	-4.003502
1	-1.424912	0.076860	-3.202281	1	-1.119226	-0.212374	-3.182442
6	-3.319437	3.863240	1.220041	6	-3.104488	3.971407	0.808223
1	-3.041869	2.891341	1.626646	1	-2.793178	3.058977	1.317567
6	-3.047827	5.209621	-0.863695	6	-2.685945	5.140894	-1.360605
1	-2.947446	5.114930	-1.943070	1	-2.570407	4.957248	-2.427080
7	-2.653749	-0.754310	3.954355	7	-3.090674	-0.551947	3.869707
7	-5.725559	0.524822	2.321932	7	-5.825495	0.959072	1.880845
7	-4.779345	-1.868036	-2.901109	7	-4.587551	-2.025086	-2.964115
7	-2.526785	-4.010578	-0.897376	7	-2.467138	-4.060695	-0.717565
7	-2.094087	2.087352	-3.316232	7	-1.727684	1.794246	-3.503336
7	-3.091087	3.878504	-0.234250	7	-2.807841	3.867045	-0.631287
15	-2.326822	-0.120787	0.000278	15	-2.278301	-0.124282	-0.036281
1	-3.973185	5.747064	-0.636876	1	-3.589073	5.736127	-1.198214
1	-2.198678	5.774209	-0.467352	1	-1.819299	5.695928	-0.989398
1	-4.366451	4.100283	1.437018	1	-4.170348	4.172923	0.961040
1	-2.680781	4.620197	1.682711	1	-2.526271	4.801701	1.221160
1	-2.644157	4.094037	-3.698279	1	-2.126171	3.796250	-4.058201
1	-0.995970	3.648286	-4.229726	1	-0.493641	3.205775	-4.481239
1	-2.240385	0.533888	-4.742343	1	-1.919420	0.107852	-4.766823
1	-0.588191	1.087801	-4.382548	1	-0.253293	0.648764	-4.455821
1	-2.135435	-5.532524	-2.312416	1	-2.033335	-5.700209	-1.979301
1	-3.048751	-6.041859	-0.869712	1	-3.060098	-6.067572	-0.570037
1	-1.228668	-3.192939	0.551930	1	-1.203107	-3.163014	0.714700
1	-0.549271	-4.524248	-0.390574	1	-0.545365	-4.607650	-0.060237
1	-6.258649	-3.250578	-3.519275	1	-6.063353	-3.428223	-3.543658
1	-5.176647	-2.660147	-4.806352	1	-4.928978	-2.935628	-4.826576
1	-5.040218	0.170920	-2.442951	1	-4.815810	0.046262	-2.663701
1	-5.167860	-0.235221	-4.177200	1	-4.920753	-0.485199	-4.364540
1	-7.311552	0.230798	0.967082	1	-7.291743	0.749575	0.381458
1	-6.814966	1.925284	1.183494	1	-6.659441	2.398982	0.587754
1	-5.853210	0.445936	4.430118	1	-6.149612	1.028162	3.967749
1	-7.265237	-0.222716	3.565215	1	-7.532458	0.422083	3.012365
1	-0.870084	-1.080959	2.864972	1	-1.247922	-1.105651	2.992087
1	-0.642110	-0.491647	4.518565	1	-1.126640	-0.425798	4.619896
1	-2.809910	-0.056434	5.939472	1	-3.408872	0.297243	5.777176
1	-3.093691	-1.801986	5.720957	1	-3.771929	-1.441812	5.644375
78	0.052575	-0.079416	0.186617	78	0.042494	-0.125684	0.420116
17	0.261980	-1.637535	-1.611515	17	0.448146	-1.710722	-1.316604
17	-0.301664	1.595140	1.876413	17	-0.455592	1.565023	2.069009
6	2.870460	-1.054817	0.669735	6	2.655754	-1.024006	1.432510
1	2.563393	-2.084209	0.541301	1	2.250980	-2.024496	1.518169
6	2.043440	0.055485	0.316633	6	2.030557	0.002900	0.803089
6	2.856451	1.194884	0.040735	6	2.860029	1.141870	0.385530
6	4.224896	0.834232	0.123283	6	4.223127	0.838143	0.313116
6	2.477699	2.542662	-0.234212	6	2.411267	2.449227	0.081301
6	5.248165	1.799912	0.006229	6	5.193944	1.828985	0.013779
6	4.338855	-0.616596	0.494030	6	4.558311	-0.553972	0.745319

6	3.457066	3.480344	-0.414114	6	3.324330	3.425151	-0.250687
1	1.426813	2.805807	-0.275866	1	1.351493	2.671350	0.133620
6	4.846232	3.151929	-0.299638	6	4.717499	3.157101	-0.288207
6	3.906254	-0.839875	1.921976	6	4.114348	-0.862640	2.102454
6	5.278464	-1.592587	-0.117896	6	5.201810	-1.539610	-0.051002
1	3.196381	4.512976	-0.629464	1	2.988114	4.433189	-0.478677
6	4.404987	-2.008086	2.625904	6	4.606677	-2.116485	2.706644
1	3.634412	0.032551	2.509282	1	4.086803	-0.009515	2.784424
6	5.653311	-2.744357	0.627384	6	5.596445	-2.775605	0.571139
6	5.205989	-2.906255	1.996175	6	5.293549	-3.013960	1.965568
1	4.173053	-2.116716	3.680944	1	4.404371	-2.293150	3.758698
1	5.582135	-3.765896	2.545390	1	5.657746	-3.934539	2.413432
6	5.846185	4.136225	-0.464238	6	5.659985	4.168999	-0.607821
6	7.182734	3.817899	-0.312693	6	7.010237	3.901089	-0.609942
1	7.938878	4.587447	-0.435418	1	7.721610	4.685787	-0.848030
1	5.551149	5.154223	-0.702523	1	5.297579	5.166698	-0.839892
6	7.577675	2.498487	0.012026	6	7.481592	2.602470	-0.291438
1	8.630901	2.270459	0.141867	1	8.549801	2.408595	-0.283495
6	6.633681	1.507952	0.166911	6	6.600321	1.590367	0.010839
1	6.940880	0.499549	0.419722	1	6.979613	0.604774	0.257908
6	5.759559	-1.427899	-1.421361	6	5.513586	-1.312549	-1.417595
1	5.479104	-0.548709	-1.993315	1	5.213911	-0.378619	-1.880064
6	6.603838	-2.382586	-1.987312	6	6.199617	-2.267192	-2.144094
6	6.977866	-3.519234	-1.259057	6	6.592794	-3.472273	-1.528885
1	7.637913	-4.257693	-1.703100	1	7.140022	-4.213690	-2.103574
1	6.975148	-2.239197	-2.997503	1	6.442215	-2.089332	-3.186787
6	6.507647	-3.695001	0.036130	6	6.294397	-3.722433	-0.194184
1	6.800261	-4.570741	0.609010	1	6.606179	-4.654749	0.267520

III_b E = -3377.76946 Nimag = 0 Tc = 0.746182				TS3_b E = -3377.757346 Nimag = 1 (-1010.34) Tc = 0.744655			
6	3.522424	-0.607676	-1.257959	6	-3.509191	-0.405140	1.399151
6	4.563981	-0.412593	-2.154423	6	-4.416870	-0.026715	2.379241
6	3.682515	-1.514400	-2.304061	6	-3.677982	-1.230989	2.509318
6	4.012774	-3.121692	-4.112634	6	-4.025102	-2.690328	4.436984
1	5.014866	-2.700394	-4.177932	1	-4.952893	-2.136394	4.572254
6	2.093888	-3.326583	-2.529015	6	-2.327665	-3.230976	2.688280
1	2.350963	-4.371188	-2.329827	1	-2.740918	-4.236836	2.568401
6	6.338191	-0.027739	-3.801076	6	-5.945402	0.676962	4.161786
1	6.434360	0.873732	-4.412590	1	-5.847805	1.608438	4.726303
6	6.052627	1.470275	-1.828671	6	-5.662857	2.029254	2.086044
1	5.445706	1.602901	-0.932003	1	-5.163128	2.018552	1.116482
6	3.056035	-1.063335	1.497506	6	-3.235756	-1.130793	-1.328905
6	2.812667	-2.126851	2.364090	6	-3.065508	-2.219682	-2.181932
6	4.005295	-1.356079	2.466804	6	-4.308143	-1.523667	-2.119253
6	6.026730	-0.030500	2.524386	6	-6.358971	-0.252466	-1.964721
1	6.981604	-0.467979	2.215389	1	-7.218434	-0.661825	-1.424594
6	5.665471	-1.834286	4.208986	6	-6.221318	-2.219422	-3.491639
1	4.876718	-2.444866	4.644150	1	-5.602535	-3.085986	-3.715361
6	0.762679	-3.398415	2.119619	6	-0.958511	-3.420754	-2.160230
1	0.753285	-4.439047	1.782016	1	-0.876712	-4.471135	-1.864822
6	2.424476	-4.001527	3.881138	6	-2.781041	-4.092635	-3.725422
1	3.461419	-3.844648	4.172781	1	-3.722193	-3.745804	-4.148047
6	2.813161	1.591322	0.423683	6	-2.780931	1.600723	-0.504726
6	2.700815	2.879488	-0.097674	6	-2.451556	2.902142	-0.129193
6	2.711863	2.668031	1.301913	6	-2.714638	2.588333	-1.484903
6	2.526672	4.548713	2.856688	6	-2.479221	4.303264	-3.212580
1	3.268442	4.772804	3.628633	1	-3.310362	4.648495	-3.833887

6	2.466874	2.181728	3.659632	6	-2.930033	1.924494	-3.801416
1	2.121368	1.210839	3.303085	1	-3.201888	0.969978	-3.353235
6	2.375838	3.102713	-2.491865	6	-1.685291	3.266591	2.144737
1	2.180251	2.030855	-2.442292	1	-0.697591	3.667343	2.389421
6	2.514677	5.129522	-1.040062	6	-1.907098	5.184517	0.557104
1	2.834507	5.454018	-0.051294	1	-2.442683	5.478619	-0.344615
7	3.315390	-2.602873	-2.922883	7	-3.394880	-2.329003	3.154663
7	5.580652	0.299940	-2.580231	7	-5.282221	0.836839	2.855108
7	5.147754	-1.084431	3.050650	7	-5.547054	-1.350819	-2.509842
7	2.066939	-3.123119	2.753989	7	-2.328273	-3.183222	-2.658102
7	2.589053	3.115130	2.526523	7	-2.754810	2.933861	-2.745841
7	2.565830	3.660958	-1.139662	7	-2.066698	3.739808	0.799848
15	2.377732	-0.138239	0.080375	15	-2.433597	-0.121424	-0.043200
1	3.189306	5.559737	-1.785447	1	-2.328461	5.731390	1.404709
1	1.497285	5.482316	-1.235169	1	-0.846354	5.436955	0.463237
1	3.256042	3.313927	-3.108028	1	-1.619416	2.178108	2.167462
1	1.503967	3.580236	-2.947622	1	-2.406347	3.630088	2.884084
1	2.743329	5.149823	1.975482	1	-2.362216	4.974659	-2.364204
1	1.530271	4.797735	3.233902	1	-1.559897	4.307933	-3.806218
1	3.423583	2.098231	4.186653	1	-3.715122	2.255530	-4.487293
1	1.716463	2.573417	4.350760	1	-1.991288	1.801836	-4.349917
1	1.764487	-3.800917	4.730644	1	-2.025953	-4.108923	-4.515960
1	2.300780	-5.042537	3.571252	1	-2.902446	-5.103939	-3.325730
1	0.599494	-2.717970	1.285043	1	-0.748372	-2.766651	-1.315065
1	-0.034713	-3.240236	2.850533	1	-0.240470	-3.203016	-2.954879
1	6.502244	-2.470336	3.903276	1	-7.169948	-2.564169	-3.070491
1	6.013814	-1.124620	4.964284	1	-6.420101	-1.660095	-4.410956
1	5.552125	0.451262	1.668376	1	-5.753750	0.352436	-1.287993
1	6.217907	0.713995	3.303488	1	-6.724217	0.373854	-2.784546
1	7.099870	1.325967	-1.543747	1	-6.747400	2.037643	1.937587
1	5.981757	2.365725	-2.454402	1	-5.378603	2.931995	2.636265
1	5.809828	-0.783184	-4.379270	1	-5.472190	-0.122504	4.728475
1	7.337210	-0.390330	-3.539057	1	-7.007627	0.454606	4.019525
1	1.653953	-2.861952	-1.647911	1	-1.919888	-2.867141	1.746400
1	1.365123	-3.271941	-3.342073	1	-1.521032	-3.247611	3.425991
1	3.443703	-2.881348	-5.016200	1	-3.338620	-2.482401	5.263703
1	4.098220	-4.207445	-4.022488	1	-4.257115	-3.758164	4.424697
78	0.062614	-0.239205	-0.323149	78	-0.095562	-0.291012	0.221168
17	-0.202359	-0.045886	2.066561	17	-0.052333	-0.044313	-2.179227
17	0.421087	-0.260901	-2.682239	17	-0.269504	-0.398151	2.595752
6	-2.467899	-1.416131	-1.210051	6	2.461811	-1.544837	0.913146
1	-1.838603	-2.173931	-1.665059	1	1.840661	-2.323612	1.339772
6	-1.964102	-0.319229	-0.614437	6	1.938621	-0.380597	0.369022
6	-2.876725	0.774270	-0.269365	6	2.840328	0.668074	0.018854
6	-4.299249	0.616520	-0.362610	6	4.266531	0.503781	0.171151
6	-2.366937	2.029472	0.145573	6	2.344290	1.931524	-0.444563
6	-5.156036	1.789438	-0.283536	6	5.094216	1.702947	0.199316
6	-4.791846	-0.729001	-0.511565	6	4.798726	-0.828404	0.310441
6	-3.190944	3.105129	0.370887	6	3.170267	2.996581	-0.637944
1	-1.296677	2.121444	0.286067	1	1.283801	2.006755	-0.651552
6	-4.585892	3.039189	0.118477	6	4.546682	2.941241	-0.257766
6	-3.960581	-1.606441	-1.392909	6	3.928118	-1.816181	0.900977
6	-5.943199	-1.282346	0.131743	6	6.099399	-1.290959	-0.140790
1	-2.771162	4.051657	0.702780	1	2.778817	3.935710	-1.020933
6	-4.415177	-3.011234	-1.592428	6	4.424560	-3.117042	1.301433
1	-4.123901	-1.142897	-2.399203	1	3.375833	-1.286210	1.892997
6	-6.358248	-2.625808	-0.187752	6	6.562380	-2.584978	0.269915
6	-5.578934	-3.449982	-1.083900	6	5.710039	-3.451347	1.036851
1	-3.795411	-3.647888	-2.217908	1	3.748926	-3.803143	1.803322
1	-5.930330	-4.457925	-1.285093	1	6.096291	-4.420309	1.339860

6	-5.396360	4.200652	0.193942	6	5.342309	4.110387	-0.253279
6	-6.722581	4.157390	-0.177013	6	6.622779	4.090049	0.262800
1	-7.337290	5.050639	-0.130018	1	7.223392	4.994235	0.275882
1	-4.944801	5.133070	0.521591	1	4.917214	5.035348	-0.633354
6	-7.270503	2.947544	-0.655257	6	7.133303	2.895886	0.810668
1	-8.301162	2.922241	-0.995960	1	8.116283	2.890459	1.271448
6	-6.509091	1.795402	-0.707665	6	6.389833	1.731462	0.775634
1	-6.957119	0.888734	-1.097087	1	6.802632	0.832800	1.216642
6	-6.639893	-0.601016	1.174251	6	6.896463	-0.571054	-1.067448
1	-6.294323	0.371814	1.496765	1	6.537925	0.368099	-1.467753
6	-7.732946	-1.167951	1.793966	6	8.117642	-1.058772	-1.492714
6	-8.186854	-2.443178	1.399874	6	8.607760	-2.286253	-1.006166
1	-9.061090	-2.877016	1.876095	1	9.577495	-2.651711	-1.329337
1	-8.242652	-0.633892	2.589379	1	8.699677	-0.492212	-2.212905
6	-7.498755	-3.161607	0.432698	6	7.831077	-3.040947	-0.146061
1	-7.824032	-4.162094	0.163502	1	8.177287	-4.011826	0.196617

IV_b E = -3377.8053985 NImag = 0 Tc = 0.747367				TS4_b E = -3377.7797285 Nimag = 1 (-994.42) Tc = 0.744794			
6	-3.443527	-0.410558	1.462485	6	3.564102	-0.395510	-1.328630
6	-4.435168	-0.094589	2.381573	6	4.536409	-0.018521	-2.245790
6	-3.515707	-1.144746	2.645374	6	3.778482	-1.202430	-2.445293
6	-3.690379	-2.451209	4.702929	6	4.202317	-2.628081	-4.383500
1	-4.690487	-2.026821	4.775817	1	5.147252	-2.091676	-4.454632
6	-1.876208	-2.880827	3.043679	6	2.396553	-3.165956	-2.745191
1	-2.133049	-3.943488	3.000947	1	2.777286	-4.186133	-2.641051
6	-6.124214	0.509140	4.052868	6	6.183201	0.683271	-3.920630
1	-6.207464	1.492370	4.524091	1	6.135845	1.626659	-4.471590
6	-5.987118	1.690205	1.861331	6	5.809702	2.000511	-1.836425
1	-5.435407	1.693512	0.920263	1	5.250964	1.985031	-0.899668
6	-3.220745	-1.242878	-1.243805	6	3.136294	-1.170812	1.369193
6	-3.067439	-2.417825	-1.977875	6	2.907100	-2.276129	2.187229
6	-4.253152	-1.635112	-2.085606	6	4.159041	-1.593516	2.208694
6	-6.208851	-0.220425	-2.234573	6	6.231717	-0.348161	2.194042
1	-7.140903	-0.517337	-1.743351	1	7.109531	-0.759758	1.686103
6	-6.088921	-2.326873	-3.561742	6	5.984789	-2.345336	3.667729
1	-5.529196	-3.256582	-3.639000	1	5.342844	-3.206988	3.838445
6	-1.057687	-3.740254	-1.678283	6	0.795197	-3.459540	2.024022
1	-1.068223	-4.757621	-1.275788	1	0.719299	-4.506561	1.715823
6	-2.803632	-4.452097	-3.308716	6	2.522346	-4.176506	3.674589
1	-3.699119	-4.103271	-3.819157	1	3.431862	-3.837446	4.166923
6	-2.848701	1.525397	-0.561887	6	2.770527	1.587861	0.582455
6	-2.693364	2.871010	-0.229897	6	2.473312	2.901578	0.220089
6	-2.783179	2.469310	-1.585485	6	2.648697	2.551593	1.581699
6	-2.656986	4.118097	-3.390179	6	2.296112	4.222055	3.332779
1	-3.436423	4.251661	-4.145715	1	3.101354	4.573152	3.984129
6	-2.684636	1.666006	-3.867484	6	2.725517	1.829619	3.888346
1	-2.378370	0.731902	-3.396323	1	3.136507	0.919472	3.452882
6	-2.244685	3.424443	2.089326	6	1.858554	3.337567	-2.087511
1	-1.350480	3.951743	2.432758	1	0.896564	3.762128	-2.388064
6	-2.426699	5.227297	0.371172	6	1.997591	5.208308	-0.435509
1	-2.809964	5.417737	-0.629811	1	2.474091	5.469472	0.508504
7	-3.082051	-2.113298	3.403452	7	3.508542	-2.279190	-3.130210
7	-5.443993	0.656634	2.753150	7	5.447863	0.832473	-2.651269
7	-5.438437	-1.417552	-2.600853	7	5.375665	-1.444876	2.671434
7	-2.369484	-3.470788	-2.298534	7	2.136695	-3.241829	2.601670
7	-2.724427	2.743764	-2.863716	7	2.612205	2.866192	2.850086
7	-2.494375	3.788522	0.681844	7	2.153337	3.767524	-0.706796

15	-2.420390	-0.154563	-0.022327	15	2.427871	-0.119065	0.066037
1	-3.041100	5.774126	1.091553	1	2.483959	5.770425	-1.237069
1	-1.392475	5.576875	0.445950	1	0.936389	5.474119	-0.407972
1	-2.056559	2.354204	2.181034	1	1.778456	2.251368	-2.145226
1	-3.094543	3.730253	2.708353	1	2.634541	3.708660	-2.764844
1	-2.814766	4.838538	-2.589870	1	2.186562	4.905211	2.492938
1	-1.678931	4.288772	-3.849902	1	1.359877	4.195818	3.898589
1	-3.661555	1.567758	-4.352995	1	3.386075	2.192379	4.680315
1	-1.938774	1.923475	-4.623679	1	1.736498	1.612519	4.303022
1	-2.004723	-4.576228	-4.044896	1	1.716756	-4.212763	4.412750
1	-3.001466	-5.415123	-2.828601	1	2.673158	-5.177624	3.259624
1	-0.862549	-3.016111	-0.888767	1	0.642139	-2.797415	1.173075
1	-0.272934	-3.648090	-2.433295	1	0.034793	-3.239582	2.777566
1	-7.099064	-2.553598	-3.209389	1	6.949491	-2.694970	3.289314
1	-6.150782	-1.850253	-4.544876	1	6.142026	-1.808910	4.608384
1	-5.620492	0.404945	-1.561688	1	5.670472	0.283954	1.504342
1	-6.454072	0.347709	-3.137483	1	6.566973	0.251192	3.046140
1	-7.044887	1.486963	1.665514	1	6.882967	1.978087	-1.622350
1	-5.903223	2.671767	2.338548	1	5.582258	2.919945	-2.385322
1	-5.547419	-0.141216	4.707409	1	5.729468	-0.096575	-4.528912
1	-7.127331	0.096145	3.907206	1	7.230851	0.437760	-3.720621
1	-1.488283	-2.536340	2.086375	1	1.956154	-2.823163	-1.810028
1	-1.106519	-2.717002	3.802572	1	1.625401	-3.135581	-3.519503
1	-3.062529	-2.077198	5.517598	1	3.567227	-2.388634	-5.242077
1	-3.767800	-3.538525	4.781239	1	4.411105	-3.700708	-4.380976
78	-0.048364	-0.238821	0.197164	78	0.118758	-0.247034	-0.328227
17	0.008696	-0.469670	-2.192565	17	-0.078653	-0.080056	2.062500
17	-0.221075	0.176460	2.544786	17	0.395838	-0.289959	-2.695548
6	2.519516	-1.454619	1.083771	6	-2.502549	-1.505092	-1.079136
1	1.924587	-2.359525	0.908367	1	-1.841480	-2.280919	-1.455316
6	1.963096	-0.297500	0.328770	6	-1.925592	-0.300523	-0.561844
6	2.829602	0.690399	-0.110086	6	-2.845302	0.745142	-0.150767
6	4.262346	0.533528	0.107065	6	-4.255137	0.525763	-0.217248
6	2.345598	1.932271	-0.674586	6	-2.343556	2.018198	0.249845
6	5.050248	1.735941	0.176319	6	-5.117375	1.695663	-0.203003
6	4.814698	-0.801197	0.268606	6	-4.750816	-0.841212	-0.351385
6	3.163938	3.000148	-0.833564	6	-3.184851	3.065941	0.489966
1	1.298703	1.975838	-0.952584	1	-1.271202	2.125627	0.369990
6	4.511707	2.964992	-0.335472	6	-4.577875	2.957207	0.210434
6	3.973119	-1.758914	0.862153	6	-3.899114	-1.786052	-0.983122
6	6.145347	-1.210601	-0.158528	6	-6.029862	-1.324409	0.128772
1	2.799099	3.926307	-1.268758	1	-2.796741	4.024096	0.825632
6	4.478956	-3.006398	1.278308	6	-4.385327	-3.052607	-1.423572
1	2.337772	-1.218207	2.149480	1	-2.119039	-0.457176	-1.834221
6	6.635021	-2.487083	0.276389	6	-6.497994	-2.606059	-0.320371
6	5.791307	-3.340458	1.034887	6	-5.669186	-3.422950	-1.148595
1	3.823636	-3.704254	1.792607	1	-3.716753	-3.714458	-1.966956
1	6.181601	-4.297831	1.369563	1	-6.055625	-4.376937	-1.495406
6	5.298267	4.132227	-0.299983	6	-5.412556	4.100826	0.258364
6	6.550310	4.124846	0.293580	6	-6.721285	4.036952	-0.169573
1	7.139428	5.036434	0.327691	1	-7.350620	4.921200	-0.144781
1	4.898827	5.050848	-0.720206	1	-4.992002	5.040747	0.605403
6	7.049451	2.945368	0.883024	6	-7.228903	2.823612	-0.681924
1	8.006924	2.958744	1.393745	1	-8.238738	2.786757	-1.078754
6	6.321552	1.775267	0.815931	6	-6.451271	1.683678	-0.692588
1	6.710427	0.878711	1.281463	1	-6.863443	0.772754	-1.106213
6	6.948040	-0.480213	-1.070897	6	-6.802388	-0.647722	1.110650
1	6.580984	0.447689	-1.491441	1	-6.434970	0.276334	1.538193
6	8.189614	-0.943772	-1.462063	6	-8.002436	-1.162644	1.555950
6	8.702631	-2.158740	-0.959328	6	-8.503176	-2.374784	1.033522

1	9.687128	-2.500320	-1.262852	1	-9.459977	-2.758194	1.374250
1	8.774535	-0.367246	-2.172472	1	-8.563543	-0.632830	2.319588
6	7.929794	-2.920892	-0.111946	6	-7.755693	-3.086344	0.118668
1	8.287302	-3.881438	0.248417	1	-8.108228	-4.043700	-0.254409

V_b			
E = -3377.8342203 Nimag = 0			
Tc = 0.750013			
6	-3.536999	0.371984	-0.806682
6	-4.830964	0.096309	-1.230337
6	-3.999925	0.973262	-1.976304
6	-4.845821	2.049957	-3.999439
1	-5.831367	1.789278	-3.616650
6	-2.497556	2.400262	-3.225789
1	-2.625223	3.483531	-3.307622
6	-7.074623	-0.447264	-2.051564
1	-7.427993	-1.455793	-2.282866
6	-6.220537	-1.377614	0.099180
1	-5.364787	-1.334031	0.774240
6	-2.057202	1.543547	1.304174
6	-1.416750	2.737879	1.628123
6	-2.615815	2.344746	2.292212
6	-4.630855	1.571599	3.382830
1	-5.595171	2.023237	3.129669
6	-3.624546	3.760373	4.026217
1	-2.894835	4.495823	3.694089
6	0.563417	3.399702	0.388935
1	0.582687	4.290174	-0.246244
6	-0.297918	4.817920	2.250654
1	-0.976407	4.801694	3.101398
6	-2.462550	-1.318080	1.241899
6	-2.604487	-2.705643	1.192587
6	-2.145424	-2.070226	2.373130
6	-1.528645	-3.406431	4.327207
1	-2.032973	-3.316329	5.293549
6	-1.152128	-0.943283	4.273037
1	-1.156547	-0.096178	3.589116
6	-3.082144	-3.730152	-0.955577
1	-2.419684	-4.454563	-1.437774
6	-2.877895	-5.134728	1.100606
1	-2.982552	-5.068406	2.182486
7	-3.813417	1.783914	-2.980394
7	-5.967335	-0.540487	-1.081552
7	-3.555198	2.554113	3.180895
7	-0.455157	3.597040	1.440202
7	-1.665292	-2.139651	3.586900
7	-2.863302	-3.786384	0.502562
15	-2.046580	0.104106	0.197192
1	-3.734080	-5.684877	0.701906
1	-1.959059	-5.671030	0.844272
1	-2.840006	-2.740399	-1.344239
1	-4.119094	-3.996553	-1.184109
1	-1.975831	-4.223441	3.764922
1	-0.468075	-3.617986	4.492577
1	-1.764277	-0.736101	5.156738
1	-0.120821	-1.128219	4.585994
1	0.729320	4.861430	2.622260

1	-0.493960	5.700822	1.634735
1	0.329054	2.515260	-0.200817
1	1.543168	3.260014	0.851989
1	-4.624369	4.195698	3.943594
1	-3.434214	3.495668	5.070761
1	-4.456197	0.698426	2.752527
1	-4.651749	1.263739	4.432857
1	-7.113772	-1.015646	0.618205
1	-6.392798	-2.413202	-0.210877
1	-6.729079	0.017715	-2.972699
1	-7.899777	0.132548	-1.626290
1	-1.815916	2.154333	-2.412658
1	-2.080763	2.005530	-4.156303
1	-4.630562	1.479432	-4.908301
1	-4.836214	3.116679	-4.236009
78	-0.107590	-0.358381	-0.908884
17	0.927644	-0.018290	1.237138
17	-1.270030	-0.859196	-2.936166
6	1.951951	0.147198	-2.454720
1	1.338584	0.460985	-3.294126
6	1.788722	-1.158590	-1.923911
6	2.826888	-1.695377	-1.065532
6	3.926693	-0.881899	-0.687872
6	2.784132	-3.070554	-0.711538
6	5.125585	-1.550193	-0.206955
6	3.805320	0.556472	-0.900424
6	3.836680	-3.657442	-0.064140
1	1.909226	-3.653362	-0.987922
6	5.045380	-2.937484	0.155797
6	2.917247	1.022748	-1.926527
6	4.498572	1.568919	-0.132542
1	3.800052	-4.708412	0.209707
6	2.994242	2.374747	-2.403854
1	1.244003	-1.885700	-2.523867
6	4.555035	2.914678	-0.632724
6	3.834541	3.271230	-1.820115
1	2.384000	2.653972	-3.258904
1	3.932891	4.280971	-2.208779
6	6.195453	-3.611557	0.638525
6	7.416614	-2.975803	0.690653
1	8.297344	-3.504602	1.041346
1	6.105109	-4.655361	0.926302
6	7.525939	-1.644059	0.235558
1	8.498775	-1.162575	0.209957
6	6.413221	-0.950534	-0.196408
1	6.540613	0.058965	-0.564648
6	5.058028	1.317366	1.150636
1	4.953953	0.333630	1.590031
6	5.717182	2.306326	1.852122
6	5.862123	3.597378	1.301134
1	6.413624	4.359998	1.842841
1	6.131871	2.087588	2.831408
6	5.278046	3.895349	0.084480
1	5.353727	4.896972	-0.329909

I_c E = -3074.5681265 Nimag = 0 Tc = 0.570397	TSI_c E = -3074.5681265 Nimag = 1 (-227.55) Tc = 0.571162
6 -3.488898 -0.624963 0.003133	6 -3.424681 1.095436 -0.097072

6	-4.313940	-0.825296	-1.090260	6	-3.343180	2.445118	0.196325
6	-4.177038	-1.820553	-0.101714	6	-3.871633	2.009896	-1.034204
6	-5.227020	-4.006318	-0.341569	6	-4.504583	3.586549	-2.780084
1	-5.955597	-4.458508	0.337828	1	-5.496003	3.705569	-3.227245
6	-3.707858	-3.494007	1.572923	6	-4.593760	1.120300	-3.158247
1	-3.365474	-2.644829	2.163580	1	-4.680503	0.187945	-2.601221
6	-4.257707	0.886002	-2.806054	6	-2.186412	3.013232	2.248024
1	-3.887199	0.698207	-3.818360	1	-1.238865	3.560737	2.257060
6	-5.745729	-1.103577	-3.048405	6	-3.159030	4.803381	0.804396
1	-6.154358	-1.939763	-2.481630	1	-3.838247	4.948845	-0.035472
7	-4.433845	-3.013536	0.386681	7	-4.379455	2.237472	-2.225492
7	-4.765166	-0.375611	-2.240074	7	-2.939706	3.374793	1.035458
15	-2.039994	0.287903	0.608449	15	-2.723477	-0.533179	0.289356
1	-6.564772	-0.429627	-3.319017	1	-3.605524	5.251835	1.697716
1	-5.277808	-1.479094	-3.964857	1	-2.208306	5.305627	0.594099
1	-3.434430	1.271949	-2.204560	1	-1.965960	1.945613	2.256271
1	-5.065604	1.623884	-2.850210	1	-2.764999	3.280714	3.138428
1	-5.759512	-3.531176	-1.164955	1	-4.381277	4.329342	-1.992176
1	-4.575616	-4.791305	-0.741854	1	-3.743082	3.751221	-3.550825
1	-4.387807	-4.103464	2.174356	1	-5.518908	1.300011	-3.712975
1	-2.841366	-4.089323	1.267980	1	-3.750777	1.043645	-3.852484
78	-0.441109	-0.219024	-0.990804	78	-0.428935	-0.199689	-0.101421
17	-0.631177	-2.544442	-0.394409	17	-0.958290	0.399869	-2.376156
17	-0.400610	1.997179	-1.847702	17	0.157115	-0.526346	2.176747
6	0.901063	-0.651242	-2.613203	6	1.921042	1.098838	-0.829160
1	0.550093	-0.424818	-3.605763	1	1.722009	2.122841	-1.073690
6	1.935804	-0.999897	-2.003141	6	1.626972	-0.105624	-0.499804
6	3.025165	-1.490610	-1.266092	6	2.614081	-1.173968	-0.363612
6	3.991842	-0.608875	-0.737869	6	3.941669	-0.754171	-0.488413
6	3.135209	-2.908866	-1.076859	6	2.302058	-2.535383	-0.131851
6	5.095317	-1.152097	-0.017279	6	5.004898	-1.699297	-0.404738
6	3.855447	0.865211	-0.942185	6	4.172674	0.699864	-0.745087
6	4.189561	-3.427170	-0.379523	6	3.313633	-3.460510	-0.040081
1	2.359520	-3.545107	-1.487533	1	1.263925	-2.825993	-0.017533
6	5.194559	-2.575920	0.163331	6	4.675965	-3.079034	-0.173701
6	4.252194	1.423125	-2.143898	6	4.022386	1.183634	-2.054811
6	3.319097	1.702111	0.091430	6	4.652274	1.593138	0.285060
1	4.276691	-4.500115	-0.232212	1	3.081636	-4.506637	0.141442
6	4.146371	2.814076	-2.375341	6	4.323807	2.527198	-2.385810
1	4.661565	0.783034	-2.920713	1	3.713479	0.492124	-2.832917
6	3.211552	3.111213	-0.152697	6	4.947443	2.951400	-0.063335
6	3.637463	3.639143	-1.400353	6	4.773497	3.385073	-1.410429
1	4.470714	3.222449	-3.327833	1	4.209842	2.863428	-3.411602
1	3.552043	4.708970	-1.572335	1	5.017138	4.415538	-1.657561
6	6.298223	-3.103644	0.878115	6	5.726286	-4.031149	-0.084193
6	7.268618	-2.270976	1.393190	6	7.041528	-3.648815	-0.219382
1	8.110385	-2.689924	1.937079	1	7.834677	-4.387514	-0.149734
1	6.368802	-4.179890	1.010736	1	5.470450	-5.072758	0.092374
6	7.179711	-0.869528	1.212315	6	7.366710	-2.290068	-0.452479
1	7.954578	-0.225196	1.616619	1	8.407342	-1.998370	-0.561485
6	6.121591	-0.322848	0.523396	6	6.375753	-1.339084	-0.542923
1	6.059575	0.749921	0.379572	1	6.636002	-0.300840	-0.722815
6	2.877936	1.195849	1.345687	6	4.835625	1.174567	1.625261
1	2.955741	0.131453	1.544767	1	4.607416	0.149167	1.895194
6	2.367170	2.036637	2.310810	6	5.294319	2.060514	2.580281
6	2.268736	3.429069	2.071177	6	5.590514	3.398741	2.237650
1	1.876699	4.083577	2.844928	1	5.955547	4.082105	2.998754
1	2.042929	1.630346	3.265055	1	5.430263	1.725028	3.604176
6	2.680756	3.949713	0.864864	6	5.418786	3.834940	0.940737
1	2.610970	5.017466	0.672284	1	5.645443	4.862898	0.669655

6	-2.650720	1.999059	0.802730	6	-3.367627	-0.874449	1.968301
6	-4.016271	2.321640	0.797481	6	-4.425393	-0.148358	2.537994
6	-1.698437	3.005431	1.033080	6	-2.811182	-1.953982	2.673622
6	-4.425634	3.638291	1.016746	6	-4.917349	-0.495962	3.797399
1	-4.766026	1.553118	0.630885	1	-4.876551	0.682806	2.003259
6	-2.116601	4.315540	1.259134	6	-3.313205	-2.300519	3.926972
1	-0.638591	2.772695	1.019208	1	-1.977876	-2.507739	2.255468
6	-3.476513	4.634993	1.248002	6	-4.362632	-1.572205	4.491696
1	-5.484241	3.881642	1.010423	1	-5.736300	0.070967	4.230887
1	-1.375279	5.089842	1.431800	1	-2.874912	-3.134327	4.466958
1	-3.795905	5.659096	1.418020	1	-4.746757	-1.842384	5.471032
6	-1.773587	-0.307644	2.321307	6	-3.606568	-1.715525	-0.797160
6	-2.746560	-0.064492	3.307229	6	-4.979267	-1.959567	-0.610848
6	-0.580176	-0.957291	2.665404	6	-2.903461	-2.415095	-1.788884
6	-2.533305	-0.489587	4.617415	6	-5.641265	-2.877572	-1.424079
1	-3.659322	0.469786	3.058849	1	-5.525722	-1.449756	0.177512
6	-0.370136	-1.370997	3.982981	6	-3.572588	-3.340886	-2.592623
1	0.167546	-1.148462	1.904587	1	-1.847363	-2.223218	-1.939326
6	-1.343946	-1.142780	4.956079	6	-4.937486	-3.569742	-2.414958
1	-3.287963	-0.300375	5.375351	1	-6.701273	-3.062845	-1.276263
1	0.555642	-1.874791	4.244971	1	-3.022786	-3.881471	-3.357343
1	-1.176610	-1.466363	5.979449	1	-5.453713	-4.291613	-3.041405

Π_c E = -3074.5709825 Nimag = 0 Tc = 0.576077				$TS2_c$ E = -3074.5521281 Nimag = 1 (-154.03) Tc = 0.574553			
6	-3.337174	1.225974	-0.045565	6	-3.360668	1.183978	0.097472
6	-3.163822	2.516316	0.421757	6	-3.497508	2.269761	-0.748145
6	-3.581148	2.285207	-0.901232	6	-3.461538	2.450538	0.644721
6	-3.839609	4.110434	-2.492791	6	-3.212228	2.614894	3.038302
1	-4.734965	4.383199	-3.059112	1	-3.824705	3.130502	3.783330
6	-4.124652	1.730165	-3.185413	6	-3.432777	4.670580	1.641605
1	-4.365479	0.754619	-2.764180	1	-3.712032	5.001269	0.641148
6	-2.223540	2.722394	2.643217	6	-3.296817	1.797319	-3.114870
1	-1.186604	3.052991	2.761935	1	-3.065184	0.797994	-2.746626
6	-2.801053	4.758154	1.320086	6	-3.735422	4.122808	-2.321224
1	-3.362755	5.073164	0.440848	1	-4.055903	4.675420	-1.437916
7	-3.923786	2.702771	-2.101025	7	-3.475860	3.210461	1.719952
7	-2.786536	3.297800	1.412008	7	-3.535228	2.712859	-1.988523
15	-2.838962	-0.504557	0.194739	15	-2.750432	-0.522798	0.216577
1	-3.283010	5.173047	2.210990	1	-2.808664	4.562085	-2.707701
1	-1.778898	5.148018	1.256251	1	-4.512663	4.208401	-3.087530
1	-2.238621	1.633965	2.591556	1	-2.445380	2.157664	-3.701197
1	-2.809420	3.056442	3.505630	1	-4.183708	1.757980	-3.756135
1	-3.777360	4.743586	-1.607858	1	-4.138195	5.093926	2.362885
1	-2.955467	4.279061	-3.118307	1	-2.424744	5.035271	1.871354
1	-4.954192	2.069770	-3.811993	1	-3.475032	1.557605	3.022405
1	-3.214153	1.643943	-3.787544	1	-2.151257	2.712620	3.290341
78	-0.389518	-0.360218	0.093485	78	-0.438415	-0.310851	-0.429793
17	-0.632159	0.807458	-2.011440	17	-0.174566	1.393803	1.265740
17	-0.105571	-1.347842	2.235766	17	-0.625625	-1.827162	-2.257532
6	2.306259	0.998705	-0.257680	6	1.993247	0.946314	-1.520170
1	1.929765	1.943125	0.113173	1	1.401304	1.815811	-1.774907
6	1.571385	-0.235075	-0.084574	6	1.540104	-0.128438	-0.861866
6	2.507786	-1.321317	-0.089882	6	2.520637	-1.167549	-0.456636
6	3.826436	-0.833299	-0.212448	6	3.873513	-0.795048	-0.380073
6	2.244995	-2.721239	-0.051895	6	2.152777	-2.488703	-0.119917
6	4.919236	-1.717081	-0.377131	6	4.891421	-1.742911	-0.049269
6	3.800565	0.665575	-0.284417	6	4.142450	0.612788	-0.730164

6	3.296394	-3.592592	-0.148599	6	3.109071	-3.416067	0.238655
1	1.225776	-3.068380	0.071091	1	1.104815	-2.760114	-0.157844
6	4.638794	-3.129884	-0.317419	6	4.484455	-3.084847	0.272865
6	3.167830	1.132677	-1.588250	6	3.532406	1.035575	-1.992874
6	4.746855	1.580313	0.408303	6	4.784494	1.553837	0.109549
1	3.125891	-4.664833	-0.105993	1	2.811252	-4.429952	0.493268
6	3.510323	2.468442	-2.074190	6	3.866066	2.394053	-2.471786
1	2.919887	0.380259	-2.330691	1	3.646738	0.282197	-2.782794
6	4.944873	2.887300	-0.108710	6	5.032284	2.880603	-0.394731
6	4.316862	3.285509	-1.359939	6	4.575812	3.254817	-1.711854
1	3.128017	2.771647	-3.044287	1	3.495785	2.685187	-3.451056
1	4.560881	4.272927	-1.744902	1	4.808525	4.254577	-2.068097
6	5.716389	-4.040147	-0.441859	6	5.472996	-4.052064	0.602607
6	7.005342	-3.589316	-0.639364	6	6.809617	-3.730840	0.591293
1	7.819000	-4.302129	-0.737864	1	7.556374	-4.479474	0.838115
1	5.510331	-5.105678	-0.387489	1	5.148693	-5.059276	0.850854
6	7.277528	-2.202954	-0.724313	6	7.216232	-2.420373	0.238084
1	8.295093	-1.864257	-0.894280	1	8.274565	-2.177182	0.208465
6	6.259219	-1.285742	-0.594354	6	6.287244	-1.454613	-0.076801
1	6.470530	-0.224464	-0.661010	1	6.625506	-0.464100	-0.361732
6	5.397845	1.200576	1.587731	6	5.183364	1.229218	1.438602
1	5.245590	0.202126	1.986197	1	4.959170	0.242748	1.826285
6	6.231985	2.095133	2.257478	6	5.832728	2.158893	2.222441
6	6.429736	3.385382	1.754070	6	6.104105	3.444166	1.708213
1	7.080088	4.081374	2.275468	1	6.621706	4.170284	2.328740
1	6.725873	1.785407	3.173793	1	6.129651	1.907564	3.235517
6	5.792638	3.772936	0.580668	6	5.707373	3.799185	0.426394
1	5.947142	4.771934	0.180550	1	5.907610	4.798409	0.050514
6	-3.741650	-0.972045	1.719369	6	-3.983537	-1.450885	-0.775056
6	-4.803715	-0.214769	2.240320	6	-5.236227	-0.924734	-1.130972
6	-3.371900	-2.168976	2.355263	6	-3.660760	-2.767340	-1.143376
6	-5.481095	-0.644909	3.382393	6	-6.149242	-1.701513	-1.846087
1	-5.114616	0.706167	1.755016	1	-5.510266	0.087261	-0.845640
6	-4.059399	-2.597032	3.490560	6	-4.581296	-3.541120	-1.849721
1	-2.538672	-2.751778	1.979193	1	-2.686608	-3.176422	-0.900628
6	-5.110256	-1.836629	4.007670	6	-5.823209	-3.010827	-2.204458
1	-6.301110	-0.052000	3.775666	1	-7.115658	-1.285132	-2.116315
1	-3.764029	-3.521732	3.977119	1	-4.320550	-4.556543	-2.132790
1	-5.638470	-2.171282	4.895765	1	-6.534764	-3.615154	-2.759772
6	-3.677009	-1.425332	-1.154284	6	-3.101308	-1.008417	1.954238
6	-5.066023	-1.642279	-1.133318	6	-2.027779	-1.218894	2.832710
6	-2.907322	-1.949872	-2.204088	6	-4.417982	-1.202363	2.407156
6	-5.676066	-2.360272	-2.160862	6	-2.272361	-1.607800	4.151861
1	-5.666659	-1.268365	-0.309254	1	-1.011874	-1.063724	2.486298
6	-3.525480	-2.672981	-3.226696	6	-4.654606	-1.583890	3.727037
1	-1.836281	-1.780493	-2.225273	1	-5.255327	-1.073596	1.727378
6	-4.906033	-2.876449	-3.207875	6	-3.581506	-1.787318	4.600360
1	-6.749131	-2.527404	-2.138338	1	-1.436677	-1.771587	4.826087
1	-2.924335	-3.079050	-4.034951	1	-5.674173	-1.734081	4.070605
1	-5.383087	-3.443070	-4.002534	1	-3.768418	-2.092841	5.626056

III_c E = -3074.5659039 Nimag = 0 Tc = 0.576788	TS3_c E = -3074.5561176 Nimag = 1 (-929.98) Tc = 0.575077						
6	-3.317074	1.224304	-0.150769	6	-3.781785	-0.077987	0.934994
6	-3.232099	2.279979	-1.040696	6	-3.946314	0.403859	2.222781
6	-3.441803	2.515917	0.330007	6	-4.365919	-0.894222	1.884883
6	-3.632726	2.766471	2.721550	6	-4.929794	-3.158022	1.227093
1	-4.323000	3.362241	3.324915	1	-4.272556	-3.974725	1.545719

6	-3.460789	4.772221	1.244960	6	-5.309369	-2.392721	3.565405
1	-3.523273	5.074972	0.199812	1	-5.285740	-1.501567	4.191122
6	-2.640491	1.706270	-3.317957	6	-2.959428	2.550445	2.684099
1	-2.583897	0.702916	-2.896265	1	-2.947129	2.645629	1.598328
6	-3.057071	4.082444	-2.679594	6	-4.081700	1.254418	4.496610
1	-3.491367	4.687949	-1.884257	1	-4.446175	2.209743	4.883576
7	-3.603976	3.319812	1.358840	7	-4.876004	-2.066430	2.206771
7	-3.018682	2.675730	-2.278366	7	-3.791719	1.399642	3.068920
15	-2.837289	-0.504065	0.136901	15	-2.828899	0.104111	-0.603195
1	-2.047321	4.445335	-2.902195	1	-4.857433	0.503077	4.647840
1	-3.676092	4.187056	-3.576338	1	-3.178337	0.965640	5.046673
1	-1.658527	1.971235	-3.722949	1	-1.934834	2.405256	3.041178
1	-3.379580	1.724111	-4.125639	1	-3.388496	3.456607	3.120278
1	-4.264682	5.260990	1.803161	1	-6.331610	-2.784483	3.541744
1	-2.495322	5.091640	1.653813	1	-4.648514	-3.150724	4.000711
1	-3.979093	1.733736	2.691171	1	-5.955907	-3.533651	1.155694
1	-2.630492	2.794502	3.161450	1	-4.608168	-2.798352	0.250495
78	-0.399200	-0.414267	-0.118932	78	-0.486372	-0.123797	-0.113021
17	-0.375078	1.340989	1.541761	17	-0.031656	-0.036391	-2.457275
17	-0.385754	-1.977489	-1.913149	17	-0.803779	-0.335003	2.264564
6	2.302388	0.897469	-0.557251	6	1.959219	-1.522100	0.702689
1	1.888717	1.880658	-0.373147	1	1.285915	-2.290188	1.065404
6	1.567003	-0.304100	-0.227770	6	1.510947	-0.306448	0.217374
6	2.510111	-1.352853	0.034595	6	2.481458	0.723239	0.003129
6	3.830068	-0.858547	-0.051221	6	3.887494	0.498625	0.217250
6	2.259641	-2.730180	0.300896	6	2.047574	2.029897	-0.398811
6	4.942351	-1.726285	0.055645	6	4.753130	1.664271	0.360926
6	3.795854	0.600613	-0.402336	6	4.360064	-0.857430	0.296619
6	3.324600	-3.572956	0.473463	6	2.911495	3.079120	-0.471408
1	1.237486	-3.086570	0.348693	1	0.999744	2.150838	-0.644863
6	4.672216	-3.110934	0.352869	6	4.264742	2.948049	-0.028507
6	3.269213	0.802718	-1.817268	6	3.418674	-1.843189	0.773828
6	4.668241	1.653119	0.182198	6	5.661245	-1.346657	-0.133389
1	3.161333	-4.625686	0.687254	1	2.564199	4.055283	-0.799715
6	3.643248	2.031935	-2.516381	6	3.845118	-3.198757	1.078767
1	3.097473	-0.083817	-2.421209	1	2.884733	-1.376330	1.765861
6	4.895073	2.847229	-0.550971	6	6.047265	-2.688294	0.184929
6	4.376199	2.988638	-1.903172	6	5.122704	-3.573217	0.841857
1	3.354376	2.136686	-3.558268	1	3.115112	-3.889378	1.490558
1	4.646443	3.891363	-2.446135	1	5.451060	-4.582378	1.074712
6	5.765985	-3.998006	0.501536	6	5.095057	4.086766	0.101892
6	7.063221	-3.555802	0.342905	6	6.348118	3.987846	0.671414
1	7.889810	-4.251584	0.454586	1	6.972283	4.869844	0.780470
1	5.566335	-5.040657	0.733456	1	4.712433	5.049763	-0.225715
6	7.328049	-2.202225	0.024805	6	6.798320	2.740364	1.148487
1	8.353669	-1.872903	-0.111937	1	7.759321	2.666959	1.649103
6	6.292855	-1.305606	-0.113951	6	6.020476	1.608742	0.995368
1	6.499253	-0.269933	-0.359089	1	6.382113	0.665485	1.386205
6	5.220090	1.516909	1.461285	6	6.525859	-0.597009	-0.971028
1	5.047037	0.605467	2.025293	1	6.221993	0.384954	-1.308587
6	5.982373	2.542736	2.018794	6	7.741049	-1.105460	-1.389470
6	6.207554	3.722752	1.301891	6	8.155246	-2.389492	-0.988403
1	6.801637	4.521145	1.736370	1	9.118580	-2.776362	-1.306878
1	6.398615	2.421721	3.014605	1	8.374330	-0.510471	-2.040639
6	5.669610	3.868361	0.028288	6	7.310259	-3.169906	-0.221886
1	5.845654	4.779985	-0.537252	1	7.594565	-4.182540	0.051215
6	-3.918483	-1.421894	-1.023469	6	-3.416001	1.737108	-1.209038
6	-5.057538	-0.854839	-1.617834	6	-4.661655	2.274320	-0.839742
6	-3.606987	-2.768266	-1.275376	6	-2.590397	2.454879	-2.090535
6	-5.870235	-1.621883	-2.454111	6	-5.073062	3.509844	-1.341455

1	-5.321463	0.181327	-1.424971	1	-5.315411	1.732781	-0.161385
6	-4.428480	-3.531017	-2.104844	6	-3.012838	3.686598	-2.593204
1	-2.717435	-3.212472	-0.842849	1	-1.630904	2.042663	-2.387304
6	-5.557243	-2.960560	-2.696892	6	-4.249064	4.217033	-2.219540
1	-6.749578	-1.174723	-2.909037	1	-6.037070	3.916344	-1.048811
1	-4.178228	-4.570162	-2.296200	1	-2.370387	4.231979	-3.278411
1	-6.191032	-3.557158	-3.346596	1	-4.570932	5.177719	-2.611210
6	-3.493258	-0.896333	1.805750	6	-3.576155	-1.165657	-1.698082
6	-2.594401	-1.113392	2.861124	6	-4.863279	-1.018013	-2.240755
6	-4.875826	-1.014213	2.032781	6	-2.828884	-2.318392	-1.985702
6	-3.077475	-1.433604	4.132060	6	-5.401270	-2.022104	-3.044823
1	-1.527661	-1.017725	2.690455	1	-5.438593	-0.116305	-2.052681
6	-5.350068	-1.327530	3.305584	6	-3.374779	-3.321067	-2.790077
1	-5.579231	-0.879810	1.216039	1	-1.819277	-2.413494	-1.598588
6	-4.450885	-1.538006	4.355907	6	-4.658994	-3.175156	-3.317411
1	-2.376875	-1.602909	4.944453	1	-6.394693	-1.900253	-3.467038
1	-6.419042	-1.419324	3.475295	1	-2.788323	-4.206630	-3.016964
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IV_c E = -3074.606658 Nimag = 0 Tc = 0.576675				TS4_c E = -3074.5809796 Nimag = 1(-906.31) Tc = 0.575310			
6	-3.748882	0.042262	0.972161	6	-3.797615	-0.012177	0.894524
6	-3.913020	0.710895	2.173753	6	-4.019478	0.570652	2.130997
6	-4.292882	-0.636812	2.046342	6	-4.425449	-0.752341	1.878584
6	-4.798190	-2.988753	1.750230	6	-4.981606	-3.056857	1.372932
1	-4.115739	-3.731634	2.177634	1	-6.008867	-3.426263	1.287945
6	-5.163201	-1.888836	3.953651	6	-5.447436	-2.113411	3.629407
1	-5.161591	-0.912638	4.436519	1	-5.413637	-1.183633	4.195375
6	-2.997723	2.935996	2.291974	6	-3.059041	2.754346	2.471295
1	-2.990400	2.862151	1.204549	1	-2.959569	2.742727	1.386151
6	-4.064828	1.895725	4.292641	6	-4.288453	1.609573	4.315442
1	-4.471016	2.883150	4.527818	1	-5.060709	0.858535	4.483518
7	-4.760181	-1.760026	2.552722	7	-4.953076	-1.894639	2.269387
7	-3.782700	1.827508	2.857368	7	-3.902741	1.629036	2.902957
15	-2.845184	0.006305	-0.604583	15	-2.803901	0.054153	-0.627447
1	-4.806044	1.144099	4.565435	1	-3.421060	1.393598	4.950044
1	-3.149349	1.736956	4.874470	1	-4.693649	2.588375	4.586040
1	-1.968126	2.888685	2.660899	1	-2.065032	2.667909	2.921713
1	-3.461645	3.881606	2.585442	1	-3.533130	3.689991	2.780442
1	-6.171519	-2.311904	4.008319	1	-6.481051	-2.473143	3.593348
1	-4.470756	-2.550482	4.485982	1	-4.828593	-2.861046	4.137788
1	-5.815027	-3.394945	1.754099	1	-4.616876	-2.775055	0.386041
1	-4.499476	-2.773158	0.725198	1	-4.348660	-3.853229	1.779517
78	-0.453635	-0.128096	-0.140802	78	-0.500562	-0.135299	-0.056884
17	-0.073512	-0.416461	-2.483548	17	0.047418	-0.271001	-2.373181
17	-0.735860	0.098958	2.238562	17	-0.863519	-0.139134	2.326373
6	1.988635	-1.481873	0.878771	6	2.034035	-1.522237	0.810398
1	1.381450	-2.355629	0.611414	1	1.329804	-2.297139	1.102325
6	1.513354	-0.280758	0.144693	6	1.517153	-0.289176	0.328001
6	2.460883	0.706997	-0.181045	6	2.500182	0.756732	0.044769
6	3.851469	0.498232	0.123758	6	3.890414	0.512010	0.205439
6	2.032438	1.986927	-0.682420	6	2.042657	2.051342	-0.332817
6	4.673699	1.668473	0.293417	6	4.768885	1.666005	0.310230
6	4.351467	-0.870693	0.281293	6	4.348206	-0.872428	0.313781
6	2.883663	3.045917	-0.732895	6	2.910448	3.098735	-0.455303
1	1.000079	2.077094	-0.999282	1	0.982959	2.176484	-0.524706
6	4.195934	2.939405	-0.175283	6	4.275427	2.953987	-0.074558
6	3.445361	-1.817969	0.770710	6	3.431274	-1.830465	0.809412

6	5.684685	-1.312200	-0.090618	6	5.652194	-1.361021	-0.094970
1	2.557132	4.005937	-1.122489	1	2.555548	4.076346	-0.770420
6	3.879781	-3.109885	1.146904	6	3.852731	-3.137853	1.193869
1	1.698645	-1.281756	1.929341	1	1.558940	-0.475013	1.586306
6	6.103328	-2.626403	0.301622	6	6.054946	-2.680733	0.298299
6	5.186931	-3.485709	0.966274	6	5.144893	-3.528464	0.999592
1	3.162112	-3.803995	1.576501	1	3.123066	-3.814318	1.630338
1	5.522228	-4.473939	1.270027	1	5.478769	-4.515890	1.305615
6	5.016109	4.082827	-0.034185	6	5.125363	4.086740	0.004254
6	6.231754	4.006831	0.615061	6	6.396275	3.982915	0.524863
1	6.843506	4.897020	0.730186	1	7.033759	4.859281	0.596384
1	4.657068	5.032749	-0.420514	1	4.738825	5.048648	-0.322199
6	6.667805	2.779348	1.161030	6	6.852005	2.736140	1.005372
1	7.598928	2.735130	1.717584	1	7.829398	2.662068	1.473181
6	5.912671	1.638834	0.996097	6	6.062397	1.610137	0.896783
1	6.252156	0.707444	1.430786	1	6.429931	0.671313	1.290581
6	6.564803	-0.567530	-0.921054	6	6.510142	-0.646589	-0.974285
1	6.248684	0.390242	-1.314422	1	6.192047	0.309933	-1.368000
6	7.808348	-1.054280	-1.267813	6	7.728219	-1.162482	-1.364641
6	8.249277	-2.311903	-0.800517	6	8.161982	-2.418337	-0.888065
1	9.236731	-2.676132	-1.067807	1	9.131744	-2.806795	-1.184915
1	8.450337	-0.465536	-1.916751	1	8.353469	-0.599961	-2.051601
6	7.403694	-3.084893	-0.038009	6	7.332570	-3.164772	-0.079491
1	7.706069	-4.075664	0.291147	1	7.631511	-4.155340	0.252713
6	-3.461311	1.526370	-1.430954	6	-3.349821	1.643875	-1.366649
6	-4.699457	2.111609	-1.112534	6	-4.603576	2.214703	-1.085157
6	-2.665462	2.100990	-2.436362	6	-2.485054	2.288194	-2.267322
6	-5.132653	3.253651	-1.787475	6	-4.984875	3.411097	-1.693767
1	-5.330126	1.680595	-0.339578	1	-5.287015	1.730518	-0.392753
6	-3.109923	3.239026	-3.111083	6	-2.877698	3.480862	-2.876701
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6	-4.338723	3.817863	-2.788309	6	-4.122590	4.044700	-2.591220
1	-6.090594	3.698601	-1.533549	1	-5.955299	3.844540	-1.469102
1	-2.490732	3.673072	-3.890693	1	-2.205354	3.969212	-3.576001
1	-4.678272	4.705207	-3.314739	1	-4.421470	4.974629	-3.066317
6	-3.606365	-1.417940	-1.476791	6	-3.529917	-1.286680	-1.646879
6	-4.921712	-1.367944	-1.967882	6	-4.813198	-1.176484	-2.207897
6	-2.846690	-2.586426	-1.641763	6	-2.778038	-2.453497	-1.854075
6	-5.474642	-2.482525	-2.596828	6	-5.342844	-2.230835	-2.950567
1	-5.507789	-0.458261	-1.876325	1	-5.391562	-0.265921	-2.082250
6	-3.407262	-3.699352	-2.272554	6	-3.315614	-3.506067	-2.598145
1	-1.817461	-2.611950	-1.298994	1	-1.771421	-2.521827	-1.454506
6	-4.719044	-3.649417	-2.747002	6	-4.595861	-3.396926	-3.143585
1	-6.490339	-2.437257	-2.979178	1	-6.333002	-2.138580	-3.387558
1	-2.811702	-4.597685	-2.406025	1	-2.725714	-4.402780	-2.763762
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6	-4.623748	0.653358	-1.063109				
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1	-5.485243	3.656205	-0.651599				
6	-6.167007	1.804804	-2.566120				
1	-6.465543	0.791982	-2.831704				
6	-4.107586	-3.128925	-1.102959				
1	-3.482108	-2.897038	-0.242029				

6	-5.871828	-2.130369	-2.555127
1	-6.542730	-1.272828	-2.607008
7	-5.137880	1.773493	-1.524601
7	-4.892843	-1.943274	-1.480919
15	-2.205914	0.039887	0.771567
1	-5.365379	-2.261462	-3.518215
1	-6.466526	-3.022130	-2.340119
1	-3.466660	-3.429115	-1.937688
1	-4.793994	-3.940820	-0.846405
1	-7.042333	2.354681	-2.204791
1	-5.776475	2.304765	-3.458951
1	-3.892996	2.941715	-0.288683
1	-4.213365	3.627526	-1.901244
78	-0.376769	-0.319903	-0.558615
17	0.932090	0.231473	1.343855
17	-1.651201	-0.893857	-2.513311
6	1.484507	-0.020897	-2.228868
1	0.794956	0.215696	-3.032453
6	1.525767	-1.313396	-1.699074
6	2.653709	-1.724402	-0.906653
6	3.703468	-0.810677	-0.641224
6	2.742030	-3.084898	-0.488876
6	4.980530	-1.373561	-0.228038
6	3.457594	0.609172	-0.890166
6	3.871281	-3.560612	0.109750
1	1.887540	-3.734325	-0.660961
6	5.035116	-2.740171	0.200959
6	2.437192	0.960422	-1.812976
6	4.140303	1.703788	-0.221039
1	3.929768	-4.591646	0.448324
6	2.328865	2.293865	-2.313327
1	0.891993	-2.089221	-2.119227
6	4.015329	3.031934	-0.744664
6	3.140266	3.284097	-1.844779
1	1.587910	2.496608	-3.082518
1	3.081626	4.291534	-2.248255
6	6.267270	-3.296335	0.628587
6	7.435857	-2.569638	0.560982
1	8.376789	-3.011466	0.875762
1	6.277510	-4.325969	0.977060
6	7.408665	-1.260633	0.035518
1	8.334979	-0.705598	-0.081659
6	6.215605	-0.680414	-0.344504
1	6.228680	0.317162	-0.763299
6	4.830330	1.549939	1.011163
1	4.850483	0.579015	1.488799
6	5.447253	2.617789	1.629825
6	5.414304	3.902077	1.045722
1	5.921980	4.732693	1.527665
1	5.954283	2.468189	2.578674
6	4.699658	4.102160	-0.115542
1	4.619646	5.095578	-0.549747
6	-2.564921	-1.259211	2.012120
6	-3.882999	-1.522796	2.428857
6	-1.503642	-1.993271	2.566638
6	-4.132485	-2.502765	3.389327
1	-4.716893	-0.967957	2.007504
6	-1.763911	-2.970699	3.528566
1	-0.484585	-1.789775	2.255829
6	-3.072699	-3.227490	3.940216

1	-5.152624	-2.698776	3.706607
1	-0.937655	-3.531807	3.954656
1	-3.268687	-3.990740	4.687677
6	-2.280305	1.676664	1.587296
6	-3.102493	1.898679	2.703236
6	-1.513440	2.729780	1.063584
6	-3.168052	3.168609	3.276770
1	-3.673778	1.085170	3.138831
6	-1.588926	3.998079	1.640710
1	-0.845527	2.547500	0.227660
6	-2.415420	4.218539	2.744944
1	-3.798061	3.333799	4.145858
1	-0.985647	4.806856	1.239198
1	-2.462481	5.203758	3.199862

I_d E = -3226.1714256 Nimag = 0 Tc = 0.656290	TSI_d E = -3226.1562606 Nimag = 1 (-198.66) Tc = 0.656511						
6	-3.934964	-0.072112	-0.558642	6	3.252864	-1.289384	0.953786
6	-4.770414	-0.910200	-1.288796	6	3.281100	-2.640043	1.278526
6	-4.709024	0.473004	-1.565942	6	3.758133	-1.666001	2.184617
6	-4.460653	2.834221	-2.025491	6	4.574864	0.066253	3.665219
1	-5.250391	3.574823	-1.864043	1	5.628439	0.160261	3.947637
6	-6.010941	1.447925	-3.395510	6	4.594156	-2.316025	4.392859
1	-6.404143	0.437391	-3.488367	1	4.234960	-3.301815	4.103341
6	-4.613930	-3.276620	-0.842503	6	2.336554	-4.176151	-0.326937
1	-5.403554	-3.971287	-0.545259	1	2.837054	-5.011518	-0.823488
6	-6.170261	-2.415495	-2.596188	6	3.291448	-5.018347	1.822150
1	-6.718558	-1.517486	-2.879311	1	3.969550	-4.730404	2.624500
6	-2.190307	1.617524	0.993408	6	3.021947	1.505655	0.356781
6	-2.080682	2.579784	1.987497	6	3.393824	2.813165	0.065953
6	-1.356487	2.708638	0.773557	6	2.551232	2.528598	1.168349
6	0.152396	4.591052	0.373549	6	1.701649	4.299461	2.621052
1	-0.005976	5.327886	-0.419959	1	1.737484	4.322045	3.713758
6	-0.056307	2.736162	-1.269406	6	0.894715	1.944451	2.838371
1	-0.543713	1.773357	-1.426936	1	0.993566	0.954422	2.391649
6	-3.219292	2.204856	4.095016	6	4.678070	3.211827	-1.946366
1	-2.628450	1.875983	4.956053	1	4.079205	3.483265	-2.821485
6	-1.819224	4.235910	3.768341	6	3.913028	5.121483	-0.536649
1	-1.317947	4.820095	2.999029	1	3.372696	5.355277	0.379020
7	-5.064210	1.521209	-2.275439	7	4.275776	-1.334142	3.347344
7	-5.231258	-2.114942	-1.506912	7	3.047993	-3.877765	0.928230
7	-0.504691	3.331248	0.002097	7	1.792822	2.903366	2.169905
7	-2.373941	3.003098	3.193679	7	3.996610	3.665873	-0.722154
15	-2.462199	-0.115765	0.498024	15	2.599195	-0.139354	-0.287964
1	-2.632886	4.831893	4.191642	1	4.921946	5.540334	-0.479726
1	-1.105836	3.990554	4.561829	1	3.385869	5.567630	-1.385806
1	-3.603716	1.331480	3.570695	1	4.811308	2.131251	-1.918852
1	-4.052150	2.821012	4.447468	1	5.654830	3.699548	-2.008806
1	-0.261982	4.976236	1.303476	1	2.541145	4.875894	2.234096
1	1.226831	4.418412	0.492553	1	0.759881	4.746153	2.286262
1	-0.287702	3.424701	-2.088729	1	1.131622	1.906149	3.906340
1	1.023658	2.569838	-1.226101	1	-0.142322	2.270822	2.712519
1	-5.630614	-2.810302	-3.463618	1	2.346203	-5.373930	2.245493
1	-6.886037	-3.163956	-2.247486	1	3.753625	-5.825638	1.248204

1	-4.067977	-2.949475	0.041696	1	2.354186	-3.303379	-0.979274
1	-3.919045	-3.766224	-1.531180	1	1.296989	-4.435907	-0.107853
1	-6.838814	2.142707	-3.223483	1	5.676094	-2.353197	4.556348
1	-5.502650	1.718003	-4.326757	1	4.101129	-2.024569	5.325285
1	-3.828900	2.784304	-1.138092	1	4.382695	0.691158	2.792460
1	-3.858031	3.138740	-2.888004	1	3.953508	0.400704	4.502929
78	-0.582280	-0.921400	-0.593023	78	0.286475	-0.170725	-0.503833
17	-1.831812	-1.677623	-2.484974	17	0.022972	-1.855414	1.162359
17	0.721247	-0.055693	1.234399	17	0.525407	1.652138	-2.041135
6	1.097135	-1.692179	-1.564796	6	-2.010214	-1.011545	-1.372560
1	0.877750	-1.995552	-2.586881	1	-1.937039	-1.965654	-1.851735
6	2.232250	-1.827769	-1.008914	6	-1.827586	0.036915	-0.689465
6	3.419445	-2.039697	-0.338526	6	-2.723311	1.063754	-0.184349
6	4.482038	-1.090329	-0.419780	6	-4.090962	0.774658	-0.281532
6	3.557582	-3.239343	0.449417	6	-2.272770	2.295982	0.353802
6	5.686977	-1.356434	0.285727	6	-5.045184	1.740775	0.163149
6	4.334641	0.112496	-1.286523	6	-4.515290	-0.521289	-0.893507
6	4.703502	-3.471023	1.147738	6	-3.180614	3.226503	0.795034
1	2.726977	-3.936110	0.475841	1	-1.207569	2.498751	0.370341
6	5.795075	-2.552342	1.085261	6	-4.577788	2.982202	0.716543
6	4.300132	-0.065975	-2.660660	6	-4.435884	-0.663939	-2.282501
6	4.254481	1.438231	-0.737449	6	-5.019234	-1.607334	-0.099264
1	4.810825	-4.367747	1.751044	1	-2.842538	4.178140	1.197552
6	4.220156	1.034340	-3.544010	6	-4.861687	-1.851499	-2.927412
1	4.375390	-1.069129	-3.070224	1	-4.099516	0.178955	-2.879942
6	4.177574	2.550049	-1.643352	6	-5.445723	-2.806377	-0.763066
6	4.166085	2.314900	-3.045489	6	-5.355182	-2.895435	-2.181721
1	4.220118	0.859091	-4.615447	1	-4.812942	-1.918497	-4.009954
1	4.124555	3.167071	-3.719167	1	-5.696469	-3.805422	-2.668520
6	6.999274	-2.809071	1.778642	6	-5.524449	3.943708	1.157353
6	8.067359	-1.938980	1.684299	6	-6.875664	3.702024	1.053330
1	8.988204	-2.153130	2.218693	1	-7.590739	4.446341	1.390585
1	7.076401	-3.709454	2.381228	1	-5.163133	4.880447	1.573734
6	7.978809	-0.775522	0.882653	6	-7.339626	2.483986	0.499909
1	8.833716	-0.111532	0.802685	1	-8.407428	2.305690	0.415780
6	6.820763	-0.492096	0.197372	6	-6.449905	1.527817	0.065145
1	6.762519	0.391670	-0.426517	1	-6.817251	0.600385	-0.360150
6	4.233859	1.702200	0.660435	6	-5.115628	-1.541523	1.315895
1	4.262633	0.873023	1.358984	1	-4.796549	-0.639579	1.827451
6	4.181187	2.993769	1.138443	6	-5.616533	-2.604399	2.038550
6	4.134997	4.091500	0.244246	6	-6.043108	-3.782136	1.383208
1	4.128223	5.106438	0.632803	1	-6.442163	-4.608174	1.964268
1	4.187116	3.171695	2.210119	1	-5.689462	-2.535567	3.119967
6	4.123289	3.870040	-1.115907	6	-5.956632	-3.879871	0.010865
1	4.094552	4.705798	-1.810871	1	-6.284198	-4.782119	-0.498811
6	-3.063721	-0.969684	1.996458	6	3.683356	-0.444451	-1.721812
6	-4.412231	-0.905448	2.395540	6	5.069930	-0.625098	-1.553467
6	-2.144501	-1.720788	2.748632	6	3.112484	-0.525924	-3.002461
6	-4.832189	-1.584754	3.538809	6	5.875375	-0.876144	-2.662268
1	-5.134071	-0.335555	1.816292	1	5.519684	-0.574474	-0.565146
6	-2.576192	-2.393123	3.893818	6	3.930294	-0.781008	-4.105809
1	-1.104537	-1.770773	2.442491	1	2.047310	-0.370698	-3.134184
6	-3.914035	-2.328001	4.288081	6	5.304958	-0.954959	-3.938201
1	-5.874271	-1.539949	3.841281	1	6.944387	-1.016547	-2.533073
1	-1.864869	-2.974193	4.472698	1	3.488622	-0.842049	-5.095630
1	-4.245471	-2.860263	5.174727	1	5.935495	-1.155286	-4.799323

Π_d E = -3226.1818209 Nimag = 0	TS_2d E = -3226.165082 Nimag = 1 (-106.54)
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Tc = 0.661647				Tc = 0.661196			
6	-3.297704	-1.361489	-0.894830	6	3.131688	-1.379928	1.046864
6	-3.253346	-2.704405	-1.250083	6	3.043606	-2.730110	1.362040
6	-3.855215	-1.750861	-2.098549	6	3.483247	-1.792207	2.318544
6	-4.884903	-0.051945	-3.482025	6	4.225192	-0.108713	3.891267
1	-5.961252	-0.023100	-3.681018	1	5.243674	-0.064010	4.290606
6	-4.786338	-2.414867	-4.263591	6	4.047157	-2.490109	4.596948
1	-4.348147	-3.380010	-4.015947	1	3.739063	-3.470079	4.237044
6	-2.091152	-4.201954	0.246438	6	2.155246	-4.177113	-0.349333
1	-2.511984	-5.060111	0.777283	1	2.571059	-5.093623	-0.775230
6	-3.142838	-5.065161	-1.848329	6	2.826856	-5.104951	1.872180
1	-3.923919	-4.822103	-2.568026	1	3.438087	-4.873232	2.743823
6	-3.268068	1.419087	-0.182908	6	3.142906	1.416289	0.414495
6	-3.738487	2.660022	0.230614	6	3.640409	2.679690	0.116687
6	-2.990740	2.533127	-0.962476	6	2.716526	2.498849	1.170316
6	-2.482523	4.465352	-2.368344	6	1.946672	4.371717	2.535528
1	-2.601001	4.552488	-3.451877	1	1.900101	4.421362	3.627057
6	-1.474325	2.225157	-2.823891	6	0.920046	2.103243	2.745745
1	-1.426841	1.207953	-2.433406	1	0.954250	1.101105	2.316527
6	-4.859850	2.801652	2.371268	6	5.081709	2.912077	-1.814340
1	-4.212800	3.079272	3.209547	1	5.138458	1.826861	-1.740121
6	-4.421223	4.861069	1.035583	6	4.371029	4.920080	-0.519149
1	-4.007677	5.201540	0.087792	1	3.805957	5.222558	0.361005
7	-4.470735	-1.433370	-3.217995	7	3.899620	-1.491862	3.531462
7	-2.915208	-3.930689	-0.943583	7	2.772333	-3.949326	0.968950
7	-2.391331	3.042846	-2.012359	7	1.939982	2.962789	2.121747
7	-4.344340	3.397036	1.127723	7	4.361294	3.457693	-0.652624
15	-2.587889	-0.196130	0.300813	15	2.594901	-0.198436	-0.222690
1	-5.466010	5.176986	1.109405	1	5.402813	5.271402	-0.425239
1	-3.851366	5.310491	1.855112	1	3.917017	5.372822	-1.406560
1	-4.888554	1.716751	2.279447	1	6.092032	3.330512	-1.832191
1	-5.869774	3.180017	2.552723	1	4.558951	3.187172	-2.736067
1	-3.349040	4.919012	-1.888101	1	2.865329	4.856424	2.206115
1	-1.572573	4.994148	-2.065815	1	1.081448	4.897776	2.118493
1	-1.812142	2.219799	-3.865160	1	1.086587	2.063245	3.827168
1	-0.468051	2.652809	-2.777892	1	-0.073903	2.518131	2.551028
1	-2.217965	-5.321244	-2.376058	1	1.817374	-5.382909	2.193672
1	-3.469729	-5.926307	-1.259932	1	3.279932	-5.947832	1.343804
1	-2.091282	-3.332525	0.902952	1	2.379204	-3.340275	-1.011195
1	-1.062578	-4.414542	-0.058496	1	1.070407	-4.264925	-0.240114
1	-5.871404	-2.520546	-4.365390	1	5.090966	-2.535454	4.924129
1	-4.368927	-2.076553	-5.217026	1	3.416937	-2.214566	5.448659
1	-4.666707	0.569865	-2.613175	1	4.161182	0.525863	3.006734
1	-4.353612	0.337425	-4.357228	1	3.529889	0.254213	4.656258
78	-0.183575	-0.032697	0.214145	78	0.235883	-0.078481	-0.522843
17	-0.014446	-1.783032	-1.407202	17	-0.200582	-1.822992	1.054450
17	-0.404147	1.820372	1.724805	17	0.657168	1.776636	-1.999371
6	2.624122	-0.980967	0.733172	6	-2.332987	-0.893309	-1.655735
1	2.300664	-2.013006	0.702931	1	-1.855863	-1.820474	-1.946384
6	1.800276	0.098163	0.265438	6	-1.758853	0.054025	-0.889880
6	2.640284	1.188504	-0.125943	6	-2.624649	1.127104	-0.352267
6	4.000445	0.822385	0.003111	6	-3.991195	0.832387	-0.290534
6	2.279627	2.502946	-0.543842	6	-2.167129	2.392191	0.081474
6	5.036620	1.759880	-0.214035	6	-4.946725	1.798956	0.136528
6	4.092503	-0.580576	0.528728	6	-4.355291	-0.505158	-0.831159
6	3.269739	3.405266	-0.822085	6	-3.061916	3.338162	0.534414
1	1.231873	2.772271	-0.609223	1	-1.107068	2.609506	0.021033
6	4.653138	3.073898	-0.667122	6	-4.454679	3.081457	0.571287
6	3.616111	-0.643471	1.966023	6	-3.847359	-0.744887	-2.182983
6	5.038165	-1.625145	0.054469	6	-5.014535	-1.528470	-0.113524

1	3.021645	4.412112	-1.147145	1	-2.708636	4.314474	0.856970
6	4.088898	-1.736842	2.804189	6	-4.308140	-1.975955	-2.860762
1	3.354906	0.291166	2.453756	1	-3.881305	0.139688	-2.827920
6	5.375850	-2.694079	0.927417	6	-5.383576	-2.735208	-0.810636
6	4.890799	-2.704135	2.296043	6	-5.026459	-2.909114	-2.199338
1	3.822923	-1.731526	3.856872	1	-4.034350	-2.113014	-3.902974
1	5.239617	-3.506335	2.941732	1	-5.356929	-3.814388	-2.700920
6	5.667105	4.023810	-0.931009	6	-5.380690	4.065048	1.011606
6	6.997881	3.710029	-0.736876	6	-6.733278	3.816595	1.004007
1	7.763831	4.453241	-0.937491	1	-7.431807	4.578758	1.335369
1	5.383587	5.013019	-1.279768	1	-4.999330	5.027275	1.343015
6	7.374342	2.429465	-0.267488	6	-7.222094	2.566646	0.548392
1	8.423834	2.203939	-0.105700	1	-8.292692	2.385896	0.528178
6	6.417196	1.472808	-0.012738	6	-6.356571	1.584282	0.125406
1	6.709857	0.493876	0.349240	1	-6.753970	0.640427	-0.231501
6	5.554861	-1.608263	-1.245910	6	-5.349090	-1.386285	1.263706
1	5.299250	-0.793015	-1.915808	1	-5.052277	-0.484104	1.785918
6	6.394654	-2.630320	-1.686636	6	-6.039567	-2.382768	1.921062
6	6.730338	-3.687202	-0.832183	6	-6.416552	-3.551836	1.227152
1	7.385324	-4.480973	-1.177812	1	-6.966902	-4.329248	1.749274
1	6.788597	-2.602652	-2.698172	1	-6.293971	-2.271566	2.970092
6	6.226200	-3.714578	0.462338	6	-6.091699	-3.725976	-0.112197
1	6.487540	-4.528830	1.133007	1	-6.382949	-4.635423	-0.629426
6	-3.435744	-0.660116	1.850152	6	3.716171	-0.592009	-1.611537
6	-4.794408	-1.028368	1.868218	6	5.069419	-0.920755	-1.405528
6	-2.691377	-0.661404	3.041542	6	3.187964	-0.577765	-2.913155
6	-5.400591	-1.388324	3.070344	6	5.884688	-1.224666	-2.494277
1	-5.376110	-1.038774	0.949965	1	5.485693	-0.944369	-0.401570
6	-3.309419	-1.024849	4.240610	6	4.014577	-0.883643	-3.997130
1	-1.646991	-0.367286	3.030143	1	2.148234	-0.312011	-3.073288
6	-4.657413	-1.386714	4.256422	6	5.356818	-1.205627	-3.790432
1	-6.447951	-1.675046	3.083381	1	6.927779	-1.480904	-2.333855
1	-2.733554	-1.024787	5.160993	1	3.605084	-0.869577	-5.002588
1	-5.131901	-1.671639	5.190776	1	5.994134	-1.445890	-4.636314

III_d E = -3226.1765679 NImag = 0 Tc = 0.663036				TS3_d E = -3226.1658757 NImag = 1 (-970.48) Tc = 0.661276			
6	3.201438	-0.359406	1.739181	6	3.301721	-0.287825	1.673758
6	3.054514	-1.069176	2.926783	6	3.243900	-0.966820	2.886636
6	3.444562	0.285014	2.937695	6	3.594917	0.398342	2.837517
6	4.031154	2.629729	2.844134	6	4.105275	2.755192	2.648572
1	5.010234	3.023949	3.135098	1	5.091594	3.179022	2.863547
6	3.818339	1.479864	5.042224	6	4.057634	1.660868	4.884379
1	3.569985	0.517701	5.486175	1	3.869312	0.704037	5.367501
6	2.199107	-3.322391	2.770562	6	2.448265	-3.246833	2.843328
1	2.625800	-4.254248	3.150157	1	2.927756	-4.153471	3.220844
6	2.734218	-2.317618	4.992572	6	3.079069	-2.162331	5.002233
1	3.347243	-1.541916	5.450805	1	3.693490	-1.356423	5.402645
6	3.549273	1.031583	-0.762816	6	3.481112	1.044454	-0.876348
6	4.458808	1.483323	-1.711689	6	4.341716	1.506100	-1.865131
6	3.371268	2.296589	-1.309281	6	3.238279	2.289640	-1.443806
6	3.046142	4.511302	-2.278472	6	2.807488	4.470990	-2.447313
1	2.814064	5.455142	-1.778475	1	2.569050	5.416963	-1.954389
6	1.366871	3.514826	-0.724129	6	1.215424	3.457936	-0.814325
1	1.180915	2.626483	-0.119573	1	1.069607	2.571763	-0.196059
6	6.239912	0.004204	-2.437419	6	6.151465	0.075354	-2.616387
1	7.304393	0.214102	-2.294038	1	7.211027	0.326572	-2.507511
6	5.963912	2.247194	-3.479204	6	5.763199	2.283864	-3.695438

1	5.311357	3.118017	-3.489599	1	5.075090	3.126763	-3.710132
7	3.762604	1.389952	3.578825	7	3.916468	1.528676	3.429425
7	2.774092	-2.198039	3.529657	7	3.029412	-2.083393	3.536350
7	2.675867	3.403076	-1.387955	7	2.502172	3.368845	-1.524549
7	5.500136	1.274296	-2.481215	7	5.364325	1.316803	-2.663637
15	2.649817	-0.359590	0.010618	15	2.673825	-0.357316	-0.026949
1	6.987100	2.558290	-3.245808	1	6.778049	2.641812	-3.495285
1	5.949439	1.784316	-4.470831	1	5.743837	1.796382	-4.675033
1	6.105440	-0.533669	-3.381375	1	6.010507	-0.485273	-3.545988
1	5.873810	-0.613354	-1.618820	1	5.831141	-0.538670	-1.776193
1	4.115306	4.487338	-2.488226	1	3.867808	4.471809	-2.698659
1	2.479484	4.455112	-3.213955	1	2.206438	4.382682	-3.358439
1	1.355553	4.416953	-0.104344	1	1.205832	4.365111	-0.202037
1	0.580250	3.574134	-1.481799	1	0.401574	3.495059	-1.544026
1	1.703022	-2.236597	5.353061	1	2.068628	-2.101363	5.420599
1	3.138264	-3.292078	5.278189	1	3.528755	-3.116180	5.289017
1	2.444156	-3.218400	1.714115	1	2.625738	-3.164668	1.771576
1	1.111366	-3.327180	2.886678	1	1.370290	-3.282942	3.025844
1	4.823638	1.775965	5.358713	1	5.069980	1.997537	5.129679
1	3.098214	2.226167	5.393040	1	3.335656	2.393570	5.259021
1	4.030279	2.428243	1.772410	1	4.037486	2.526642	1.584498
1	3.264369	3.376800	3.076558	1	3.337545	3.489805	2.914674
78	0.293339	-0.158851	-0.235434	78	0.300437	-0.230188	-0.166504
17	-0.127628	-0.686528	2.060120	17	0.017862	-0.718542	2.154163
17	0.673265	0.456143	-2.528016	17	0.542370	0.319108	-2.494973
6	-2.185579	-1.070905	-1.474487	6	-2.219068	-1.251260	-1.230901
1	-1.521078	-1.657269	-2.100568	1	-1.578082	-1.894180	-1.822785
6	-1.724352	-0.167357	-0.585134	6	-1.723330	-0.255545	-0.404655
6	-2.678818	0.766030	0.004061	6	-2.650941	0.672018	0.160106
6	-4.093890	0.651099	-0.222802	6	-4.068071	0.555168	-0.075121
6	-2.219133	1.837502	0.816857	6	-2.176838	1.774204	0.946782
6	-4.963204	1.768223	0.121661	6	-4.901532	1.726371	0.172244
6	-4.562370	-0.599908	-0.747002	6	-4.584338	-0.698933	-0.557864
6	-3.067592	2.807094	1.284374	6	-3.011211	2.763209	1.369445
1	-1.166837	1.858213	1.070994	1	-1.126322	1.780910	1.210327
6	-4.438740	2.841269	0.905824	6	-4.373203	2.810837	0.936827
6	-3.661124	-1.239169	-1.752530	6	-3.684955	-1.510214	-1.343270
6	-5.760275	-1.289972	-0.353528	6	-5.893258	-1.263064	-0.271030
1	-2.685958	3.603894	1.918364	1	-2.636034	3.573103	1.989954
6	-4.075575	-2.551780	-2.320419	6	-4.156768	-2.684392	-2.053541
1	-3.779775	-0.544280	-2.624711	1	-3.132310	-0.762316	-2.157099
6	-6.128332	-2.508888	-1.023497	6	-6.327356	-2.424963	-0.988779
6	-5.268822	-3.094523	-2.027634	6	-5.443278	-3.079937	-1.914364
1	-3.394968	-3.023071	-3.023926	1	-3.457237	-3.228196	-2.681261
1	-5.585418	-4.025420	-2.489523	1	-5.808309	-3.953130	-2.447577
6	-5.260690	3.946685	1.237935	6	-5.173087	3.949195	1.192778
6	-6.551241	4.033158	0.759849	6	-6.436507	4.061838	0.648146
1	-7.173279	4.887939	1.006435	1	-7.038967	4.944916	0.838046
1	-4.845353	4.740272	1.853310	1	-4.762129	4.750337	1.801237
6	-7.048576	3.017368	-0.082890	6	-6.926487	3.039809	-0.189590
1	-8.047183	3.104959	-0.500480	1	-7.895809	3.149762	-0.666340
6	-6.275097	1.914602	-0.394236	6	-6.178922	1.900414	-0.418623
1	-6.679315	1.158594	-1.057576	1	-6.573013	1.137146	-1.078122
6	-6.541349	-0.889767	0.768510	6	-6.722658	-0.791801	0.778609
1	-6.234533	-0.031820	1.350864	1	-6.385076	0.026229	1.401094
6	-7.670882	-1.587855	1.143205	6	-7.947263	-1.375354	1.042795
6	-8.075176	-2.723001	0.414320	6	-8.407777	-2.456028	0.266568
1	-8.974521	-3.259817	0.701161	1	-9.378992	-2.897162	0.468523
1	-8.244109	-1.264578	2.006262	1	-8.553482	-1.000439	1.861738
6	-7.304160	-3.179283	-0.643494	6	-7.599524	-2.976919	-0.726573

1	-7.587996	-4.082632	-1.175409	1	-7.921541	-3.842390	-1.298844
6	3.472358	-1.843739	-0.678446	6	3.509999	-1.833230	-0.714375
6	4.629967	-2.404766	-0.109237	6	4.707615	-2.344514	-0.181958
6	2.898636	-2.431986	-1.818491	6	2.906293	-2.467866	-1.813424
6	5.204145	-3.543545	-0.675508	6	5.291713	-3.480002	-0.744568
1	5.081399	-1.960826	0.774195	1	5.182562	-1.865230	0.670079
6	3.487026	-3.565577	-2.382906	6	3.504813	-3.597438	-2.374968
1	2.005092	-2.000373	-2.259263	1	1.981607	-2.075428	-2.225496
6	4.633668	-4.122997	-1.813171	6	4.691442	-4.105342	-1.841870
1	6.092918	-3.979282	-0.228454	1	6.211565	-3.877592	-0.325808
1	3.041671	-4.017399	-3.264119	1	3.036552	-4.085207	-3.224543
1	5.081065	-5.010896	-2.249998	1	5.146952	-4.990571	-2.275645

IV_a E = -3226.2152752 Nimag = 0 Tc = 0.662709				TS4_a E = -3226.1894967 Nimag = 1 (-923.97) Tc = 0.661702			
6	3.364464	-0.609360	1.550759	6	3.216524	-0.381795	1.716520
6	3.341896	-1.511224	2.610165	6	3.101322	-1.114065	2.893913
6	3.747918	-0.174114	2.805855	6	3.468454	0.248582	2.920918
6	4.373852	2.150556	3.048027	6	4.019393	2.603068	2.861303
1	5.390155	2.478196	3.289724	1	4.996196	3.005081	3.148759
6	4.366595	0.642825	5.029911	6	3.853721	1.411417	5.041520
1	4.110048	-0.369649	5.335792	1	3.143268	2.157068	5.412159
6	2.457419	-3.720958	2.183719	6	2.286646	-3.382533	2.722035
1	2.977961	-4.676556	2.288634	1	2.748552	-4.307613	3.075933
6	3.262170	-3.092799	4.461126	6	2.844921	-2.398043	4.947917
1	3.943613	-2.405536	4.961827	1	3.278274	-3.367103	5.207465
6	3.481620	1.186206	-0.704933	6	3.539939	1.048398	-0.771138
6	4.283492	1.812746	-1.652182	6	4.444258	1.522349	-1.714883
6	3.245148	2.523398	-0.999942	6	3.355829	2.325024	-1.289030
6	2.799380	4.862086	-1.534058	6	3.026617	4.561401	-2.208212
1	2.628112	5.702806	-0.857080	1	2.798943	5.493207	-1.684467
6	1.314982	3.572593	0.004288	6	1.359413	3.535808	-0.659167
1	1.236082	2.610362	0.510778	1	1.179388	2.638842	-0.066172
6	5.971738	0.511634	-2.810210	6	6.229759	0.067694	-2.478729
1	7.045881	0.711065	-2.747816	1	6.098109	-0.447700	-3.435430
6	5.593762	2.898812	-3.406443	6	5.941318	2.333057	-3.468555
1	4.962514	3.755299	-3.178181	1	5.279749	3.196980	-3.465272
7	4.150455	0.805133	3.586858	7	3.776737	1.346037	3.576683
7	3.117006	-2.724945	3.046163	7	2.848164	-2.253908	3.485630
7	2.543163	3.611105	-0.806621	7	2.660456	3.432405	-1.340620
7	5.235476	1.758649	-2.551503	7	5.482248	1.334542	-2.492559
15	2.674137	-0.336267	-0.103786	15	2.666703	-0.364563	-0.011768
1	6.643223	3.164495	-3.245824	1	6.960061	2.649160	-3.223245
1	5.451365	2.624334	-4.456261	1	5.936296	1.889225	-4.468765
1	5.733816	0.144686	-3.813701	1	5.867837	-0.571098	-1.674731
1	5.695321	-0.244397	-2.076938	1	7.292839	0.280986	-2.330845
1	3.834712	4.897439	-1.871954	1	4.094187	4.541008	-2.425659
1	2.122583	4.949460	-2.390522	1	2.453027	4.527212	-3.140367
1	1.342822	4.388771	0.732435	1	1.357654	4.426585	-0.023475
1	0.443431	3.682965	-0.647454	1	0.563606	3.612391	-1.405619
1	2.286626	-3.079030	4.958890	1	3.449638	-1.615457	5.405070
1	3.680720	-4.100489	4.521511	1	1.820418	-2.348272	5.331911
1	2.497540	-3.396246	1.145126	1	2.501421	-3.255088	1.661676
1	1.410171	-3.826768	2.480950	1	1.203029	-3.421140	2.866514
1	5.414677	0.842525	5.275158	1	3.603211	0.444534	5.473594
1	3.730624	1.346683	5.575997	1	4.865160	1.695914	5.348643
1	4.250094	2.137289	1.964708	1	4.009125	2.421172	1.786144
1	3.659795	2.853637	3.490218	1	3.244959	3.334204	3.117080

78	0.269845	-0.165085	-0.139564	78	0.322357	-0.173931	-0.248338
17	0.071078	-1.100508	2.048870	17	-0.081660	-0.789956	2.018391
17	0.460804	0.881693	-2.296128	17	0.640648	0.496521	-2.534408
6	-2.241180	-1.080754	-1.405739	6	-2.271998	-1.182022	-1.360069
1	-1.646386	-2.001635	-1.461254	1	-1.593867	-1.837887	-1.899559
6	-1.728368	-0.197832	-0.324551	6	-1.716744	-0.153395	-0.540963
6	-2.637242	0.606138	0.363575	6	-2.662945	0.757715	0.091255
6	-4.048601	0.523554	0.049377	6	-4.064485	0.582821	-0.089995
6	-2.185998	1.613470	1.294813	6	-2.177175	1.868368	0.840063
6	-4.851401	1.687979	0.325482	6	-4.924541	1.721303	0.190804
6	-4.577792	-0.695967	-0.551062	6	-4.553246	-0.698605	-0.593759
6	-3.021387	2.583066	1.745595	6	-3.024200	2.831960	1.307183
1	-1.152724	1.561500	1.617190	1	-1.113738	1.911549	1.045481
6	-4.346857	2.700021	1.210324	6	-4.400661	2.824661	0.938909
6	-3.699706	-1.424779	-1.367359	6	-3.671826	-1.465845	-1.396906
6	-5.917143	-1.219440	-0.328418	6	-5.852756	-1.275118	-0.307051
1	-2.681965	3.327608	2.460331	1	-2.648480	3.657818	1.905576
6	-4.168432	-2.490919	-2.165355	6	-4.131599	-2.585065	-2.152385
1	-1.988137	-0.553101	-2.345639	6	-6.293980	-2.405162	-1.074591
6	-6.369335	-2.303306	-1.151381	6	-5.424705	-3.002940	-2.037127
6	-5.482185	-2.885268	-2.096506	1	-3.432894	-3.100232	-2.805506
1	-3.476999	-2.998515	-2.832595	1	-5.789747	-3.842984	-2.620988
1	-5.844191	-3.696452	-2.722551	6	-5.232975	3.932103	1.239038
6	-5.148419	3.822763	1.506166	6	-6.519098	4.001973	0.749527
6	-6.376236	3.997479	0.893964	1	-7.144711	4.861408	0.970766
1	-6.975538	4.874682	1.119452	1	-4.824727	4.743985	1.835037
1	-4.772927	4.566561	2.203358	6	-7.007263	2.967376	-0.077396
6	-6.838750	3.055341	-0.048819	1	-7.997836	3.048159	-0.514718
1	-7.777743	3.223721	-0.566574	6	-6.234032	1.856197	-0.344155
6	-6.099125	1.923197	-0.318485	1	-6.628366	1.086027	-0.994163
1	-6.459443	1.213419	-1.052015	6	-6.670256	-0.856581	0.777272
6	-6.767806	-0.805391	0.729553	1	-6.324146	-0.069290	1.434335
1	-6.429669	-0.051956	1.429779	6	-7.885643	-1.457386	1.031494
6	-8.016341	-1.367572	0.907694	6	-8.357645	-2.501750	0.207345
6	-8.490447	-2.371695	0.036130	1	-9.325596	-2.952872	0.403457
1	-9.480869	-2.792724	0.178563	1	-8.480203	-1.127763	1.878158
1	-8.636736	-1.037478	1.735756	6	-7.567955	-2.970682	-0.820458
6	-7.672510	-2.836155	-0.968967	1	-7.897343	-3.806878	-1.430854
1	-7.999916	-3.641899	-1.620320	6	3.487115	-1.835023	-0.724884
6	3.435549	-1.670139	-1.096794	6	4.655784	-2.390516	-0.172740
6	4.640353	-2.296780	-0.729498	6	2.906608	-2.416509	-1.865065
6	2.768377	-2.067634	-2.268632	6	5.233643	-3.518341	-0.756552
6	5.169060	-3.311463	-1.527908	1	5.112133	-1.951841	0.710743
1	5.163714	-2.000185	0.175545	6	3.498567	-3.539423	-2.446591
6	3.311443	-3.077991	-3.064823	1	2.004681	-1.989839	-2.293042
1	1.838394	-1.585679	-2.554951	6	4.655932	-4.091864	-1.893760
6	4.505557	-3.701030	-2.695747	1	6.130694	-3.950818	-0.323251
1	6.094998	-3.799381	-1.237933	1	3.047975	-3.986854	-3.327297
1	2.794375	-3.383143	-3.969495	1	5.106167	-4.971713	-2.343619
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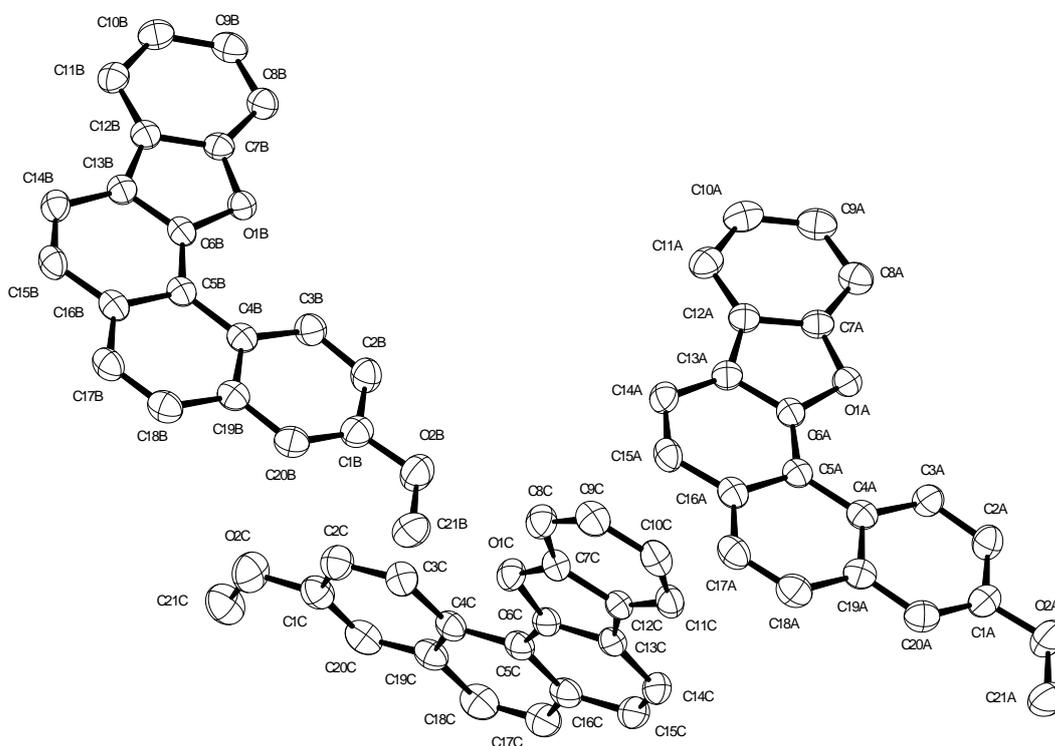
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6	-2.185772	0.769715	3.196575				
6	-3.305638	-1.213980	4.011426				
1	-4.210903	-1.191016	4.626409				

6	-2.169567	0.325917	5.604465
1	-1.568337	-0.494061	6.009722
6	-0.227998	3.639634	1.599606
1	-0.309764	4.721078	1.734376
6	-0.285586	3.438374	4.089009
1	-0.341609	4.529264	4.118435
6	-3.600679	-0.784122	0.076623
6	-4.831916	-1.180541	-0.433248
6	-3.884401	-2.141739	0.002037
6	-4.365394	-4.531011	-0.140575
1	-4.213754	-5.303488	0.617609
6	-2.117086	-3.697081	0.553660
1	-1.558706	-2.776773	0.729964
6	-6.361244	0.503443	-1.274926
1	-6.384221	0.665779	-2.357191
6	-6.931573	-1.913940	-1.446476
1	-6.536739	-2.909417	-1.253816
7	-2.543079	0.022294	4.216629
7	-0.788378	2.972784	2.789023
7	-3.505926	-3.381381	0.179523
7	-5.979587	-0.889330	-0.992603
15	-2.241092	0.428028	0.110130
1	-7.883865	-1.789405	-0.921973
1	-7.097986	-1.801589	-2.522165
1	-5.643408	1.186323	-0.823381
1	-7.357513	0.690769	-0.863337
1	-5.413685	-4.234536	-0.125976
1	-4.104463	-4.938027	-1.122974
1	-2.117997	-4.323392	1.451014
1	-1.637938	-4.237635	-0.268074
1	-0.898959	3.038538	4.895712
1	0.755781	3.127638	4.224837
1	-0.785750	3.343032	0.712199
1	0.820272	3.352372	1.475962
1	-1.585385	1.243180	5.643711
1	-3.071829	0.444513	6.212507
1	-3.587604	-1.301294	2.961784
1	-2.699574	-2.078540	4.302620
78	-0.300150	-0.504660	-0.661013
17	0.942426	0.264237	1.214823
17	-1.570071	-1.457214	-2.466882
6	1.639068	-0.544503	-2.341052
1	0.972184	-0.453964	-3.192806
6	1.563226	-1.680399	-1.511442
6	2.662372	-1.975207	-0.621358
6	3.759392	-1.083090	-0.532065
6	2.675175	-3.218562	0.071149
6	5.000214	-1.602613	0.020931
6	3.591651	0.259598	-1.085103
6	3.774235	-3.613793	0.778579
1	1.794938	-3.853920	0.014130
6	4.977456	-2.851048	0.726775
6	2.621862	0.450723	-2.113764
6	4.307304	1.438119	-0.638357
1	3.776620	-4.556697	1.318799
6	2.609279	1.647413	-2.899199
6	4.272959	2.626656	-1.441924
6	3.454567	2.675876	-2.613811
1	1.915608	1.709426	-3.733553
1	3.472733	3.571171	-3.228909

6	6.172061	-3.367011	1.289804
6	7.377327	-2.726888	1.101613
1	8.290102	-3.139213	1.520786
1	6.124601	-4.302373	1.841104
6	7.425385	-1.554766	0.317124
1	8.381536	-1.083704	0.109336
6	6.270835	-1.007918	-0.204895
1	6.345564	-0.123315	-0.823597
6	4.960838	1.516022	0.621984
1	4.923145	0.666291	1.291305
6	5.623026	2.659492	1.018666
6	5.675887	3.787214	0.171097
1	6.224555	4.672817	0.477961
1	6.107878	2.690586	1.989982
6	5.001239	3.769856	-1.031988
1	4.996853	4.647089	-1.673370
6	-2.876403	1.892480	-0.776705
6	-3.680531	2.851330	-0.131582
6	-2.548684	2.050633	-2.134018
6	-4.150706	3.955514	-0.842293
1	-3.937219	2.743109	0.918793
6	-3.030216	3.157191	-2.836189
1	-1.930688	1.312456	-2.634257
6	-3.826409	4.108120	-2.194359
1	-4.765128	4.697637	-0.341194
1	-2.775707	3.277018	-3.884793
1	-4.191002	4.971041	-2.743553
1	0.947364	-2.518357	-1.828965

X-ray Structures:

Compound 11t



Empirical formula
Color

$C_{21}H_{14}O_2$
colourless

Formula weight
Temperature
Wavelength
Crystal system
Space group
Unit cell dimensions

298.32 $g \cdot mol^{-1}$
200 K
0.71073 Å

MONOCLINIC

P2₁/n, (no. 14)

$a = 28.109(4)$ Å

$b = 4.5304(6)$ Å

$c = 33.581(5)$ Å

$\alpha = 90^\circ$.

$\beta = 90.356(3)^\circ$.

$\gamma = 90^\circ$.

Volume
Z

4276.3(10) Å³
12

Density (calculated)

1.390 $Mg \cdot m^{-3}$

Absorption coefficient
F(000)

0.088 mm^{-1}
1872 e

Crystal size
 θ range for data collection
Index ranges

1.0 x 0.06 x 0.05 mm^3
0.94 to 26.45°.

Reflections collected
Independent reflections

-35 $\leq h \leq 35$, -5 $\leq k \leq 5$, -42 $\leq l \leq 41$
84818
8791 [$R_{int} = 0.0552$]

Reflections with $I > 2\sigma(I)$
Completeness to $\sigma = 26.45^\circ$

6428
99.6 %

Absorption correction
Max. and min. transmission

Gaussian
1.00 and 0.95

Refinement method
Data / restraints / parameters

Full-matrix least-squares on F^2
8791 / 0 / 625

Goodness-of-fit on F^2

1.034

Final R indices [$I > 2\sigma(I)$]

$R_1 = 0.0411$

$wR^2 = 0.0978$

R indices (all data)

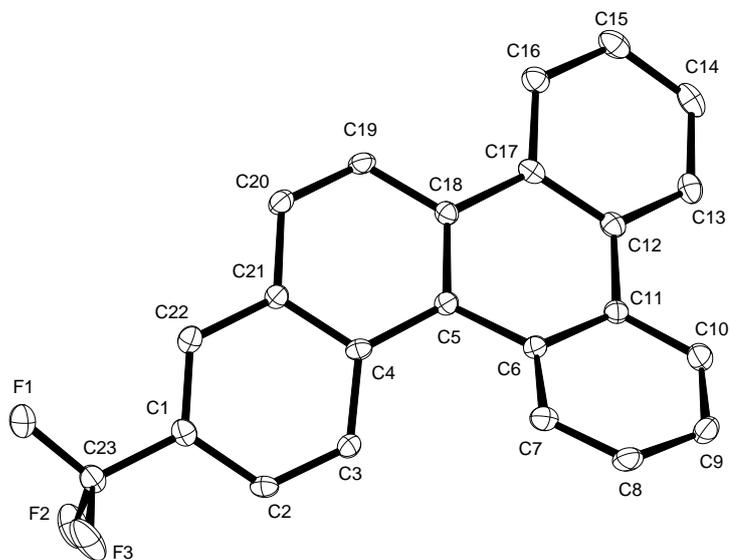
$R_1 = 0.0638$

$wR^2 = 0.1135$

Largest diff. peak and hole

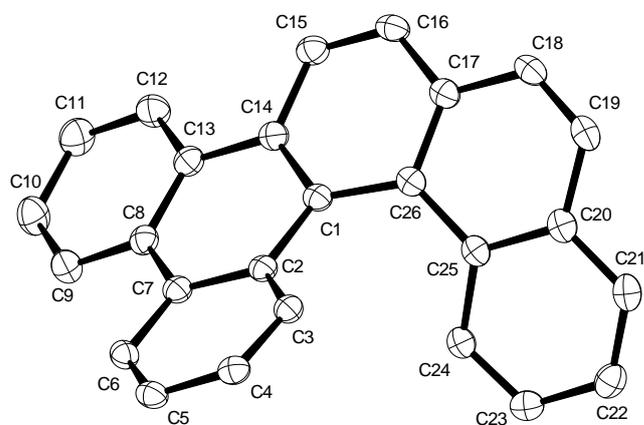
0.189 and -0.188 $e \cdot \text{Å}^{-3}$

Compound 11o



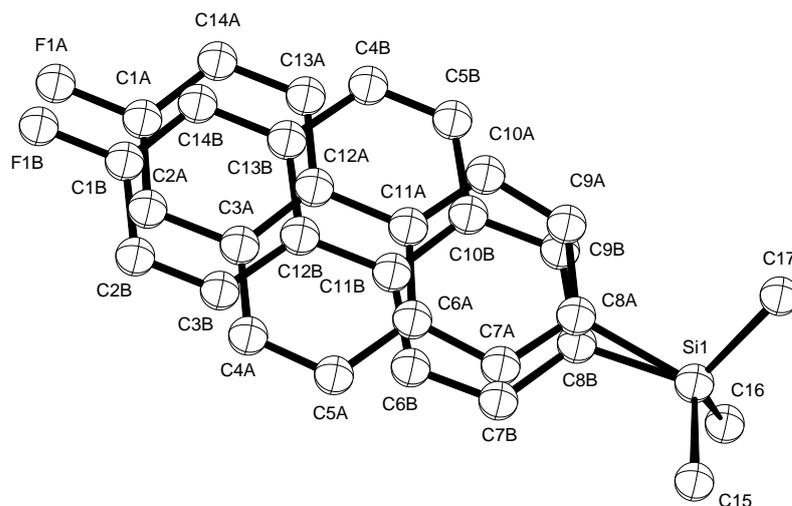
Empirical formula	$C_{23}H_{13}F_3$	
Color	colourless	
Formula weight	$346.33 \text{ g} \cdot \text{mol}^{-1}$	
Temperature	100 K	
Wavelength	0.71073 \AA	
Crystal system	MONOCLINIC	
Space group	$P2_1/c$, (no. 14)	
Unit cell dimensions	$a = 12.0407(14) \text{ \AA}$ $b = 11.2123(12) \text{ \AA}$ $c = 11.8610(16) \text{ \AA}$	$\alpha = 90^\circ$ $\beta = 106.890(11)^\circ$ $\gamma = 90^\circ$
Volume	$1532.2(3) \text{ \AA}^3$	
Z	4	
Density (calculated)	$1.501 \text{ Mg} \cdot \text{m}^{-3}$	
Absorption coefficient	0.112 mm^{-1}	
F(000)	712 e	
Crystal size	$0.14 \times 0.08 \times 0.07 \text{ mm}^3$	
θ range for data collection	2.79 to 32.03°	
Index ranges	$-17 \leq h \leq 17$, $-15 \leq k \leq 16$, $-16 \leq l \leq 17$	
Reflections collected	16304	
Independent reflections	5309 [$R_{\text{int}} = 0.0698$]	
Reflections with $I > 2\sigma(I)$	3075	
Completeness to $\theta = 27.50^\circ$	99.7 %	
Absorption correction	Gaussian	
Max. and min. transmission	0.99 and 0.99	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5309 / 0 / 235	
Goodness-of-fit on F^2	1.076	
Final R indices [$I > 2\sigma(I)$]	$R_1 = 0.0704$	$wR^2 = 0.1242$
R indices (all data)	$R_1 = 0.1466$	$wR^2 = 0.1510$
Largest diff. peak and hole	0.448 and $-0.363 \text{ e} \cdot \text{\AA}^{-3}$	

Compound 11p:



Empirical formula	$C_{26}H_{16}$	
Color	colourless	
Formula weight	$328.39 \text{ g} \cdot \text{mol}^{-1}$	
Temperature	100 K	
Wavelength	1.54178 \AA	
Crystal system	MONOCLINIC	
Space group	$P2_1/n$, (no. 14)	
Unit cell dimensions	$a = 10.0094(5) \text{ \AA}$ $b = 8.1625(4) \text{ \AA}$ $c = 20.4952(11) \text{ \AA}$	$\alpha = 90^\circ$ $\beta = 103.407(2)^\circ$ $\gamma = 90^\circ$
Volume	$1628.86(14) \text{ \AA}^3$	
Z	4	
Density (calculated)	$1.339 \text{ Mg} \cdot \text{m}^{-3}$	
Absorption coefficient	0.577 mm^{-1}	
F(000)	688 e	
Crystal size	$0.26 \times 0.19 \times 0.08 \text{ mm}^3$	
θ range for data collection	4.44 to 67.26°	
Index ranges	$-11 \leq h \leq 11$, $-9 \leq k \leq 8$, $-24 \leq l \leq 24$	
Reflections collected	36073	
Independent reflections	2895 [$R_{\text{int}} = 0.0528$]	
Reflections with $I > 2\sigma(I)$	2612	
Completeness to $\theta = 67.26^\circ$	99.0 %	
Absorption correction	Gaussian	
Max. and min. transmission	0.96 and 0.89	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2895 / 0 / 235	
Goodness-of-fit on F^2	1.079	
Final R indices [$I > 2\sigma(I)$]	$R_1 = 0.0348$	$wR^2 = 0.0908$
R indices (all data)	$R_1 = 0.0380$	$wR^2 = 0.0931$
Largest diff. peak and hole	0.150 and $-0.195 \text{ e} \cdot \text{\AA}^{-3}$	

Compound11c:



Empirical formula
Color
Formula weight
Temperature
Wavelength
Crystal system
Space group
Unit cell dimensions

C₁₇H₁₇F Si
colourless
268.40 g · mol⁻¹
100 K
1.54184 Å
ORTHOHOMBIC
P2₁2₁2₁, (no. 19)
a = 7.6774(3) Å
b = 28.5135(10) Å
c = 6.5884(2) Å

α = 90°.
β = 90°.
γ = 90°.

Volume
Z

1442.26(9) Å³
4

Density (calculated)
Absorption coefficient
F(000)

1.236 Mg · m⁻³
1.389 mm⁻¹
568 e

Crystal size
θ range for data collection
Index ranges
Reflections collected
Independent reflections

0.18 x 0.17 x 0.16 mm³
3.10 to 66.68°.
-9 ≤ h ≤ 9, -33 ≤ k ≤ 33, -7 ≤ l ≤ 7
31715
2524 [R_{int} = 0.0523]

Reflections with I > 2σ(I)
Completeness to θ = 66.68°
Absorption correction
Max. and min. transmission

2504
99.5 %
Gaussian
0.75 and 0.64

Refinement method
Data / restraints / parameters

Full-matrix least-squares on F²
2524 / 0 / 160

Goodness-of-fit on F²

1.212

Final R indices [I > 2σ(I)]

R₁ = 0.0868

wR² = 0.1966

R indices (all data)

R₁ = 0.0871

wR² = 0.1967

Absolute structure parameter

0.12(10)

Largest diff. peak and hole

0.433 and -0.519 e · Å⁻³