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Supporting Information

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Tunable Carbonyl Ylide Reactions: Selective Synthesis of Dihydrofurans and Dihydrobenzoxepines**

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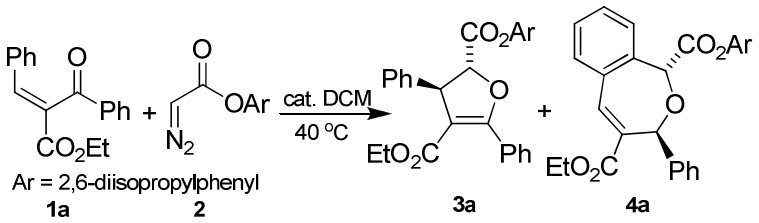
Contents

1. General information

All reactions were carried out under dry nitrogen atmosphere. Dichloromethane (DCM) was distilled over calcium hydride prior to use. $CuPF_6(CH_3CN)_4$, CuCl, and $AgSbF_6$ were purchased from Aldrich, and the diazo esters,[1] substrate,[2] and ligand[3] were prepared according to literature procedures. Powdered M.S. 4Å was preactivated for 8 hours at 250 °C under vacuum prior to use.

NMR spectra were recorded on a Varian Mercury-300 or a Varian Mercury-400 nuclear magnetic resonance spectrometer. Chemical shifts are reported in parts per million (ppm) down field from TMS, using residual $CDCl_3$ as an internal standard. The relative configurations of **3** and **4** were determined by coupling constant of their ^{1}H NMR and NOESY-1D analysis.

2. Effect of catalysts on the carbonyl ylide reaction



Ar = 2,6-diisopropylphenyl

1a **2** **3a** **4a**

cat.	con.(%)	**3a** (%)	**4a** (%)
$CuPF_6(CH_3CN)_4$ (5%)	100	29	51
$CuCl/AgSbF_6$ (5%)	88	43	16

Scheme S1. Effects of catalysts on the carbonyl ylide reaction.

3. Effect of other ligands on the carbonyl ylide reaction

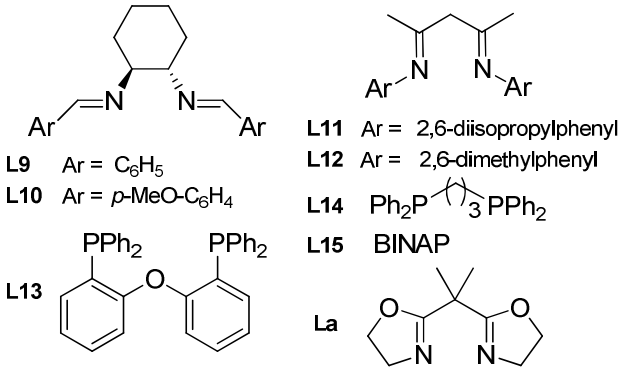
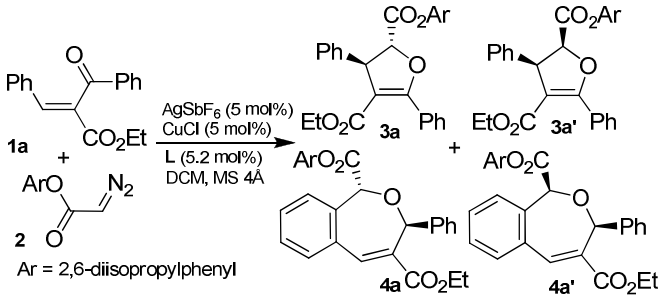


Figure S1. Other Ligands screened for the carbonyl ylide chemistry.

Table S1. Effect of other ligands on the carbonyl ylide reaction.[a]

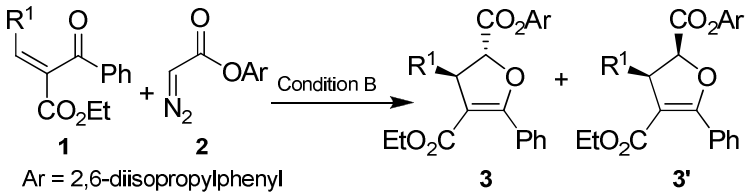


Entry	Ligand	Con.(%)[b]	**3a/3a'/4a/4a'**[b]
1	**L9**	85	56/24/20/0
2	**L10**	88	56/17/27/0
3	**L11**	27	38/39/23/0
4	**L12**	100	29/16/55/0
5	**L13**	26	47/42/11/0
6	**L14**	42	43/45/12/0
7	**L15**	79	51/27/22/0
8	**La**	100	85/6/9/0

[a] Reaction conditions：CuCl (2.5 mg, 0.025 mmol), $AgSbF_5$ (8.6 mg, 0.025 mmol), M.S. 4Å (200 mg), Ligand (0.026 mmol), DCM: 4 mL, rt, **1a** (140 mg, 0.5 mmol), **2** (492 mg, 2.0 mmol). [b] Determined by ^{1}H NMR.

4. The yield and diastereoselectivity of 3 under Condition B

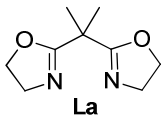
Table S2. Yield and diastereoselectivity of **3** under **Condition B**. [a]



3 + 3'	**a**	**b**	**c**	**d**	**e**	**f**	**g**	**h**	**i**	**j**
Yield (%)[a]	17	6	18	9	21	17	6	21	17	30
dr[a]	81/19	> 95/5	80/20	> 95/5	92/8	75/25	56/44	68/32	50/50	71/29

[a] Determined by ^{1}H NMR.

5. Ligand La (prepared according to literature procedures)[3f]

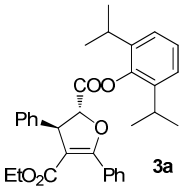


2,2'-(propane-2,2-diyl)bis(4,5-dihydrooxazole)

Yield: 39%. ^{1}H NMR (400 MHz, $CDCl_3$): δ 4.30 (t, J = 9.2 Hz, 4H), 3.89 (t, J = 9.2 Hz, 4H), 1.53 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 169.5, 67.6, 54.0, 38.2, 23.8; IR (neat, cm^{-1}): 2983, 2940, 2905, 2883, 1657, 1522, 1504, 1471, 1387, 1353, 1253, 1197, 1142, 1113; LRMS-EI (*m/z*): 182.1, 181, 167, 151, 137, 113; HRMS-EI: Calcd. for $C_9H_{14}N_2O_2$: 182.1055; Found: 182.1058.

6. General procedure for Condition A

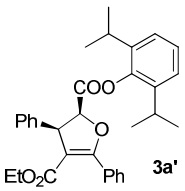
CuCl (2.5 mg, 0.025 mmol), $AgSbF_6$ (8.6 mg, 0.025 mmol), **L7** (9.6 mg, 0.026 mmol), 200 mg M.S. 4Å, and CH_2Cl_2 (2 mL) were stirred under nitrogen for 1 hour at room temperature. Then the substrate (**1**) (0.5 mmol) was added, and the mixture was stirred for another 5 min. Then, a solution of the 2,6-diisopropylphenyl diazoacetate (**2**) (492 mg, 2.0 mmol) in CH_2Cl_2 (2.0 mL) was dropwise added through a syringe pump for 9-10 hours. After another 1 h of stirring at room temperature, the mixture was filtered through a thin layer (40 mm) of silica gel (100-200 mesh), and washed with DCM to remove the catalyst. The filtrate was concentrated under reduced pressure, and the residue was purified by flash chromatography.



3a

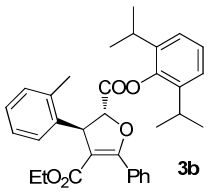
2-(2,6-diisopropylphenyl) 4-ethyl 3,5-diphenyl-2,3-dihydrofuran-2,4-dicarboxylate (3a)

^{1}H NMR (300 MHz, $CDCl_3$): δ 8.02 (dd, *J* = 1.5 Hz, 8.1 Hz, 2H), 7.47-7.16 (m, 11H), 5.29 (d, *J* = 3.3 Hz, 1H), 4.89 (d, *J* = 3.6 Hz, 1H), 4.13-3.96 (m, 2H), 2.95 (br, 2H), 1.24-1.06 (m, 15H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 169.0, 165.4, 163.8, 145.1, 141.9, 140.1, 131.1, 129.9, 128.9, 127.7, 127.6, 127.2, 126.9, 124.0, 106.9, 84.8, 60.0, 54.1, 27.6, 22.8, 13.9; IR (neat, cm^{-1}): 3064, 3029, 2966, 2932, 2871, 1772, 1757, 1710, 1632, 1600, 1494, 1456, 1447, 1385, 1366, 1344, 1313, 1248, 1188, 1165, 1144, 1067, 1044, 1030; LRMS-ESI (*m/z*): 521.3 ($M+Na^+$); HRMS-ESI: Calcd. for $C_{32}H_{35}O_5^+$: 499.2484; Found: 499.2455.



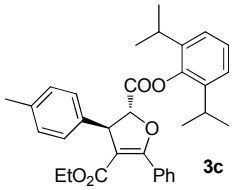
3a'

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.99 (dd, *J* = 1.6 Hz, 8.0 Hz, 2H), 7.49-7.41 (m, 5H), 7.36-7.32 (m, 3H), 7.16-7.12 (m, 1H), 7.04 (d, *J* = 7.2 Hz, 2H), 5.78 (d, *J* = 9.6 Hz, 1H), 4.86 (d, *J* = 9.6 Hz, 1H), 4.01 (q, *J* = 7.2 Hz, 2H), 1.06-0.99 (m, 15H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 166.1, 164.5, 163.9, 144.9, 140.4, 138.5, 131.1, 129.8, 128.8, 128.6, 128.6, 127.9, 127.8, 126.7, 123.9, 109.4, 83.6, 60.0, 52.5, 29.7, 26.7, 23.4, 13.9; LRMS-ESI (*m/z*): 521.5 ($M+Na^+$).



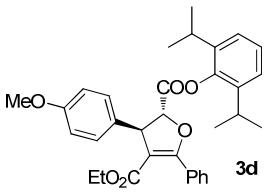
2-(2,6-diisopropylphenyl) 4-ethyl 5-phenyl-3-o-tolyl-2,3-dihydrofuran-2,4-dicarboxylate (3b)

^{1}H NMR (300 MHz, $CDCl_3$): δ 8.06 (d, *J* = 6.0 Hz, 2H), 7.45-7.16 (m, 10H), 5.19 (dd, *J* = 3.0 Hz, 10.2 Hz, 2H), 4.10-3.96 (m, 2H), 2.98 (br, 2H), 2.56 (s, 3H), 1.27-1.04 (m, 15H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 169.2, 165.6, 163.7, 145.0, 140.1, 140.0, 135.5, 131.0, 130.5, 129.9, 128.9, 127.7, 127.3, 126.9, 126.8, 126.3, 124.0, 107.0, 84.8, 59.9, 49.5, 27.5, 23.1, 19.6, 13.9; IR (neat, cm^{-1}): 3065, 2966, 2871, 1770, 1712, 1628, 1600, 1493, 1465, 1366, 1340, 1310, 1250, 1066; LRMS-ESI (*m/z*): 535.3 ($M+Na^+$); HRMS-ESI: Calcd. for $C_{33}H_{36}NaO_5^+$: 535.2460; Found: 535.2452; Anal. Calcd. for $C_{33}H_{36}O_5$: C, 77.32; H, 7.08; Found: C, 77.38; H, 7.23.



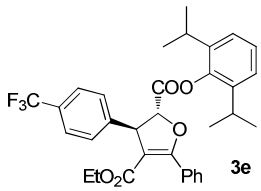
2-(2,6-diisopropylphenyl) 4-ethyl 5-phenyl-3-p-tolyl-2,3-dihydrofuran-2,4-dicarboxylate (3c)

^{1}H NMR (300 MHz, $CDCl_3$): δ 8.02 (d, *J* = 8.4 Hz, 2H), 7.42-7.15 (m, 10H), 5.28 (d, *J* = 3.6 Hz, 1H), 4.87 (d, *J* = 3.6 Hz, 1H), 4.13-3.95 (m, 2H), 2.96 (br, 2H), 2.34 (s, 3H), 1.24-1.06 (m, 15H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 169.0, 165.2, 163.7, 145.1, 140.0, 139.0, 137.2, 130.9, 129.8, 129.5, 128.9, 127.6, 127.0, 126.8, 124.0, 107.0, 84.9, 60.0, 53.7, 27.5, 22.9, 21.0, 13.9; IR (neat, cm^{-1}): 2965, 2871, 1758, 1712, 1628, 1600, 1513, 1493, 1447, 1366, 1165, 1066; LRMS-ESI (*m/z*): 535.3 ($M+Na^+$); HRMS-MALDI/DHB: Calcd. for $C_{33}H_{36}NaO_5^+$: 535.2460; Found: 535.2457.



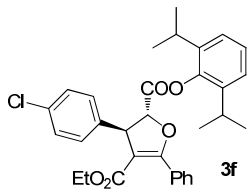
2-(2,6-diisopropylphenyl) 4-ethyl 3-(4-methoxyphenyl)-5-phenyl-2,3-dihydrofuran-2,4-dicarboxylate (3d)

^{1}H NMR (300 MHz, $CDCl_3$): δ 8.02 (dd, *J* = 0.9 Hz, 6.6 Hz, 2H), 7.43-7.16 (m, 8H), 6.91 (d, *J* = 8.4 Hz, 2H), 5.27 (d, *J* = 3.9 Hz, 1H), 4.86 (d, *J* = 3.6 Hz, 1H), 4.11-3.99 (m, 2H), 3.77 (s, 3H), 2.96 (br, 2H), 1.24-1.07 (m, 15H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 169.0, 165.0, 163.7, 159.0, 145.0, 140.0, 134.0, 130.9, 129.8, 128.9, 128.1, 127.6, 126.8, 124.0, 114.1, 107.1, 84.9, 59.9, 55.1, 53.4, 27.5, 23.1, 13.9; IR (neat, cm^{-1}): 3064, 2965, 2871, 2837, 1770, 1709, 1611, 1583, 1512, 1494, 1464, 1366, 1304, 1254, 1066, 1032; LRMS-ESI (*m/z*): 551.4 ($M+Na^+$); HRMS-ESI: Calcd. for $C_{33}H_{36}NaO_6^+$: 551.2410; Found: 551.2397.



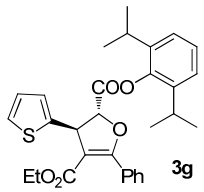
2-(2,6-diisopropylphenyl) 4-ethyl 5-phenyl-3-(4-(trifluoromethyl)phenyl)-2,3-dihydrofuran-2,4-dicarboxylate (3e)

^{1}H NMR (300 MHz, $CDCl_3$): δ 8.04 (d, *J* = 6.3 Hz, 2H), 7.67 (d, *J* = 8.1 Hz, 2H), 7.56 (d, *J* = 8.1 Hz, 2H), 7.47-7.43 (m, 3H), 7.24-7.17 (m, 3H), 5.29 (d, *J* = 3.0 Hz, 1H), 4.99 (d, *J* = 3.6 Hz, 1H), 4.14-3.97 (m, 2H), 2.95 (br, 2H), 1.25-1.06 (m, 15H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 168.7, 165.9, 163.4, 145.9, 145.0, 140.0, 131.3, 130.1, 129.9, 129.7, 128.5, 127.7, 127.6, 127.0, 125.9, 125.8, 124.1, 122.2, 106.3, 84.3, 60.1, 53.9, 27.6, 23.3, 13.8; ^{19}F NMR (282 MHz, $CDCl_3$): −62.87. IR (neat, cm^{-1}): 3067, 2966, 2933, 2872, 1758, 1713, 1619, 1600, 1494, 1466, 1447, 1422, 1386, 1366, 1326, 1159, 1113, 1067, 1019; LRMS-ESI (*m/z*): 589.3 ($M+Na^+$); HRMS-ESI: Calcd. for $C_{33}H_{34}F_3O_5^+$: 567.2353; Found: 567.2346; Anal. Calcd. for $C_{33}H_{33}F_3O_5$: C, 69.95; H, 5.87; Found: C, 70.25; H, 5.98.



2-(2,6-diisopropylphenyl) 4-ethyl 3-(4-chlorophenyl)-5-phenyl-2,3-dihydrofuran-2,4-dicarboxylate (3f)

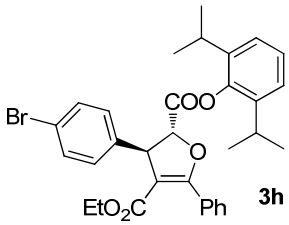
^{1}H NMR (300 MHz, $CDCl_3$): δ 8.03 (d, *J* = 6.3 Hz, 2H), 7.44-7.17 (m, 10H), 5.25 (d, *J* = 3.3 Hz, 1H), 4.87 (d, *J* = 3.3 Hz, 1H), 4.11-3.99 (m, 2H), 2.94 (br, 2H), 1.24-1.06 (m, 15H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 168.8, 165.6, 163.5, 145.0, 140.4, 139.9, 133.3, 131.2, 129.8, 129.0, 128.6, 128.5, 127.7, 126.9, 124.0, 106.5, 84.5, 60.0, 53.5, 27.5, 22.9, 13.9; IR (neat, cm^{-1}): 3065, 3028, 2966, 2932, 2871, 1773, 1757, 1712, 1627, 1600, 1577, 1492, 1466, 1447, 1413, 1385, 1366, 1311, 1284, 1189, 1144, 1068, 1031, 1015; LRMS-ESI (*m/z*): 555.2 ($M+Na^+$); HRMS-ESI: Calcd. for $C_{32}H_{34}ClO_5^+$: 533.2089; Found: 533.2089; Anal. Calcd. for $C_{32}H_{33}ClO_5$: C, 72.10; H, 6.24; Found: C, 72.05; H, 6.22.



5-phenyl-3-thiophen-2-yl-2,3-dihydro-furan-2,4-dicarboxylic acid 2-(2,6-diisopropyl-phenyl) ester 4-ethyl ester (3g)

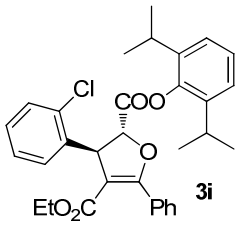
^{1}H NMR (300 MHz, $CDCl_3$): δ 8.01 (d, *J* = 6.0 Hz, 2H), δ 7.47-7.40 (m, 3H), δ 7.27-7.17 (m, 4H), δ 7.10-7.09 (m, 1H), 7.09-6.98 (m, 1H), 5.34 (d, *J* = 3.3 Hz, 1H), 5.20 (d, *J* = 3.3 Hz, 1H), 4.15-4.05 (m, 2H), 2.93 (br, 2H), 1.24-1.11 (m, 15H); ^{13}C NMR (75 MH z, $CDCl_3$): δ 168.6, 165.5, 163.5, 145.2, 145.0, 140.0, 131.2, 129.9, 128.7, 127.7, 127.1, 127.0, 124.6, 124.6, 124.0, 106.7,

84.7, 60.1, 49.1, 27.6, 22.9, 14.0; IR (neat, cm^{-1}): 2966, 2931, 2871, 1772, 1711, 1628, 1599, 1493, 1465, 1446, 1366, 1329, 1186, 1067, 1044; LRMS-ESI (*m/z*): 527.1 (M + Na^+); HRMS-MALDI/DHB: Calcd. for $C_{30}H_{32}NaO_5S^+$: 527.1863; Found: 527.1868.



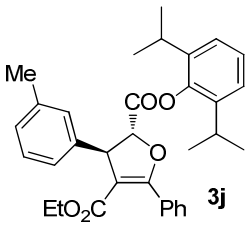
2-(2,6-diisopropylphenyl) 4-ethyl 3-(4-bromophenyl)-5-phenyl-2,3-dihydrofuran-2,4-dicarboxylate (3h)

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.01-7.98 (m, 2H), 7.53-7.42 (m, 5H), 7.30-7.17 (m, 5H), 5.23 (d, *J* = 3.2 Hz, 1H), 4.83 (d, *J* = 3.6 Hz, 1H), 4.12-3.99 (m, 2H), 2.91 (br, 2H), 1.23-1.08 (m, 15H); ^{13}C NMR (100 MH z, $CDCl_3$): δ 168.8, 165.6, 163.5, 145.0, 140.9, 140.0, 132.0, 131.2, 129.8, 128.9, 128.6, 127.7, 127.0, 124.0, 121.5, 106.5, 84.4, 60.0, 53.6, 27.5, 22.8, 13.9; IR (neat, cm^{-1}): 2966, 1770, 1708, 1630, 1488, 1262, 1164, 1068, 1011; LRMS-ESI (*m/z*): 577.3 (M + H^+); HRMS-MALDI/DHB: Calcd. for $C_{32}H_{33}O_5BrNa^+$: 599.1404; Found: 599.1409.



2-(2,6-diisopropylphenyl) 4-ethyl 3-(2-chlorophenyl)-5-phenyl-2,3-dihydrofuran-2,4-dicarboxylate (3i)

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.06-8.04 (m, 2H), 7.48-7.38 (m, 5H), 7.31-7.17 (m, 5H), 5.51 (d, *J* = 3.6 Hz, 1H), 5.21 (d, *J* = 3.2 Hz, 1H), 4.12-3.98 (m, 2H), 3.01 (br, 2H), 1.23-1.17 (m, 12 H), 1.07 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MH z, $CDCl_3$): δ 168.6, 166.7, 164.0, 145.4, 140.5, 139.3, 133.7, 131.6, 130.2, 129.2, 129.0, 128.7, 128.1, 127.8, 127.3, 124.4, 106.2, 84.7, 60.4, 50.3, 27.8, 23.9, 23.3, 14.3; IR (neat, cm^{-1}): 2967, 1765, 1708, 1630, 1494, 1468, 1445, 1366, 1309, 1264, 1169, 1143, 1069; LRMS-ESI (*m/z*): 555.3 (M + H^+); HRMS-MALDI/DHB: Calcd. for $C_{32}H_{33}O_5ClNa^+$: 555.1909; Found: 555.1893.



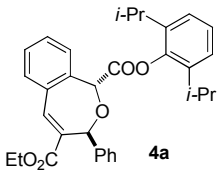
2-(2,6-diisopropylphenyl) 4-ethyl 5-phenyl-3-(m-tolyl)-2,3-dihydrofuran-2,4-dicarboxylate (3j)

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.04-8.02 (m, 2H), 7.48-7.40 (m, 3H), 7.29-7.11 (m, 7H), 5.29 (d,

J = 3.2 Hz, 1H), 4.86 (d, *J* = 3.6 Hz, 1H), 4.12-3.99 (m, 2H), 2.95 (br, 2H), 2.37 (s, 3H), 1.24-1.08 (m, 15H); ^{13}C NMR (100 MH z, $CDCl_3$): δ 169.4, 165.7, 164.2, 145.5, 142.5, 140.5, 138.9, 131.4, 130.3, 129.3, 129.1, 128.7, 128.2, 128.1, 127.3, 124.6, 124.4, 107.4, 85.2, 60.3, 54.5, 27.9, 23.2, 21.8, 14.3; IR (neat, cm^{-1}): 2966, 1771, 1708, 1629, 1493, 1446, 1258, 1193, 1164, 1067; LRMS-ESI (*m/z*): 513.4 (M + H^+); HRMS-MALDI/DHB: Calcd. for $C_{33}H_{36}O_5Na^+$: 535.2455; Found: 535.2440.

7. General procedure for Condition B

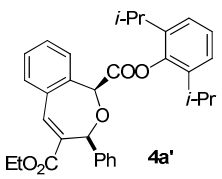
$CuPF_6(CH_3CN)_4$ (15 mg, 0.04 mmol), **L4** (21 mg, 0.042 mmol), 200 mg M.S. 4Å, and CH_2Cl_2 (2 mL) were stirred under nitrogen for 1 hour at 31 °C. Then the substrate (**1**) (0.5 mmol) was added, and the mixture was stirred for another 5 min. Then, a solution of the 2,6-diisopropylphenyl diazoacetate (**2**) (492 mg, 2.0 mmol) in CH_2Cl_2 (2.0 mL) was dropwise added through a syringe pump for 9-10 hours. After another 1 h of stirring at 31 °C, the mixture was filtered through a thin layer (40 mm) of silica gel (100-200 mesh), and washed with DCM to remove the catalyst. The filtrate was concentrated under reduced pressure, and the residue was purified by flash chromatography.



4a

1-(2,6-diisopropylphenyl) 4-ethyl 3-phenyl-1,3-dihydrobenzo[c]oxepine-1,4-dicarboxylate (4a)

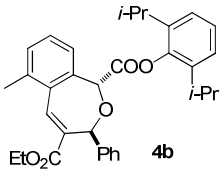
^{1}H NMR (300 MHz, $CDCl_3$): δ 7.93 (s, 1H), 7.60 (d, *J* = 7.5 Hz, 1H), 7.46-7.10 (m, 11H), 6.49 (s, 1H), 5.57 (s, 1H), 4.17-4.03 (m, 2H), 2.69 (hept, *J* = 6.9 Hz, 2H), 1.11-1.06 (m, 15H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 168.1, 166.3, 144.8, 140.1, 140.0, 139.4, 139.0, 134.4, 134.1, 132.7, 129.1, 128.9, 128.7, 128.6, 128.5, 127.0, 126.8, 123.9, 80.4, 75.9, 61.1, 27.1, 23.7, 13.8; IR (neat, cm^{-1}): 3063, 3030, 2965, 2931, 2870, 1760, 1713, 1634, 1494, 1464, 1454, 1385, 1364, 1292, 1255, 1203, 1161, 1127, 1094, 1060, 1029; LRMS-ESI (*m/z*): 521.3 (M+Na^+); HRMS-MALDI/DHB: Calcd. for $C_{32}H_{34}NaO_5^+$: 521.2298; Found: 521.2307.



4a'

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.87 (s, 1H), 7.61 (d, *J* = 7.6 Hz, 1H), 7.52 (d, *J* = 7.6 Hz, 1H),

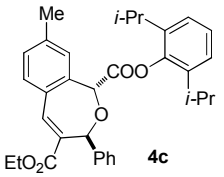
7.45 (t, *J* = 7.6 Hz, 1H), 7.39-7.35 (m, 3H), 7.30-7.27 (m, 3H), 7.24-7.22 (m, 1H), 7.19-7.17 (m, 2H), 6.22 (d, *J* = 1.6 Hz, 1H), 5.66 (s, 1H), 4.19-4.02 (m, 2H), 3.09 (hept, 2H), 1.25-1.10 (m, 15H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 168.0, 166.4, 145.4, 140.3, 138.8, 138.6, 138.3, 136.4, 134.0, 133.6, 129.1, 128.8, 128.4, 128.3, 128.2, 126.9, 125.0, 124.0, 86.7, 78.8, 61.0, 27.3, 23.3, 13.9; LRMS-ESI (*m/z*): 521.5 ($M+Na^+$).



4b

1-(2,6-diisopropylphenyl) 4-ethyl 6-methyl-3-phenyl-1,3-dihydrobenzo[c]oxepine-1,4-dicarboxylate (4b)

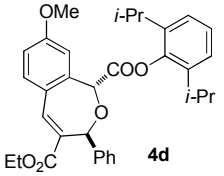
^{1}H NMR (300 MHz, $CDCl_3$): δ 8.14 (s, 1H), 7.35-7.08 (m, 11H), 6.58 (s, 1H), 5.62 (s, 1H), 4.20-4.06 (m, 2H), 2.66 (br, 2H), 2.49 (s, 3H), 1.16-1.10 (m, 12H), 0.85 (br, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 168.6, 166.2, 145.1, 140.7, 140.1, 139.3, 139.3, 135.9, 135.3, 131.4, 130.9, 129.3, 128.2, 128.0, 127.9, 126.7, 126.7, 123.8, 78.8, 61.2, 29.6, 27.3, 23.1, 20.3, 13.9; IR (neat, cm^{-1}): 3065, 3030, 2965, 2870, 1763, 1713, 1631, 1598, 1493, 1464, 1384, 1364, 1246, 1207, 1164, 1123, 1094, 1076, 1028; LRMS-ESI (*m/z*): 535.3 ($M+Na^+$); HRMS-ESI: Calcd. for $C_{33}H_{37}O_5^+$: 513.2641; Found: 513.2632.



4c

1-(2,6-diisopropylphenyl) 4-ethyl 8-methyl-3-phenyl-1,3-dihydrobenzo[c]oxepine-1,4-dicarboxylate (4c)

^{1}H NMR (300 MHz, $CDCl_3$): δ 7.92 (s, 1H), 7.52-7.11 (m, 11H), 6.43 (s, 1H), 5.51 (s, 1H), 4.19-4.00 (m, 2H), 2.71 (br, 2H), 2.38 (s, 3H), 1.10-1.06 (m, 15H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 168.1, 166.3, 144.8, 140.0, 139.9, 139.5, 139.2, 139.0, 134.3, 132.9, 129.9, 129.1, 128.9, 128.4, 128.3, 127.3, 126.6, 123.8, 80.4, 75.4, 60.8, 26.9, 23.6, 21.2, 13.7; IR (neat, cm^{-1}): 3064, 3030, 2965, 2930, 2871, 1763, 1712, 1709, 1633, 1611, 1455, 1385, 1364, 1295, 1260, 1203, 1163, 1142, 1095, 1051; LRMS-ESI (*m/z*): 535.3 ($M+Na^+$); HRMS-ESI: Cacld. for $C_{33}H_{36}NaO_5^+$: 535.2460; Found: 535.2452.

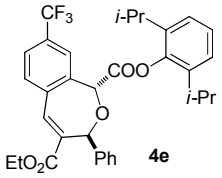


4d

1-(2,6-diisopropylphenyl) 4-ethyl 8-methoxy-3-phenyl-1,3-dihydrobenzo[c]oxepine-1,4-dicarboxylate (4d)

^{1}H NMR (300 MHz, $CDCl_3$): δ 7.90 (s, 1H), 7.54 (d, *J* = 8.4 Hz, 1H), 7.42-6.91 (m, 10H), 6.45 (s,

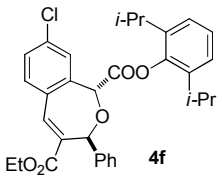
1H), 5.51 (s, 1H), 4.15-4.02 (m, 2H), 3.83 (s, 3H), 2.71 (hep, J = 6.3 Hz, 2H), 1.11-1.06 (m, 15H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 167.9, 166.4, 160.2, 144.8, 141.0, 140.0, 139.9, 138.9, 136.1, 131.0, 128.9, 128.3, 126.6, 125.3, 123.8, 113.7, 112.6, 80.4, 75.5, 60.7, 55.3, 27.0, 23.4, 13.8; IR (neat, cm^{-1}): 2966, 2870, 1759, 1709, 1606, 1568, 1505, 1458, 1289, 1259, 1204, 1164, 1123, 1046; LRMS-ESI (*m/z*): 551.3 ($M+Na^+$); HRMS-ESI: Calcd. for $C_{33}H_{37}O_6^+$: 529.2590; Found: 529.2584.



4e

1-(2,6-diisopropylphenyl) 4-ethyl 3-phenyl-8-(trifluoromethyl)-1,3-dihydrobenzo[c]oxepine-1,4-dicarboxylate (4e)

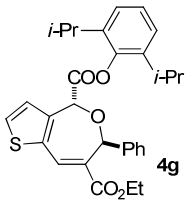
^{1}H NMR (300 MHz, $CDCl_3$): δ 7.93 (s, 1H), 7.72-7.68 (m, 3H), 7.40-7.30 (m, 5H), 7.30-7.11 (m, 3H), 6.48 (s, 1H), 5.60 (s, 1H), 4.18-4.03 (m, 2H), 2.66 (hept, J = 6.3 Hz, 2H), 1.27-0.88 (m, 15H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 167.5, 165.9, 144.8, 140.2, 140.0, 139.4, 137.3, 136.9, 136.2, 134.4, 130.9, 129.1, 128.8, 127.0, 125.5, 125.4, 124.0, 123.7, 80.8, 75.2, 61.4, 27.2, 23.8, 22.7, 13.8; ^{19}F NMR (376 MHz, $CDCl_3$): −62.67. IR (neat, cm^{-1}): 3065, 2967, 2931, 2872, 1763, 1717, 1638, 1493, 1456, 1386, 1365, 1333, 1261, 1205, 1081, 1051, 1018; LRMS-ESI (*m/z*): 589.3 ($M+Na^+$); HRMS-ESI: Calcd. for $C_{33}H_{34}F_3O_5^+$: 567.2353; Found: 567.2346.



4f

1-(2,6-diisopropylphenyl) 4-ethyl 8-chloro-3-phenyl-1,3-dihydrobenzo[c]oxepine-1,4-dicarboxylate (4f)

^{1}H NMR (300 MHz, $CDCl_3$): δ 7.88 (s, 1H), 7.53-7.11 (m, 11H), 6.44 (s, 1H), 5.50 (s, 1H), 4.17-4.02 (m, 2H), 2.68 (br, 2H), 1.09-1.04 (m, 15H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 167.6, 166.1, 144.7, 141.0, 140.1, 139.6, 137.8, 135.4, 135.3, 134.6, 131.3, 129.0, 128.7, 126.9, 126.9, 124.0, 80.7, 74.9, 61.1, 27.1, 23.7, 13.8; IR (neat, cm^{-1}): 3064, 3031, 2966, 2871, 2254, 1767, 1716, 1635, 1592, 1561, 1491, 1465, 1385, 1365, 1249, 1201, 1051, 1019; LRMS-ESI (*m/z*): 555.2 ($M+Na^+$); HRMS-ESI: Cacld. for $C_{32}H_{34}ClO5^+$: 533.2089; Found: 533.2103.

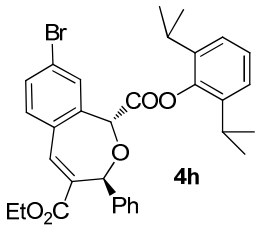


4g

4-(2,6-diisopropyl-benzoyl)-6-phenyl-4,6-dihydro-thieno[3,2-c]oxepine-7-carboxylic acid ethyl ester (4g)

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.96 (s, 1H), δ 7.43-7.33 (m, 6H), δ 7.24-7.20 (m, 1H), 7.16-7.13

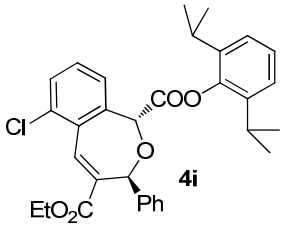
(m, 3H), 6.50 (s, 1H), 5.19 (s, 1H), 4.17 (q, 2H), 2.81 (br, 2H), 1.22-1.11 (m, 15H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 168.1, 166.0, 145.1, 142.0, 140.2, 138.0, 134.8, 130.9, 130.5, 129.3, 129.1, 129.0, 128.7, 127.9, 126.8, 124.0, 80.2, 72.7, 61.1, 27.1, 23.5, 14.1; IR (neat, cm^{-1}): 2965, 2931, 2870, 1748, 1705, 1624, 1466, 1453, 1364, 1162, 1095, 1061; LRMS-ESI (*m/z*): 527.3 ($M+Na^+$); HRMS-ESI: Cacld. for $C_{30}H_{32}NaO_5S^+$: 527.1863; Found: 527.1839.



4h

1-(2,6-diisopropylphenyl) 4-ethyl 8-bromo-3-phenyl-1,3-dihydrobenzo[c]oxepine-1,4-dicarboxylate (4h)

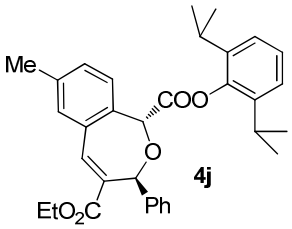
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.86 (s, 1H), 7.59-7.11 (m, 11H), 6.42 (d, J = 1.2 Hz, 1H), 5.49 (s, 1H), 4.20-4.00 (m, 2H), 2.65 (br, 2H), 1.10-1.05 (m, 15H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.6, 166.1, 144.8, 141.2, 140.1, 139.6, 137.9, 135.6, 134.8, 131.7, 129.8, 129.1, 128.7, 126.9, 124.0, 123.6, 80.7, 74.9, 61.2, 27.1, 23.7, 23.1, 13.8; IR (neat, cm^{-1}): 2966, 1766, 1712, 1635, 1587, 1455, 1385, 1365, 1253, 1201, 1159, 1094, 1050; LRMS-EI (*m/z*): 577, 530, 355, 325, 299, 218, 189, 105, 91; HRMS-EI: Cacld. for $C_{32}H_{33}O_5Br$: 576.1511; Found: 576.1514.



4i

1-(2,6-diisopropylphenyl) 4-ethyl 6-chloro-3-phenyl-1,3-dihydrobenzo[c]oxepine-1,4-dicarboxylate (4i)

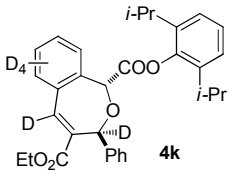
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.32 (s, 1H), 7.50-7.09 (m, 11H), 6.59 (s, 1H), 5.62 (s, 1H), 4.23-4.05 (m, 2H), 2.68 (br, 1H), 2.55 (br, 1H), 1.18-1.10 (m, 12H), 0.88 (br, 3H); ^{13}C NMR (75MHz, $CDCl_3$): δ 167.9, 165.7, 144.9, 141.1, 139.9, 137.0, 136.4, 134.4, 130.8, 130.2, 130.1, 128.4, 128.2, 127.1, 126.8, 123.9, 79.3, 76.6, 61.4, 27.3, 23.4, 13.9; IR (neat, cm^{-1}): 2966, 1764, 1713, 1442, 1385, 1365, 1247, 1182, 1162, 1121, 1094, 1065, 1019; LRMS-ESI (*m/z*): 533.3 ($M + H^+$); HRMS-MALDI/DHB: Cacld. for $C_{32}H_{33}O_5ClNa^+$: 555.1909; Found: 555.1892.



4j

1-(2,6-diisopropylphenyl) 4-ethyl 7-methyl-3-phenyl-1,3-dihydrobenzo[c]oxepine-1,4-dicarboxylate (4j)

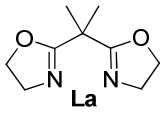
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.94 (s, 1H), 7.46-7.14 (m, 11H), 6.50 (s, 1H), 5.57 (s, 1H), 4.24-4.04 (m, 2H), 2.73 (hept, J = 7.6 Hz, 2H), 2.46 (s, 3H), 1.15-1.10 (m, 15H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 168.2, 166.3, 145.0, 140.1, 140.1, 139.2, 138.4, 136.6, 134.8, 134.2, 132.6, 129.8, 128.9, 128.5, 128.4, 127.0, 126.7, 123.9, 80.3, 75.7, 61.0, 27.0, 23.4, 20.9, 13.8; IR (neat, cm^{-1}): 2966, 1761, 1711, 1455, 1229, 1161, 1094, 1048; LRMS-ESI (*m/z*): 513.4 (M + H^+); HRMS-MALDI/DHB: Cacld. for $C_{33}H_{36}O_5Na^+$: 535.2455; Found: 535.2438.



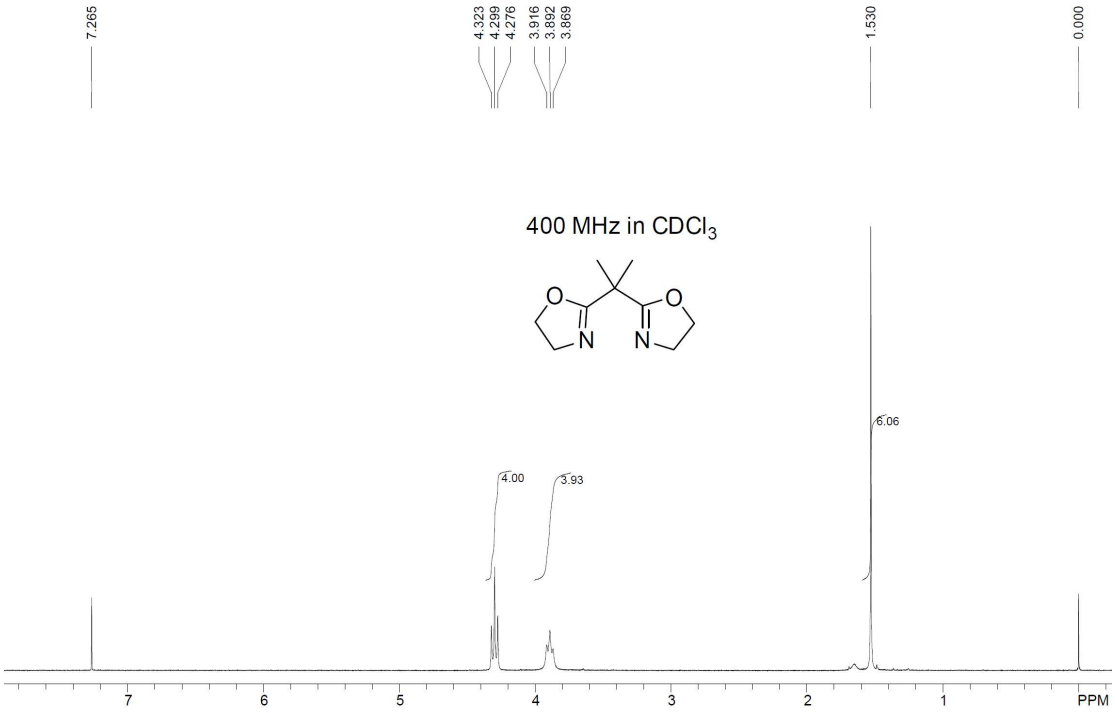
4k

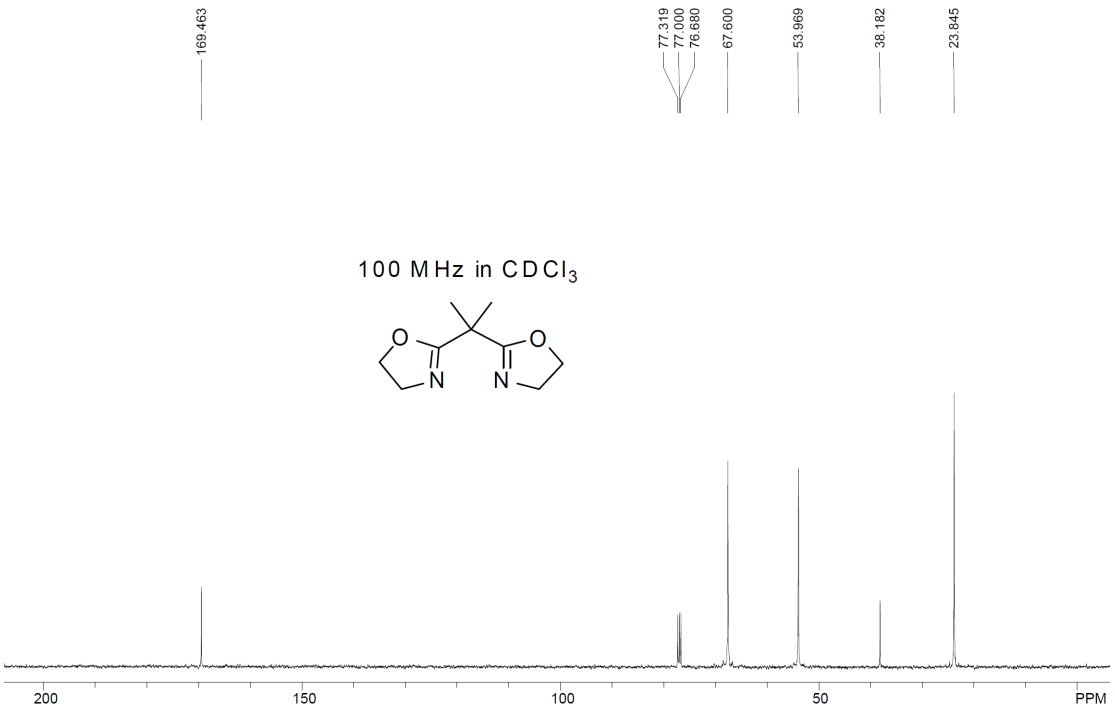
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.40-7.08 (m, 8H), 5.56 (s, 1H), 4.16-4.03 (m, 2H), 2.71 (hept, J = 7.0 Hz, 2H), 1.10-1.07 (m, 15H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 168.07, 166.24, 144.96, 140.17, 139.95, 139.39, 139.39, 138.56, 134.42, 133.60, 132.65, 128.91, 128.58, 128.52, 128.41, 128.11, 126.72, 123.91, 79.96, 75.94, 60.99, 27.09, 23.27, 22.57, 13.84; IR (neat, cm^{-1}): 2966, 2929, 2870, 1759, 1711, 1622, 1466, 1449, 1385, 1365, 1296, 1258, 1239, 1163, 1095, 1040; LRMS-ESI (*m/z*): 527.1 (M+Na^+); HRMS-ESI: Cacld. for $C_{32}H_{28}D_6NaO_5^+$: 527.2675; Found: 527.2682.

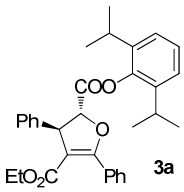
8. ^{1}H and ^{13}C NMR spectra



2,2'-(propane-2,2-diyl)bis(4,5-dihydrooxazole)

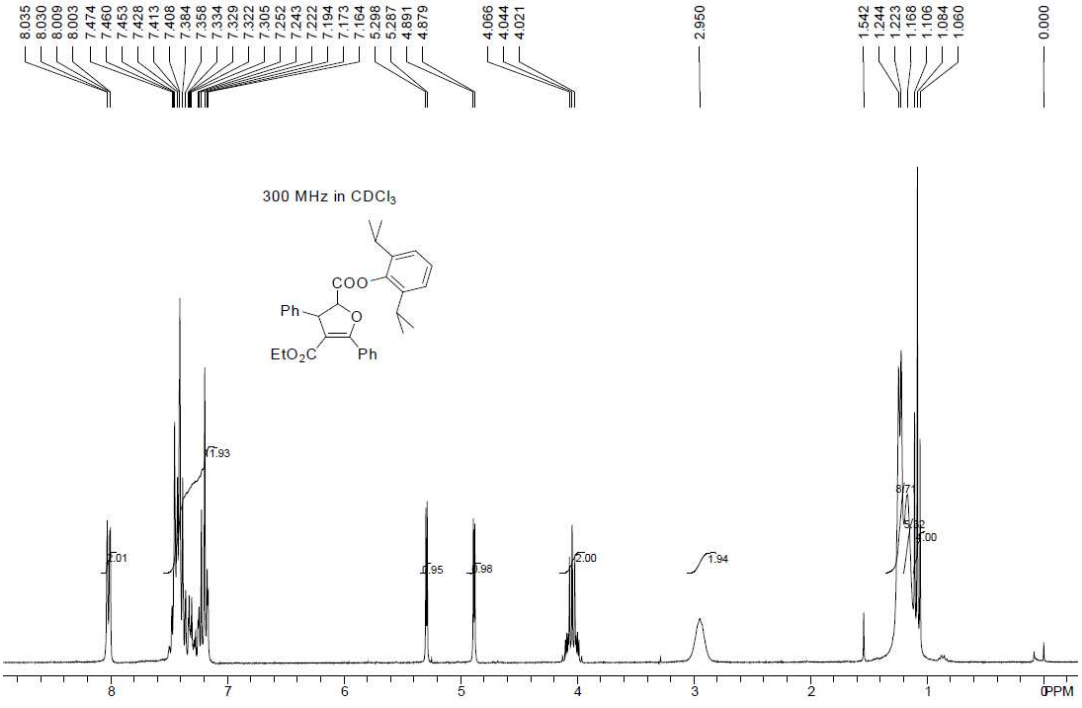


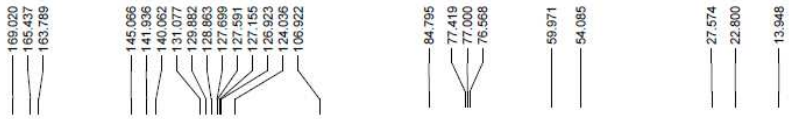


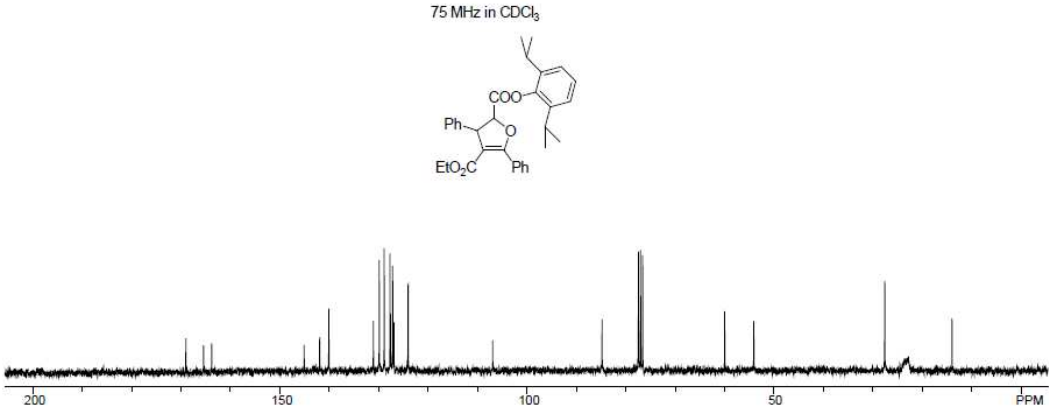


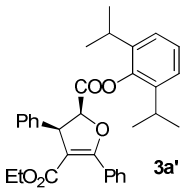
3a

Trans-2-(2,6-diisopropylphenyl) 4-ethyl 3,5-diphenyl-2,3-dihydrofuran-2,4-dicarboxylate (3a)



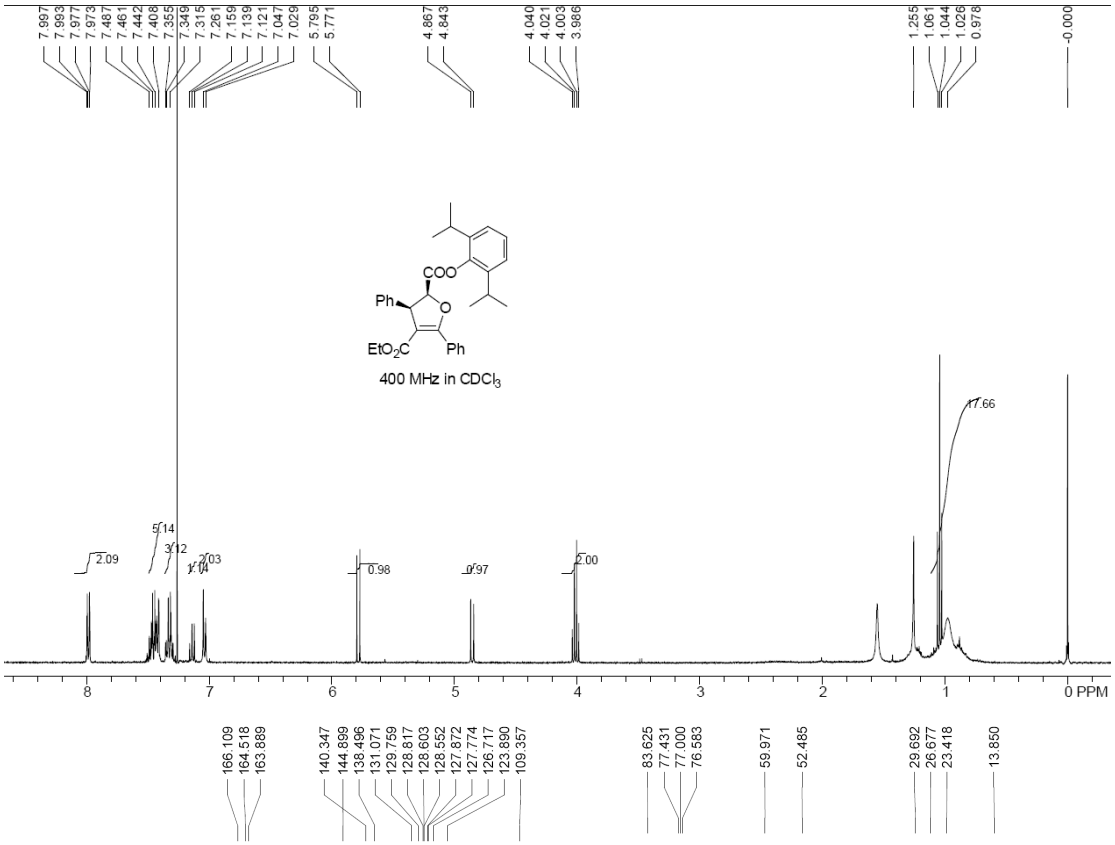


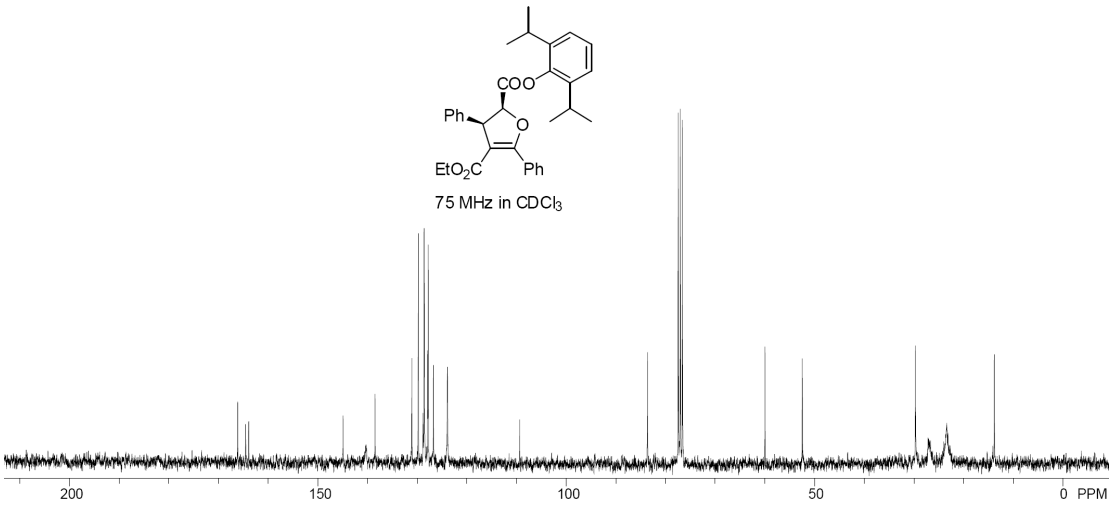


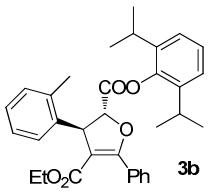


3a'

Cis-2-(2,6-diisopropylphenyl) 4-ethyl 3,5-diphenyl-2,3-dihydrofuran-2,4-dicarboxylate (3a')

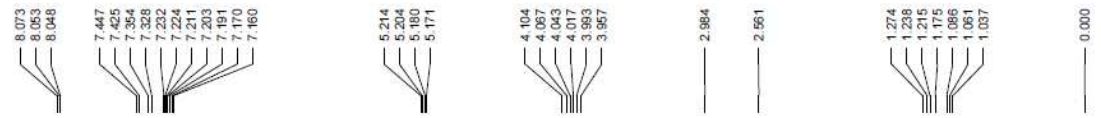


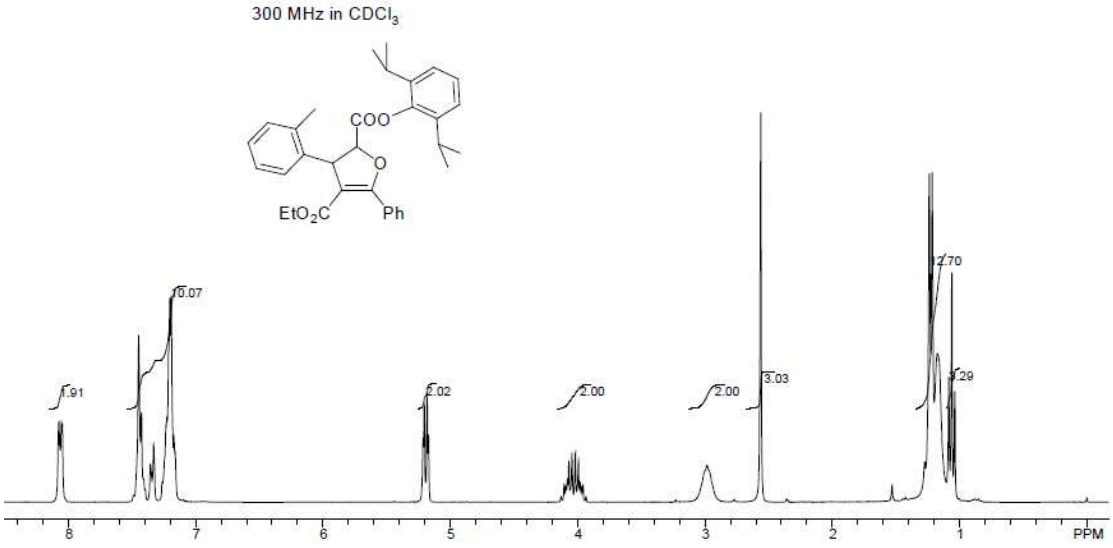


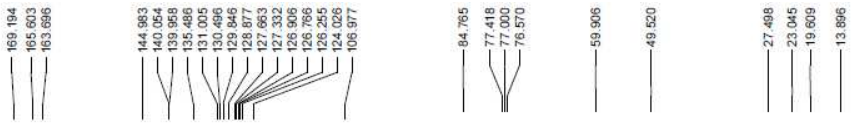


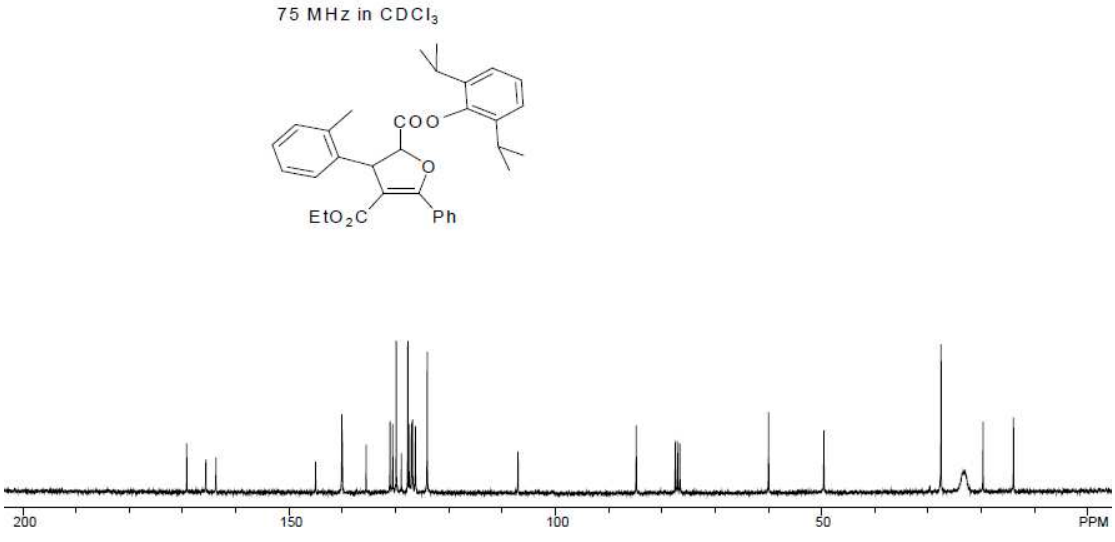
3b

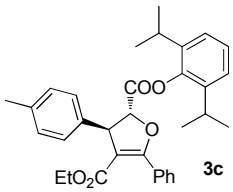
2-(2,6-diisopropylphenyl) 4-ethyl 5-phenyl-3-o-tolyl-2,3-dihydrofuran-2,4-dicarboxylate (3b)





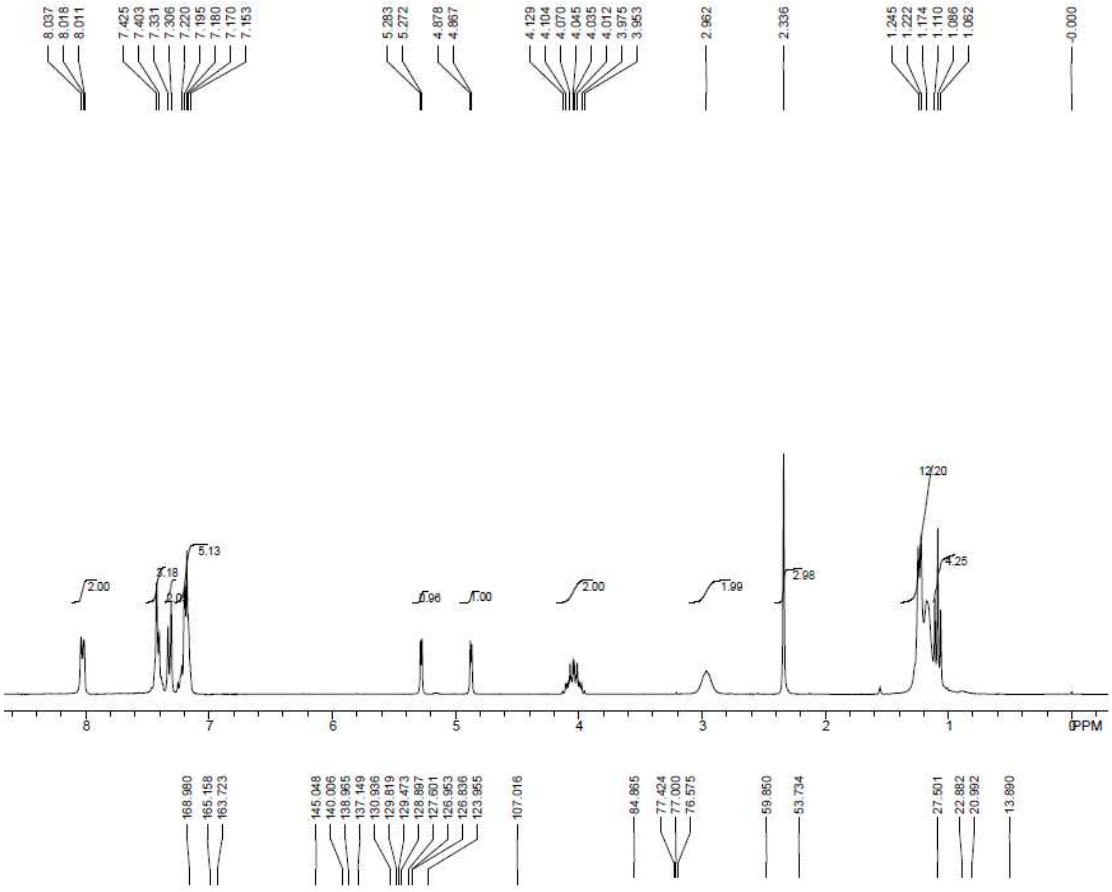




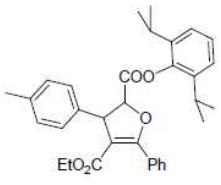


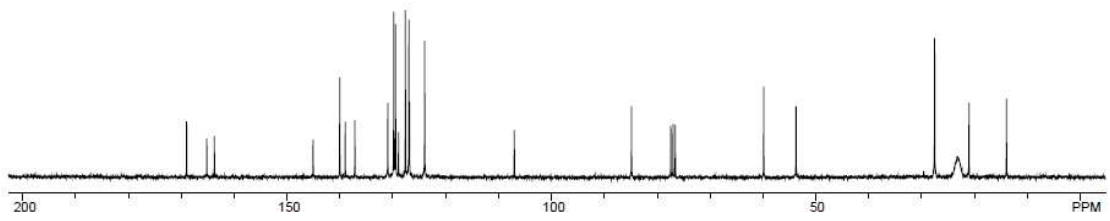
3c

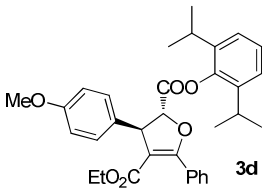
2-(2,6-diisopropylphenyl) 4-ethyl 5-phenyl-3-p-tolyl-2,3-dihydrofuran-2,4-dicarboxylate (3c)



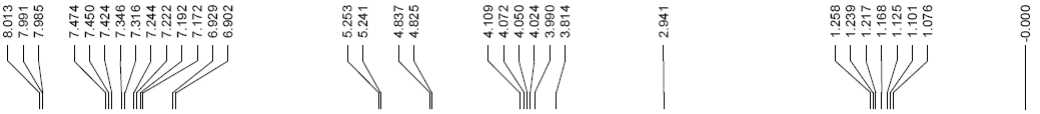
75 MHz in $CDCl_3$

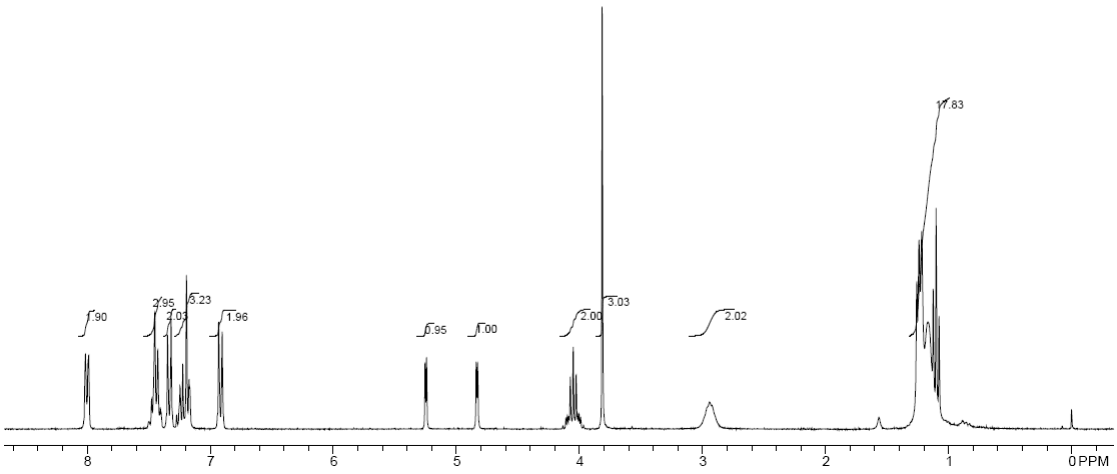




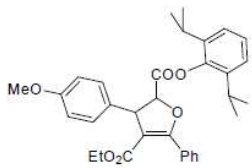


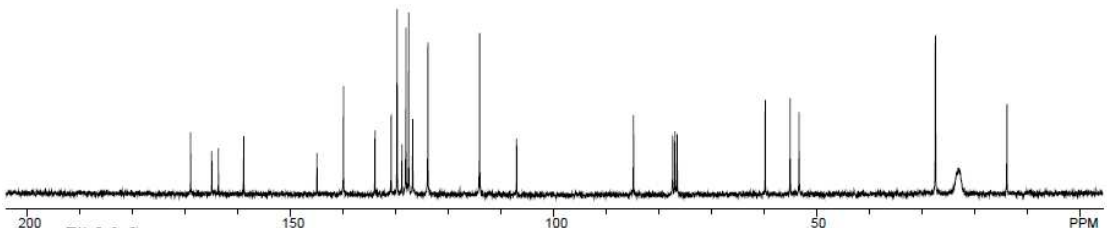
2-(2,6-diisopropylphenyl) 4-ethyl 3-(4-methoxyphenyl)-5-phenyl-2,3-dihydrofuran-2,4-dicarboxylate (3d)

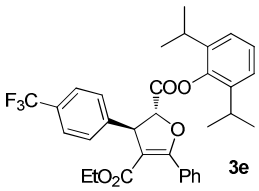




75 MHz in $CDCl_3$

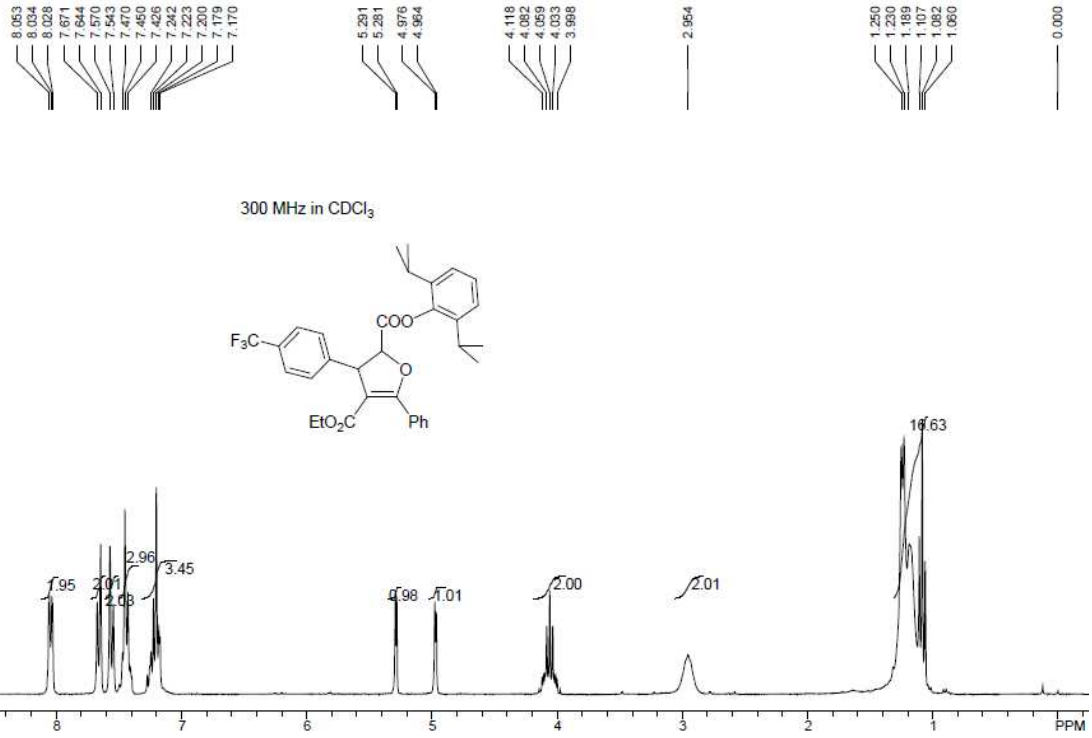


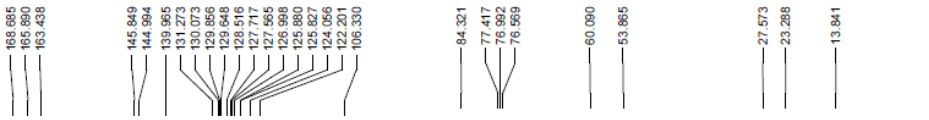


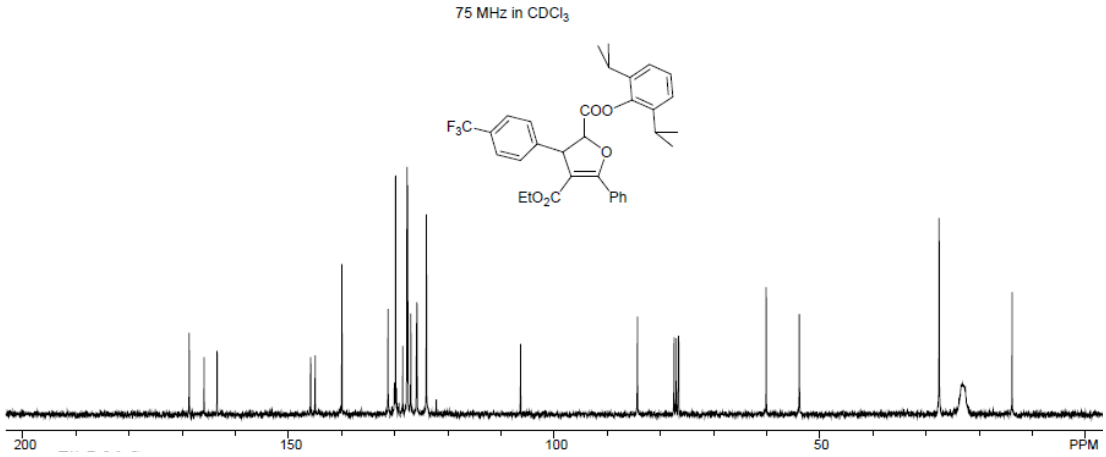


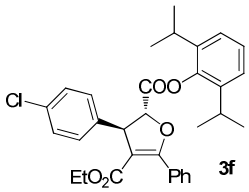
3e

2-(2,6-diisopropylphenyl) 4-ethyl 5-phenyl-3-(4-(trifluoromethyl)phenyl)-2,3-dihydrofuran-2,4-dicarboxylate (3e)

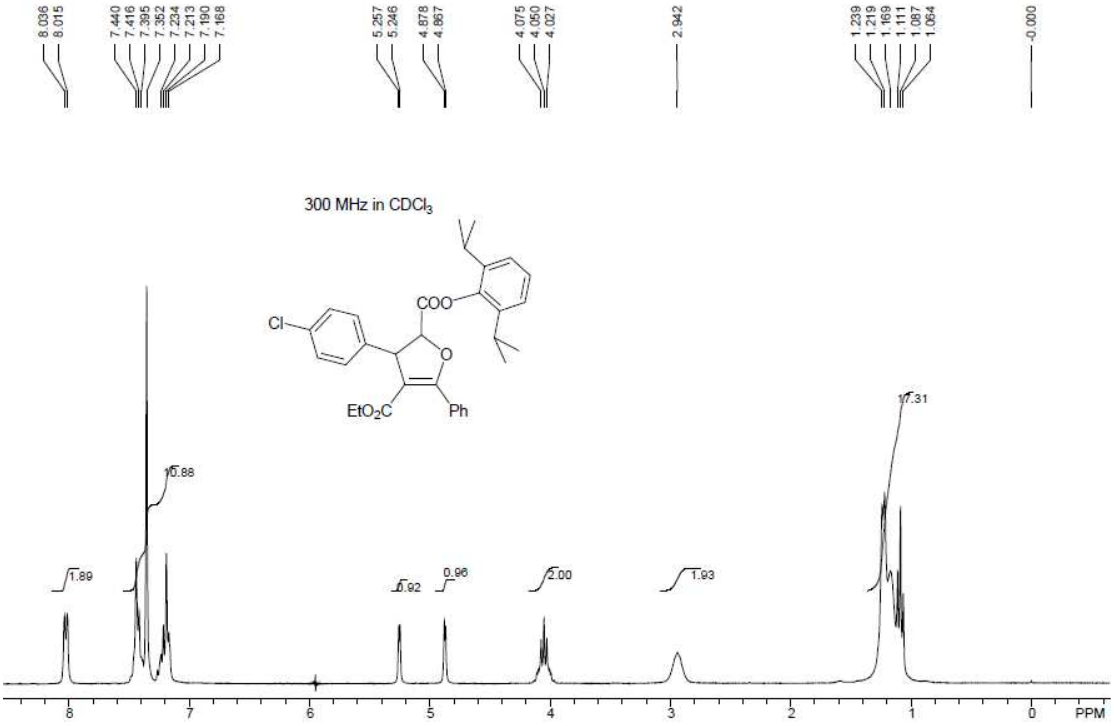


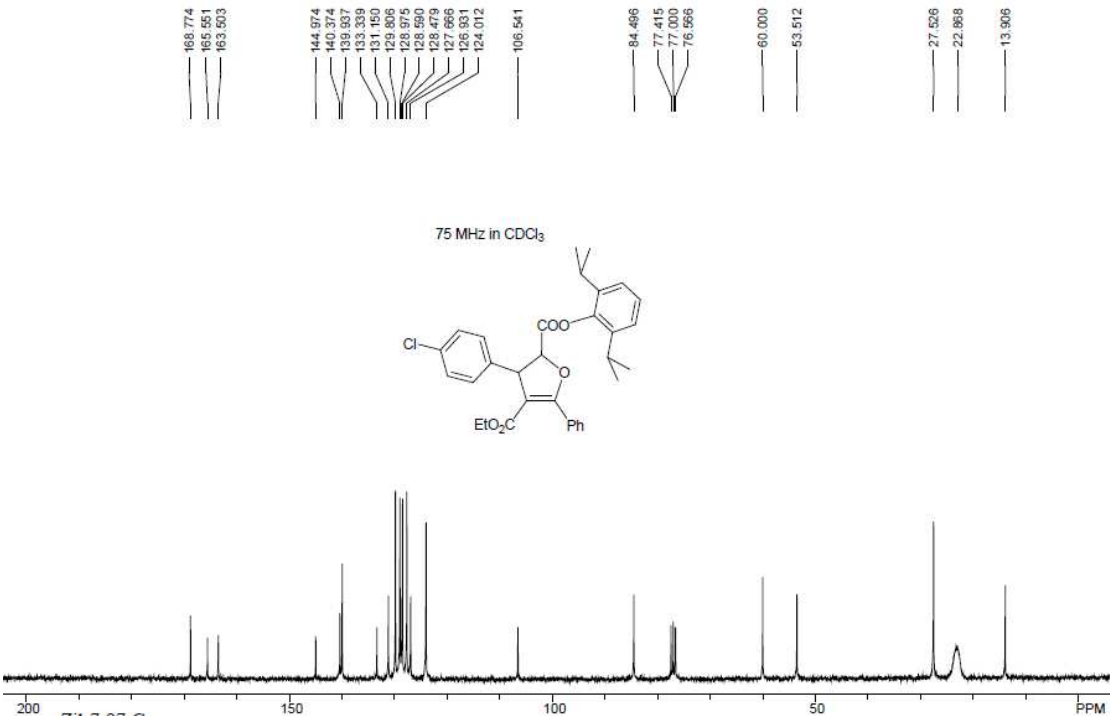


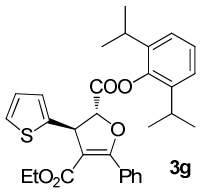




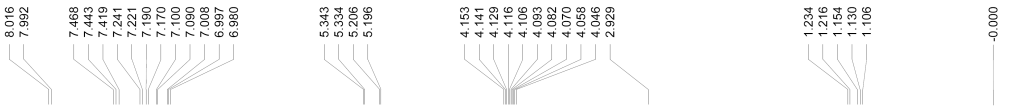
2-(2,6-diisopropylphenyl) 4-ethyl 3-(4-chlorophenyl)-5-phenyl-2,3-dihydrofuran-2,4-dicarboxylate (3f)

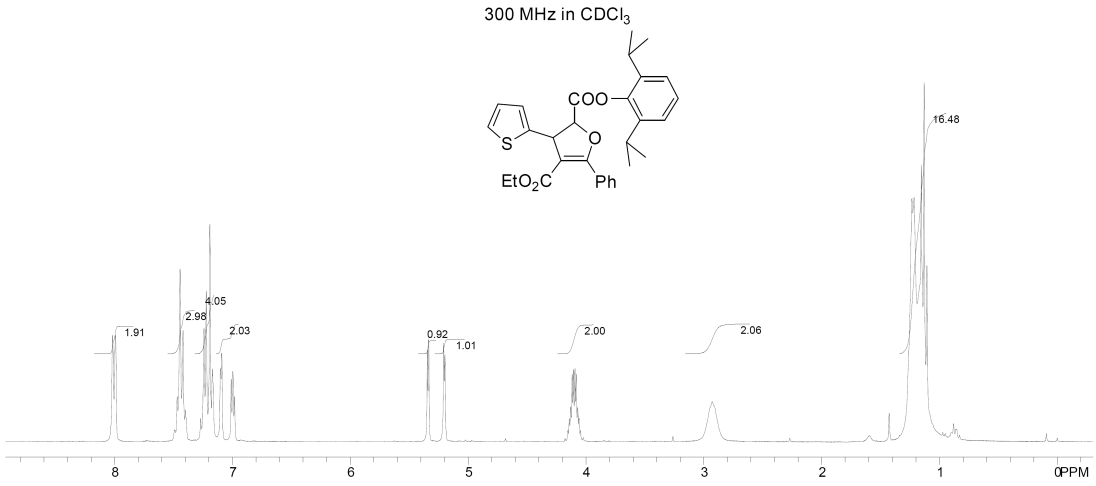


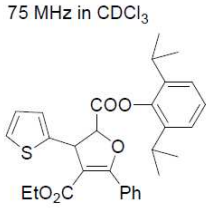


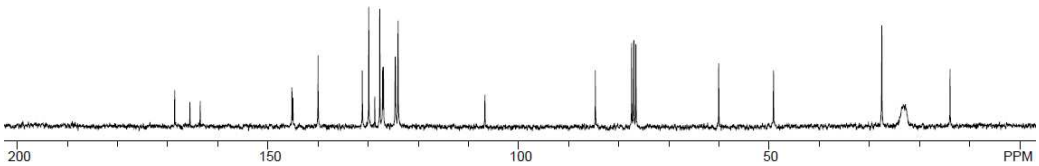


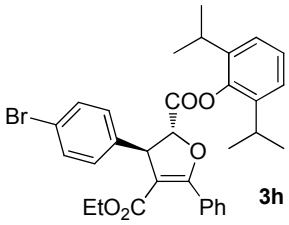
5-phenyl-3-thiophen-2-yl-2,3-dihydro-furan-2,4-dicarboxylic acid 2-(2,6-diisopropyl-phenyl) ester 4-ethyl ester (3g)





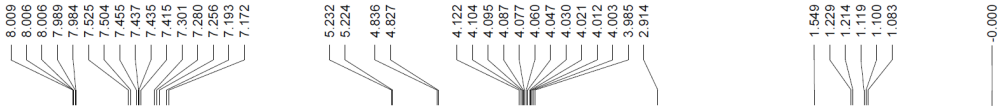


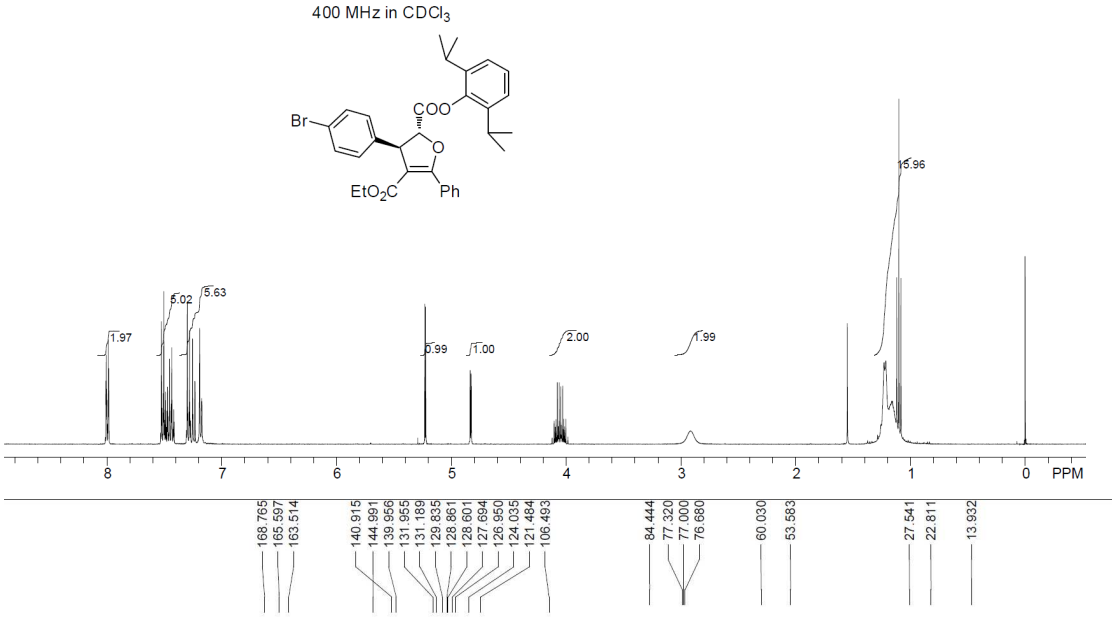


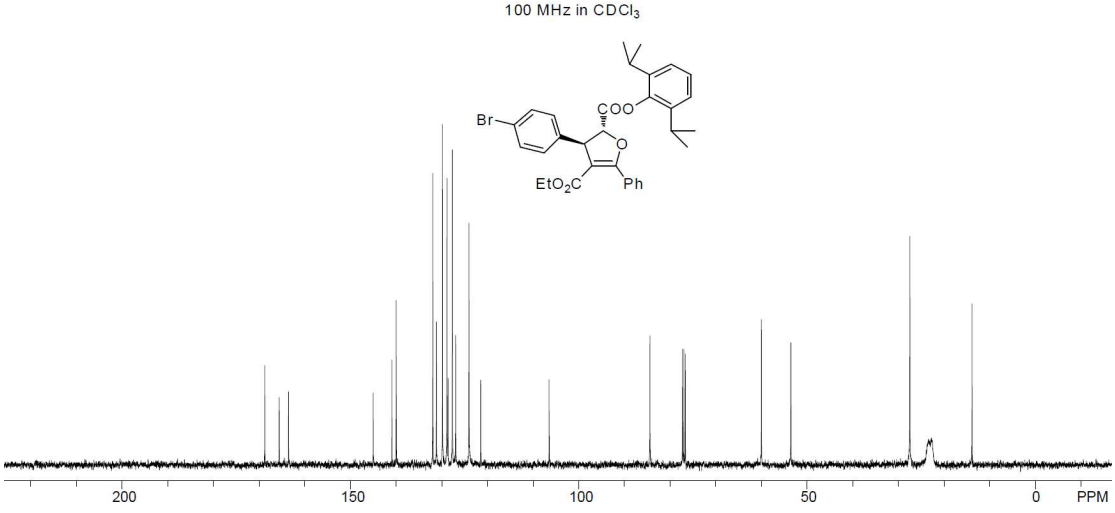


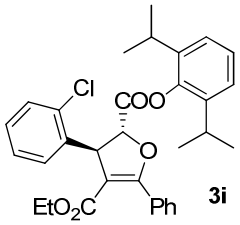
3h

2-(2,6-diisopropylphenyl) 4-ethyl 3-(4-bromophenyl)-5-phenyl-2,3-dihydrofuran-2,4-dicarboxylate (3h)



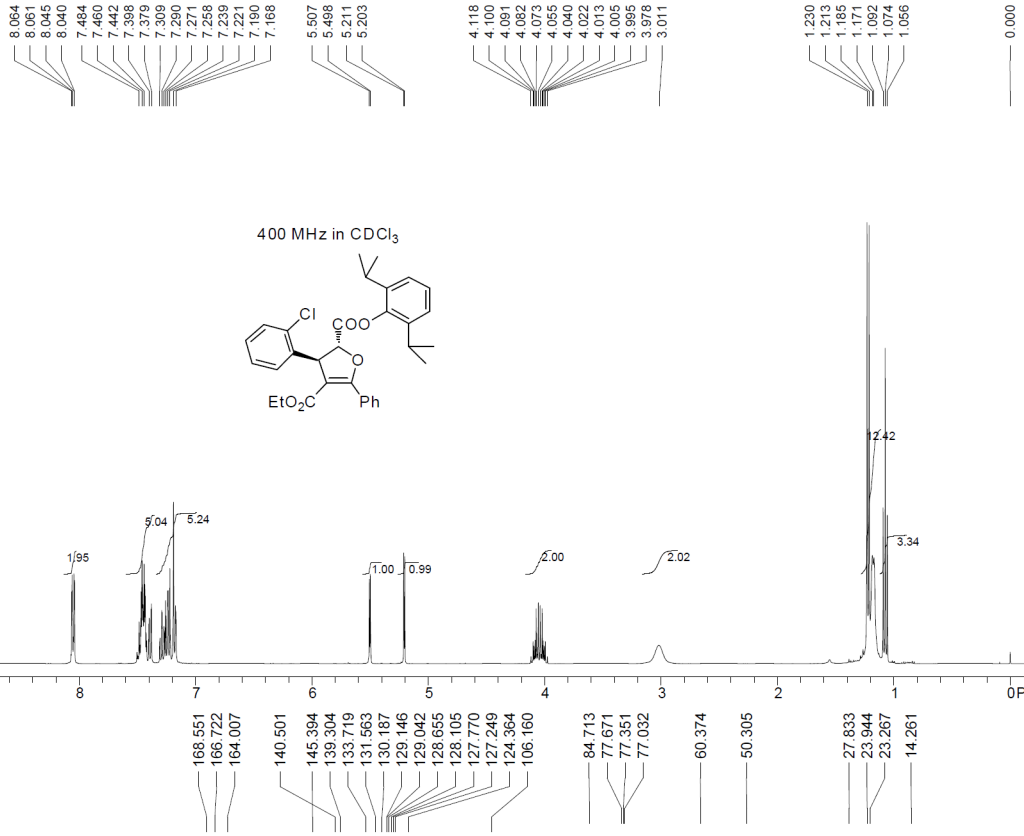


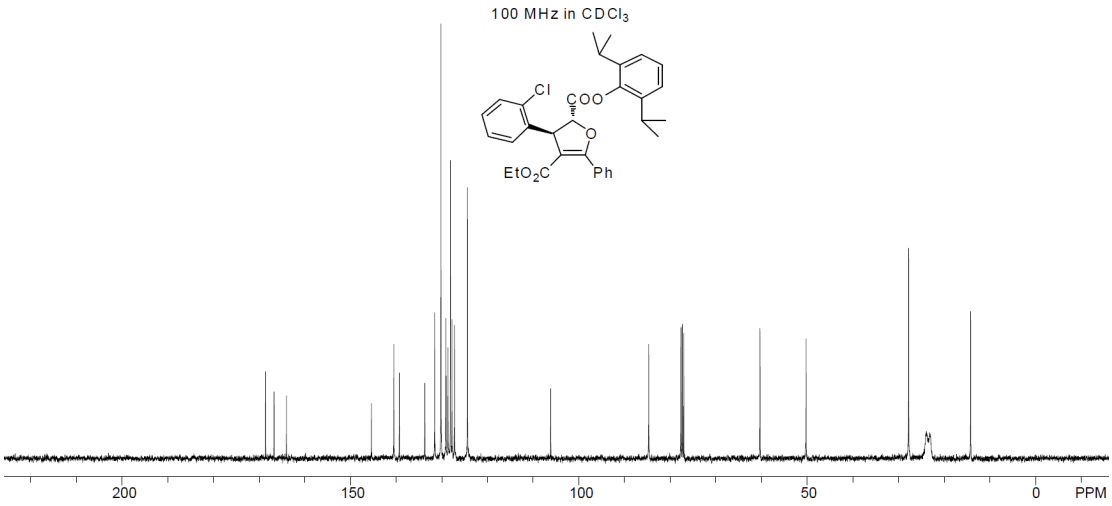


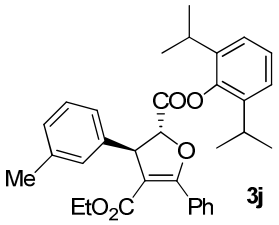


3i

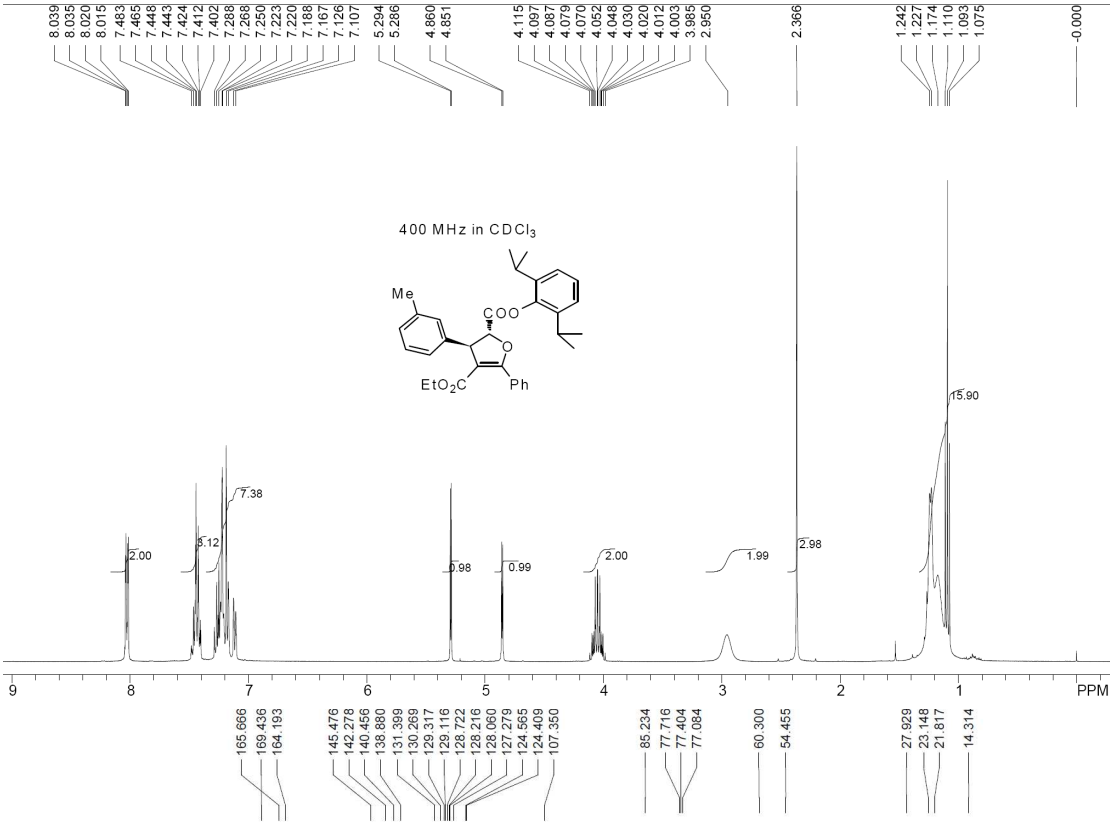
2-(2,6-diisopropylphenyl) 4-ethyl 3-(2-chlorophenyl)-5-phenyl-2,3-dihydrofuran-2,4-dicarboxylate (3i)

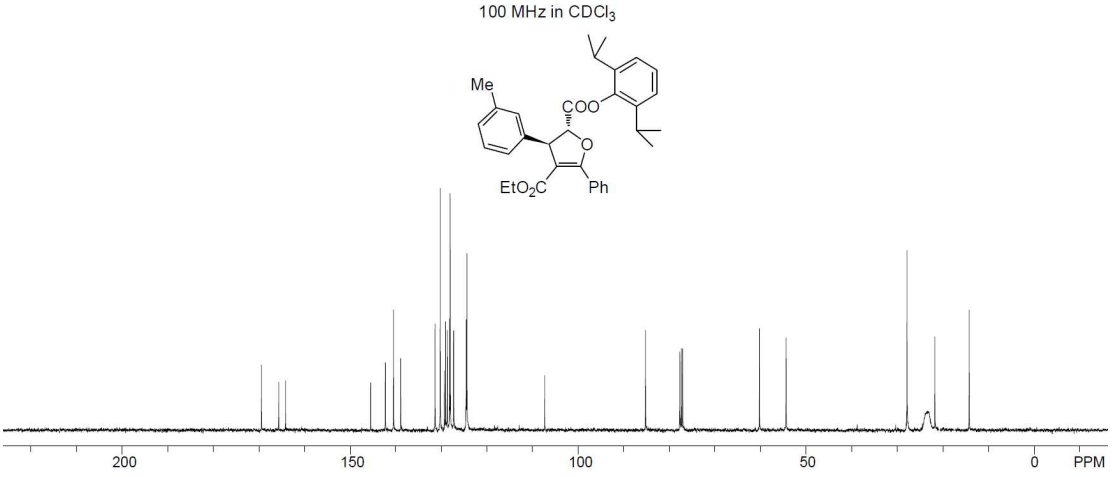


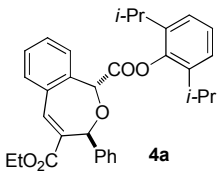




2-(2,6-diisopropylphenyl) 4-ethyl 5-phenyl-3-(m-tolyl)-2,3-dihydrofuran-2,4-dicarboxylate (3j)

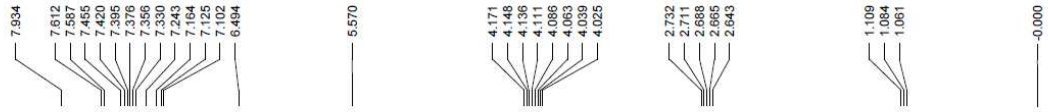


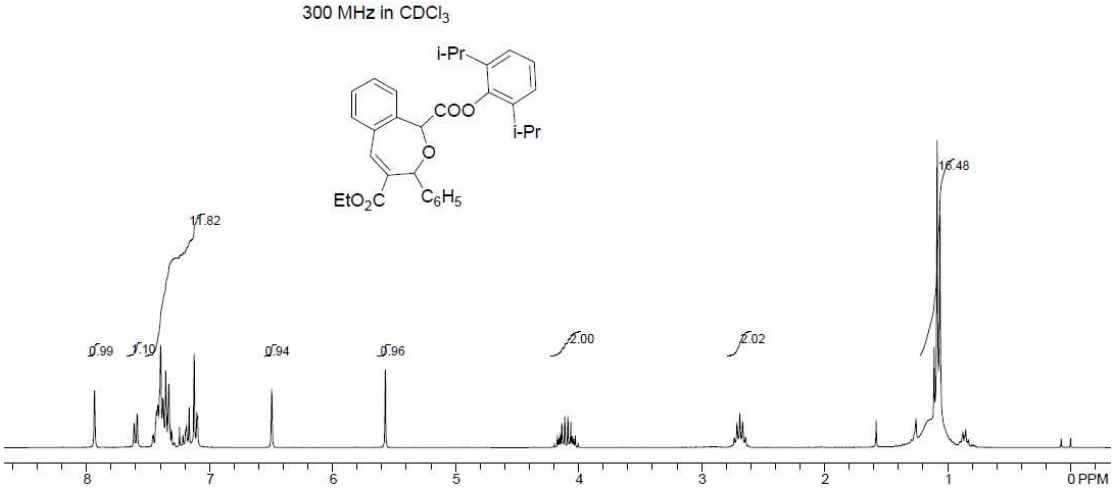


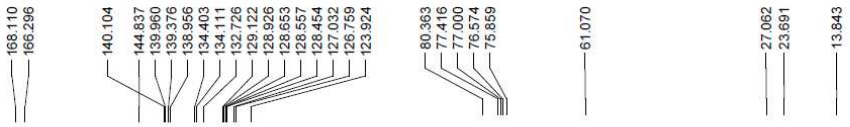


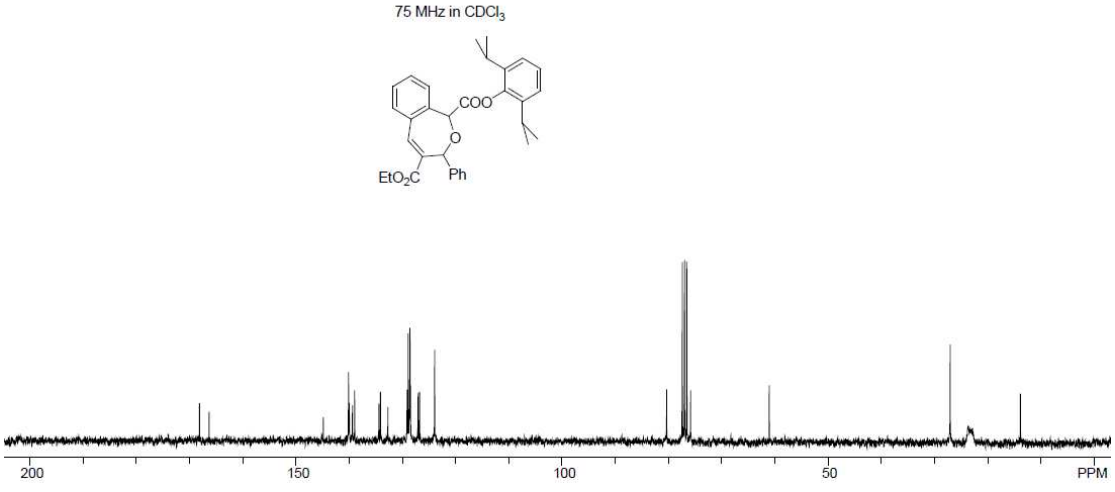
4a

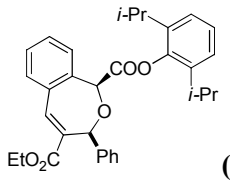
1-(2,6-diisopropylphenyl) 4-ethyl 3-phenyl-1,3-dihydrobenzo[c]oxepine-1,4-dicarboxylate (4a)







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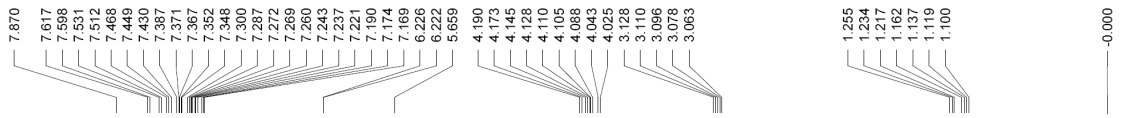
i-Pr
O
EtO2C
Ph

(4a')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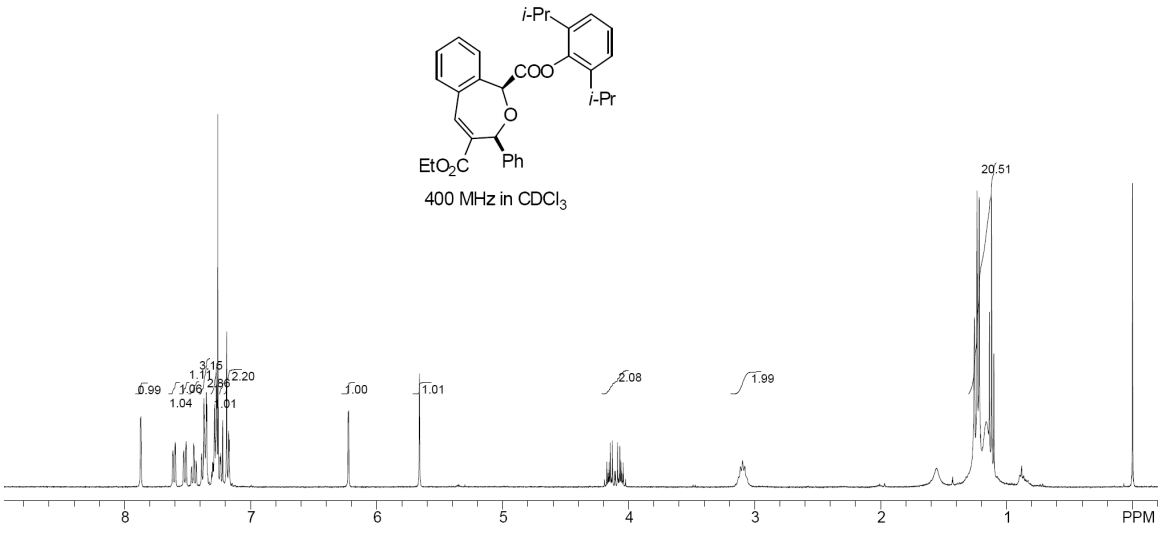
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COO
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O
EtO2C
Ph
400 MHz in CDCl3
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3.15
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7
6
5
4
3
2
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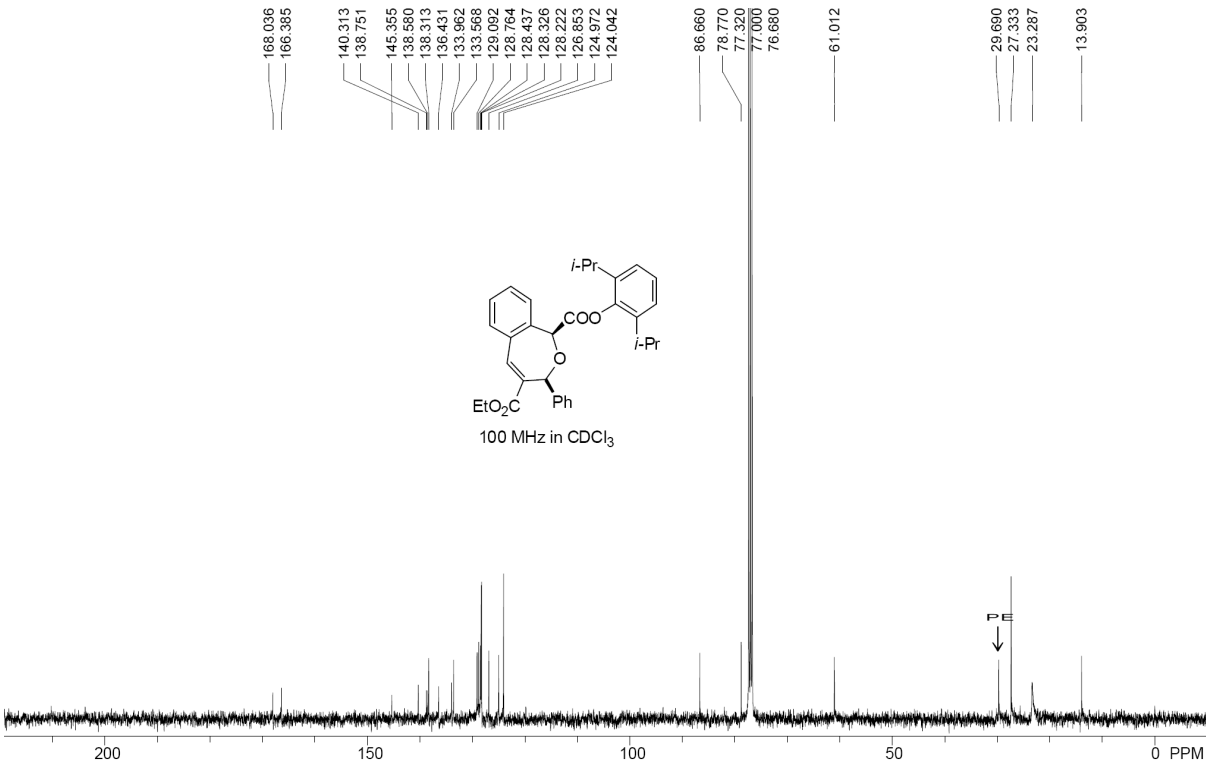
PPM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124.972
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61.012
29.690
27.333
23.287
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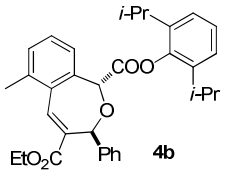
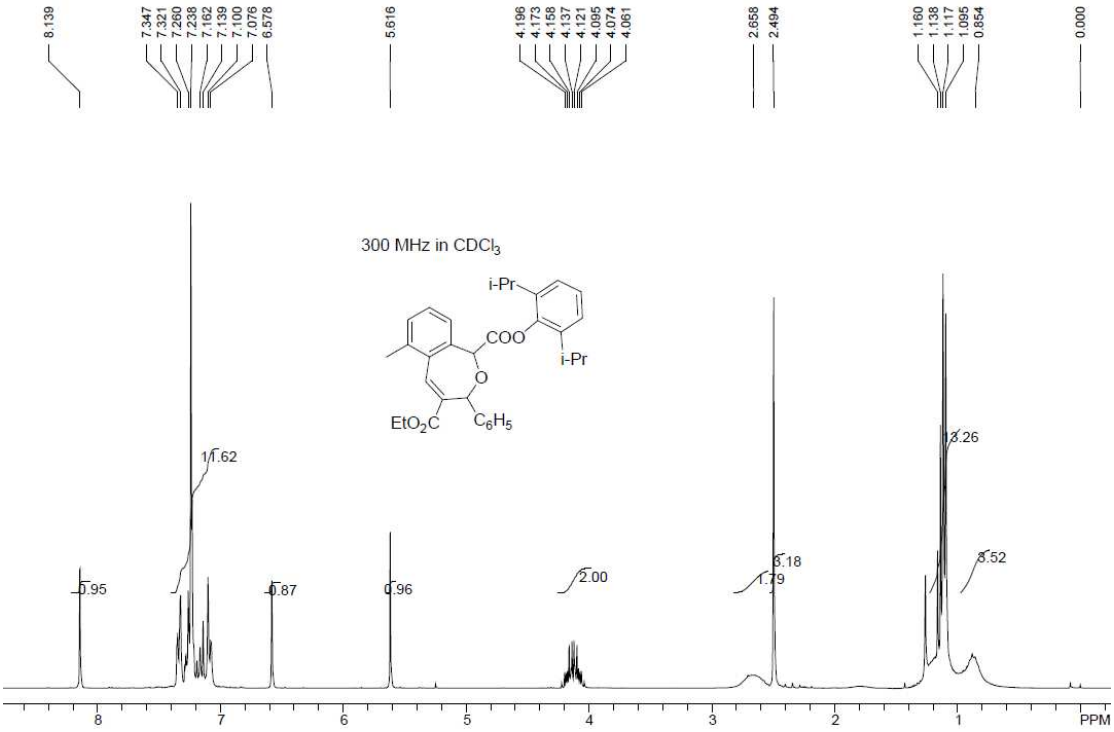
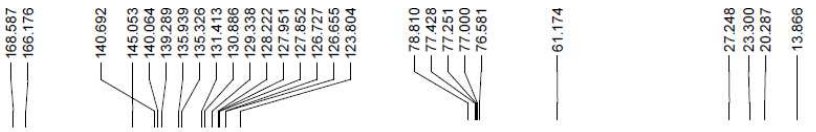
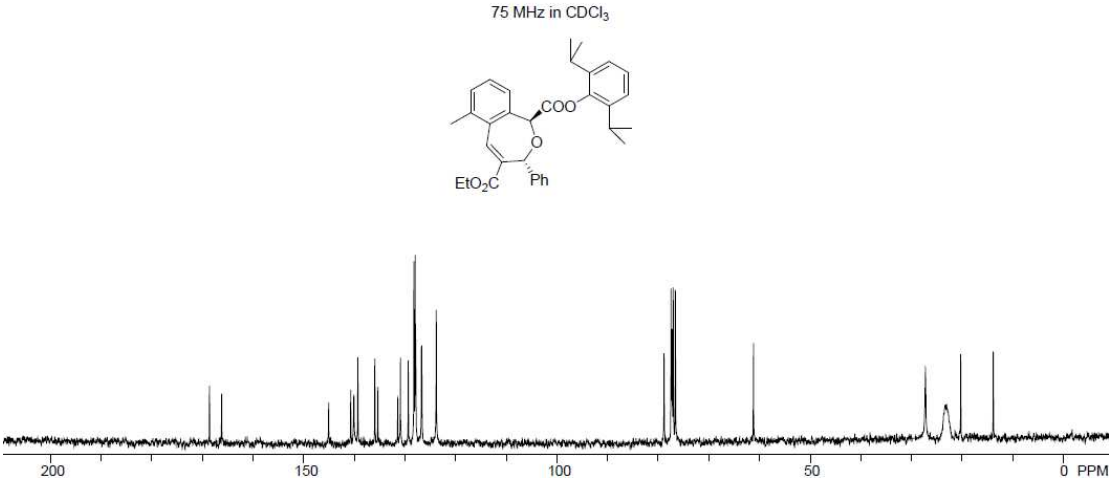


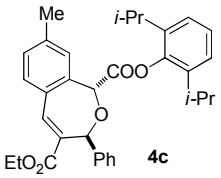
4b

1-(2,6-diisopropylphenyl) 4-ethyl 6-methyl-3-phenyl-1,3-dihydrobenzo[c]oxepine-1,4-dicarboxylate (4b)



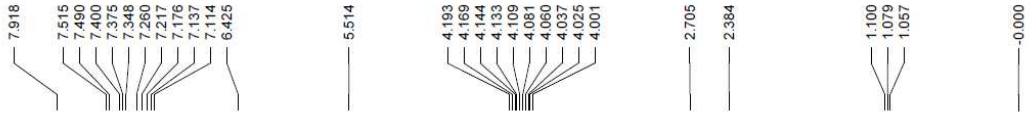


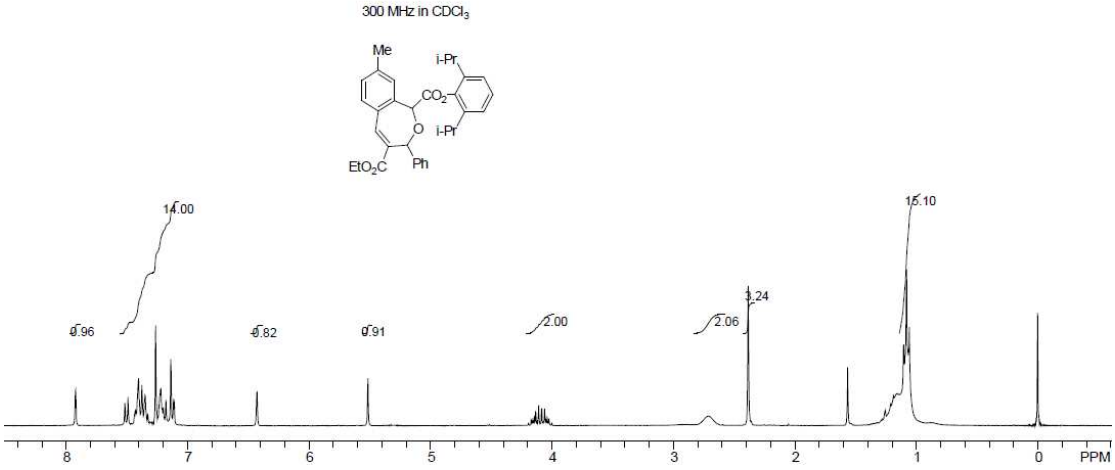


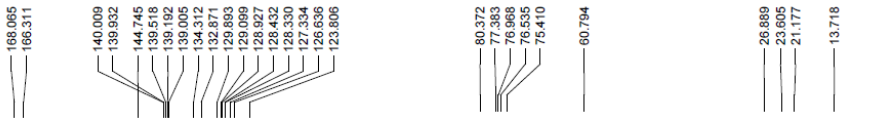


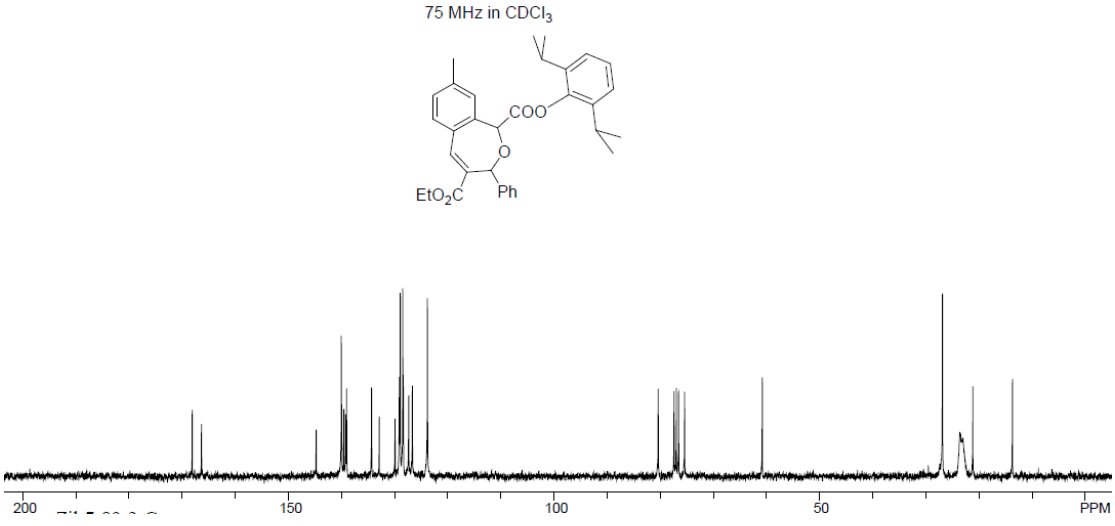
4c

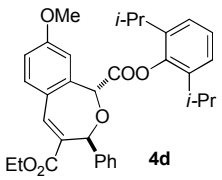
1-(2,6-diisopropylphenyl) 4-ethyl 8-methyl-3-phenyl-1,3-dihydrobenzo[c]oxepine-1,4-dicarboxylate (4c)





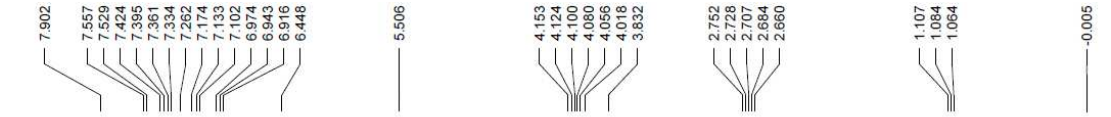


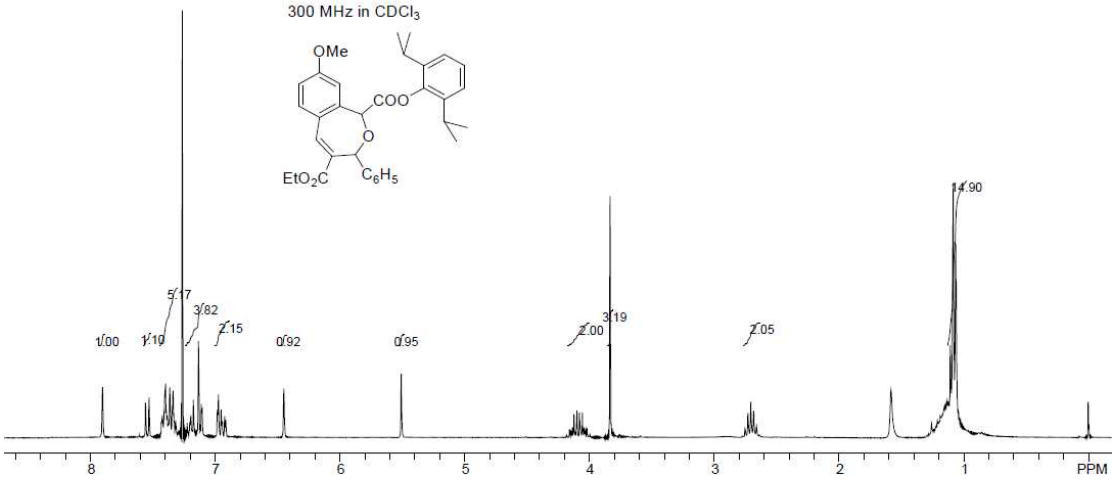


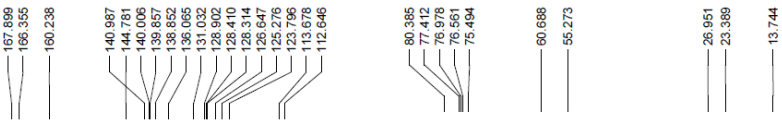


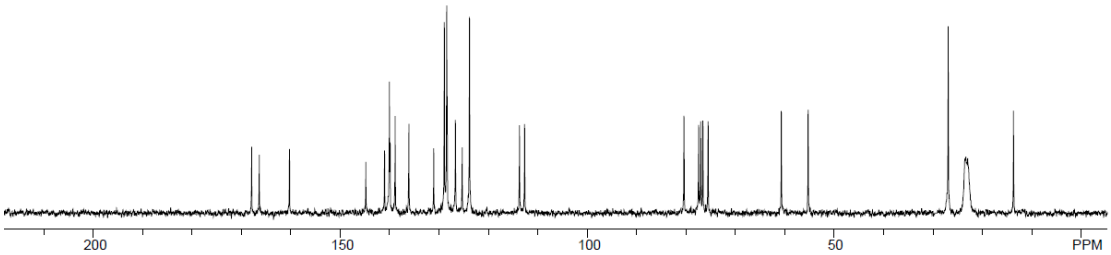
4d

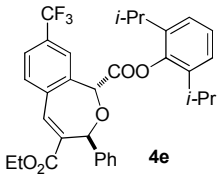
1-(2,6-diisopropylphenyl) 4-ethyl 8-methoxy-3-phenyl-1,3-dihydrobenzo[c]oxepine-1,4-dicarboxylate (4d)





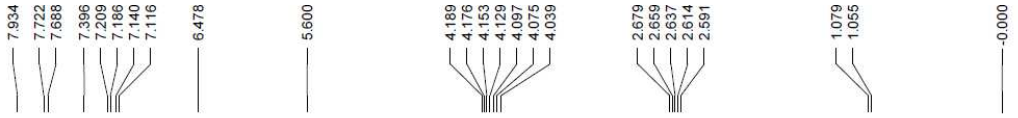


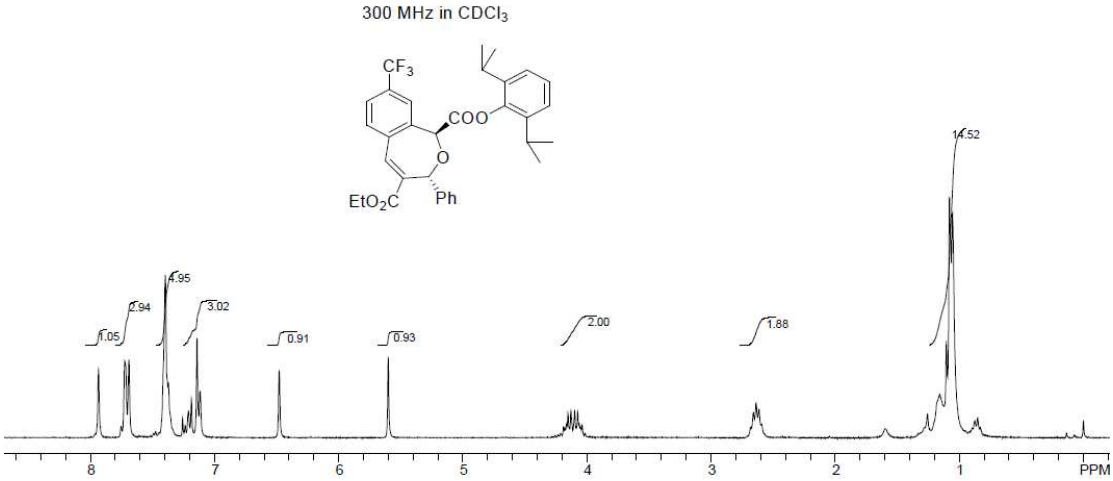


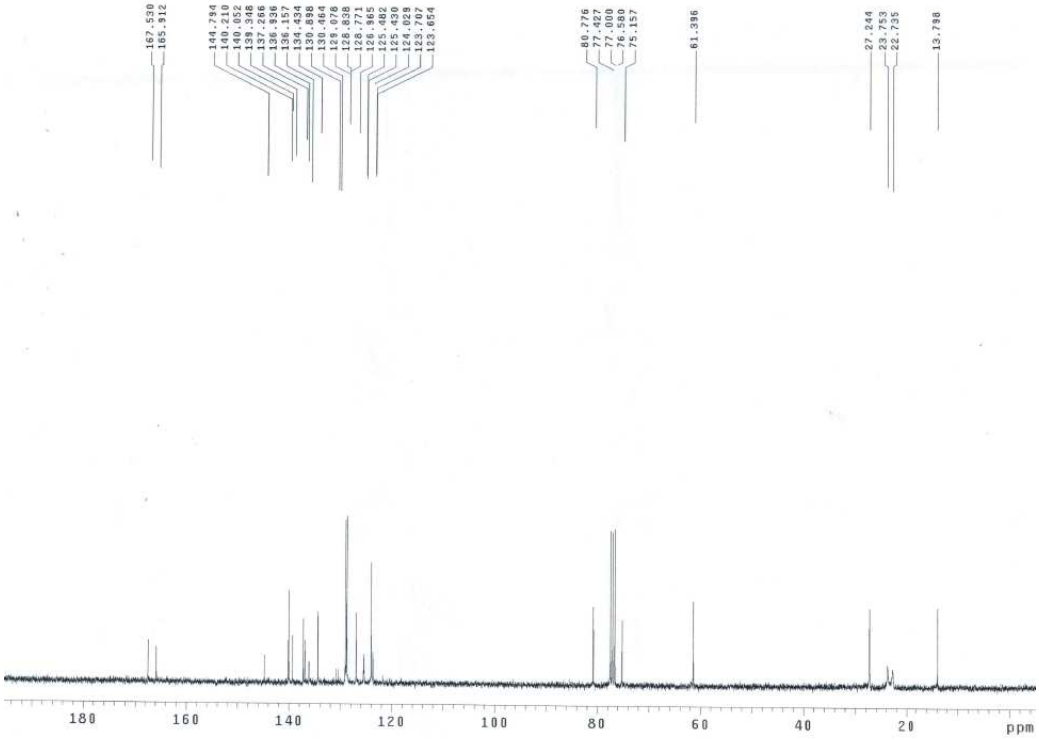


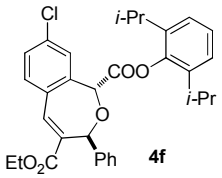
4e

1-(2,6-diisopropylphenyl) 4-ethyl 3-phenyl-8-(trifluoromethyl)-1,3-dihydrobenzo[c]oxepine-1,4-dicarboxylate (4e)



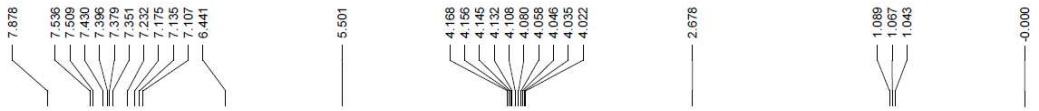


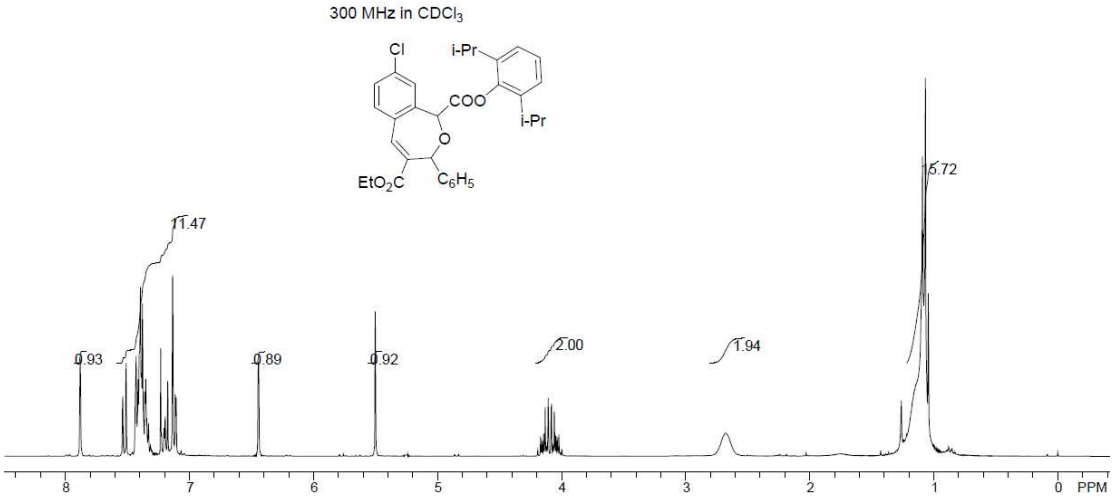


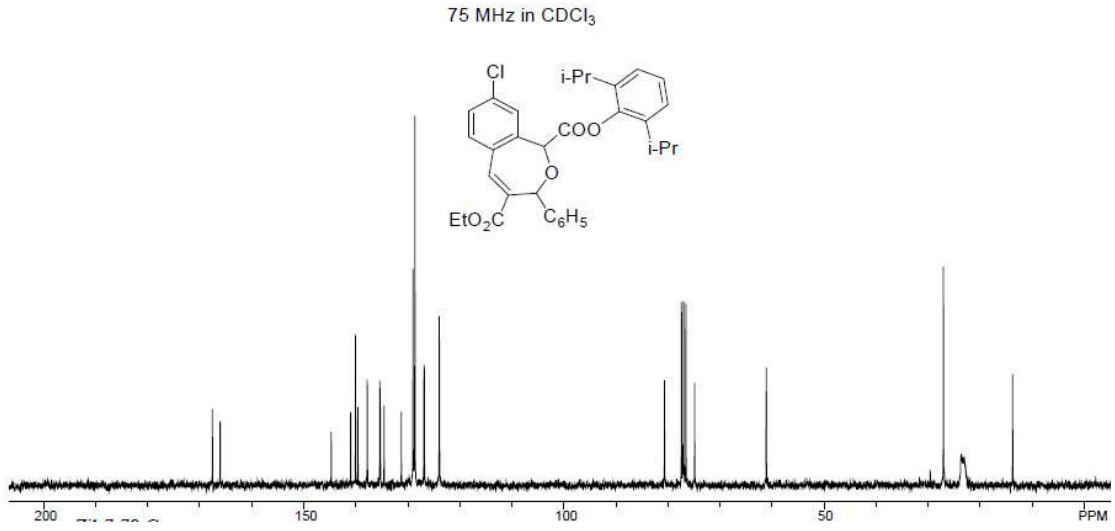


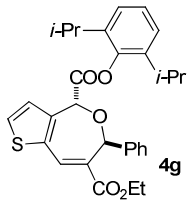
4f

1-(2,6-diisopropylphenyl) 4-ethyl 8-chloro-3-phenyl-1,3-dihydrobenzo[c]oxepine-1,4-dicarboxylate (4f)

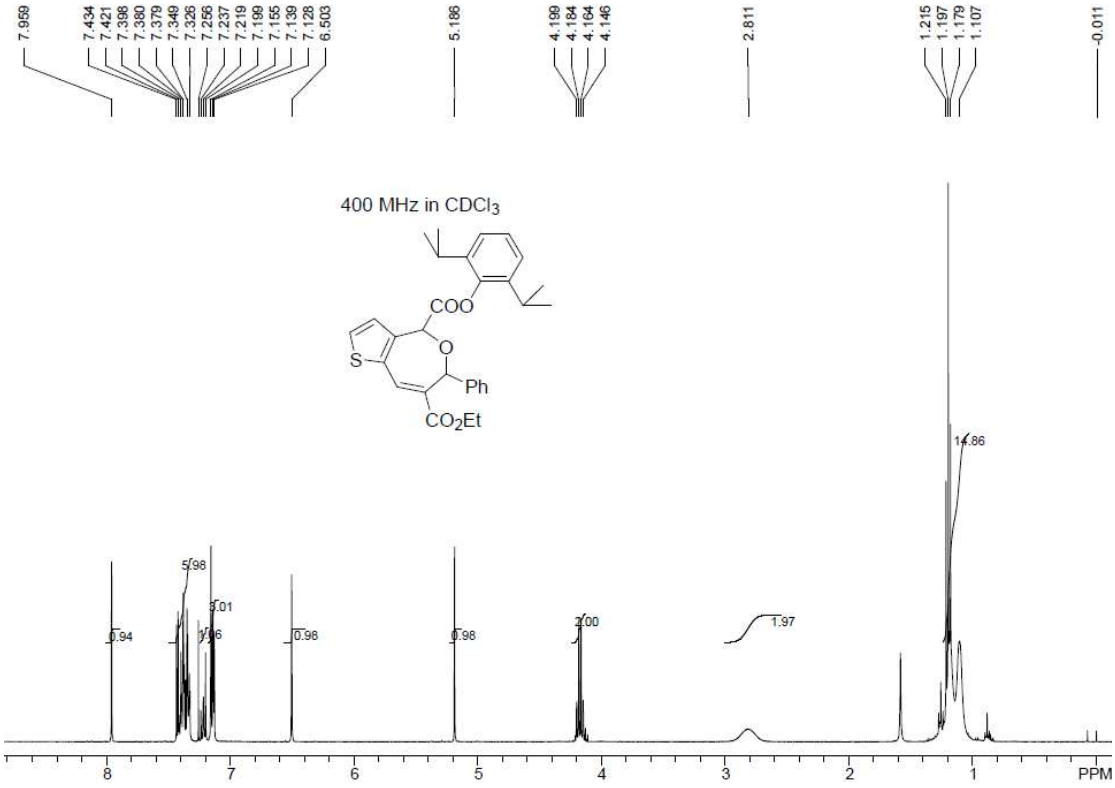


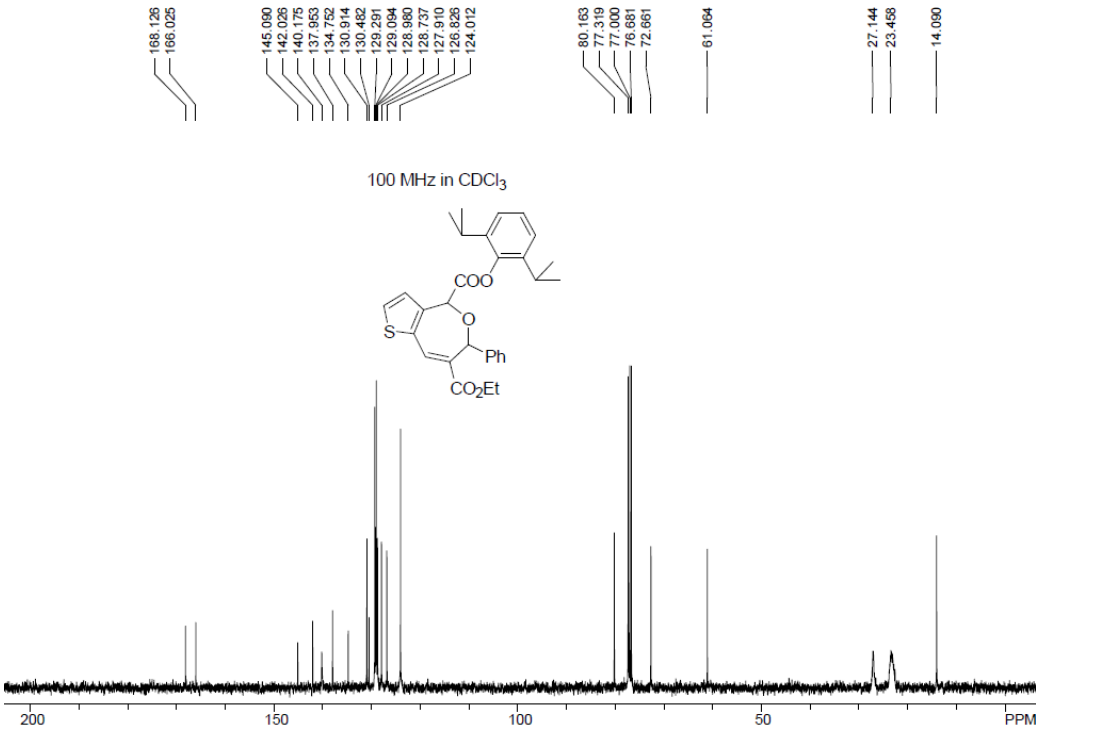


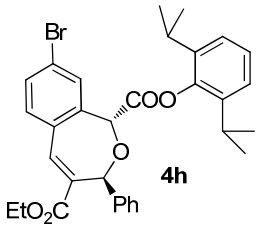




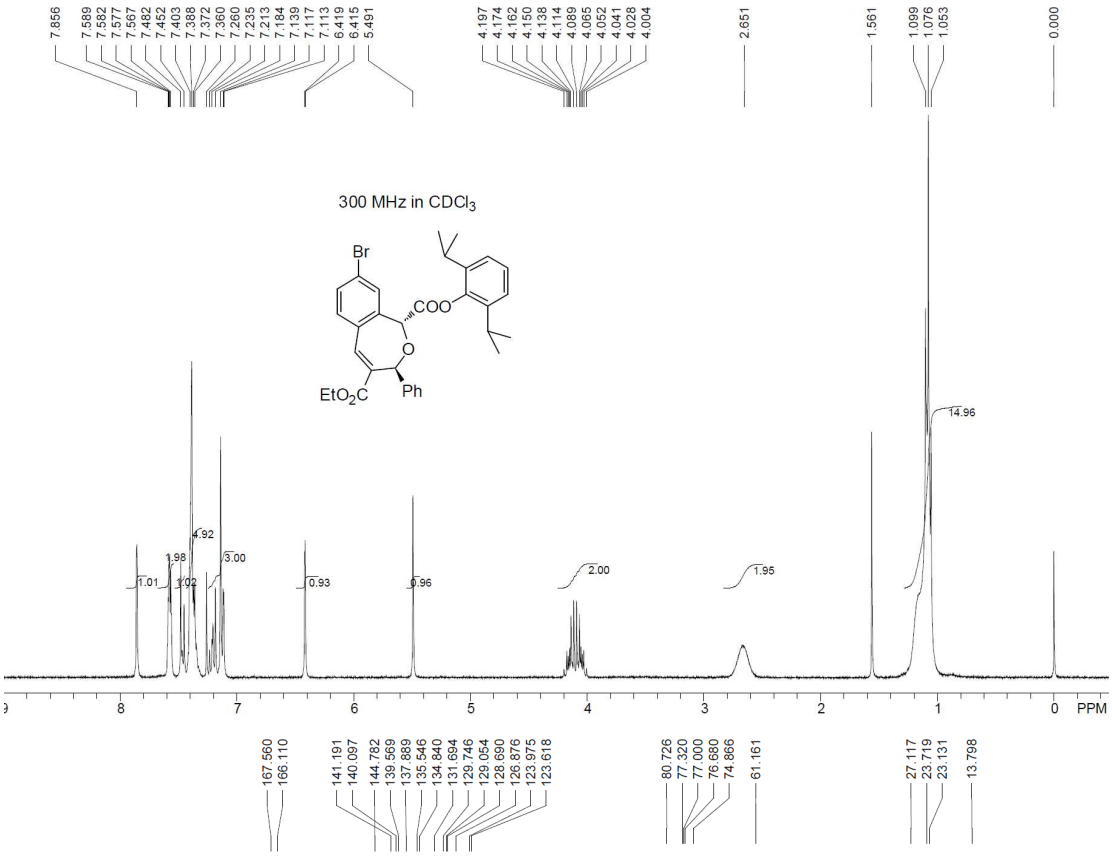
4-(2,6-diisopropyl-benzoyl)-6-phenyl-4,6-dihydro-thieno[3,2-c]oxepine-7-carboxylic acid ethyl ester (4g)

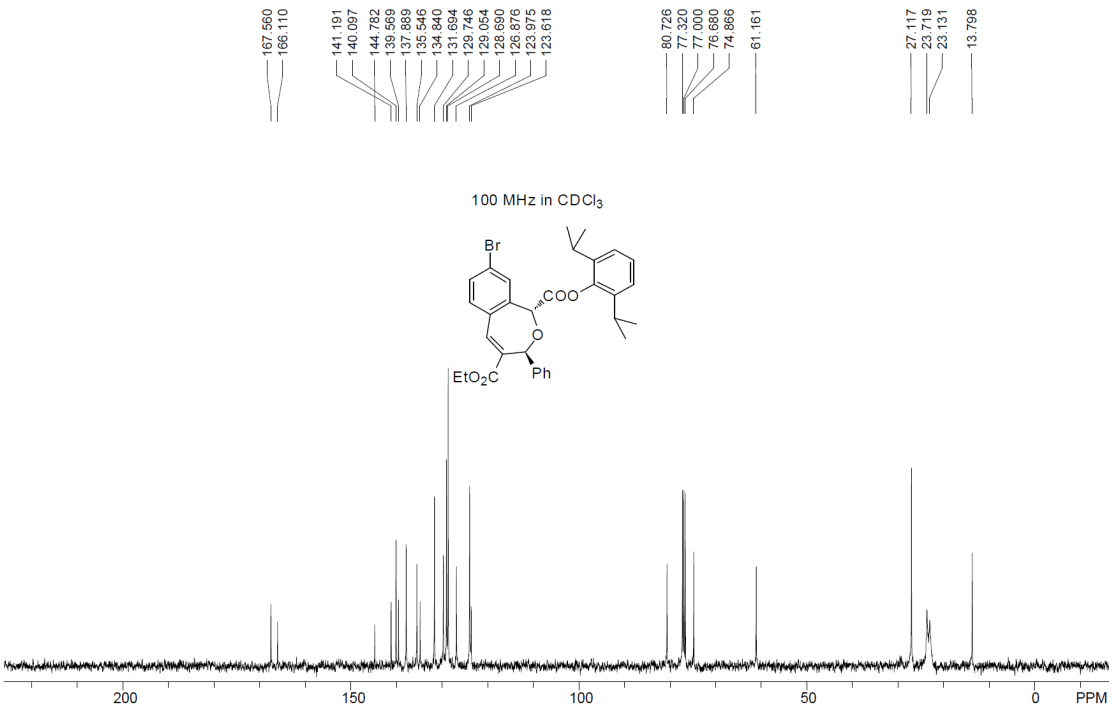


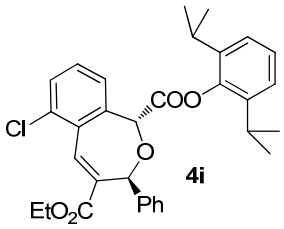




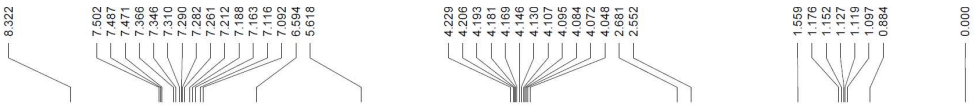
1-(2,6-diisopropylphenyl) 4-ethyl 8-bromo-3-phenyl-1,3-dihydrobenzo[c]oxepine-1,4-dicarboxylate (4h)

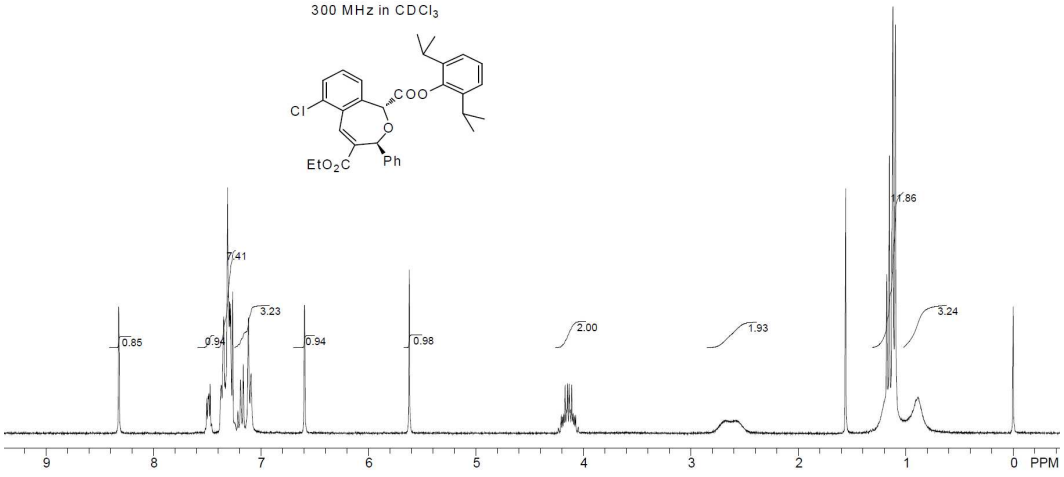


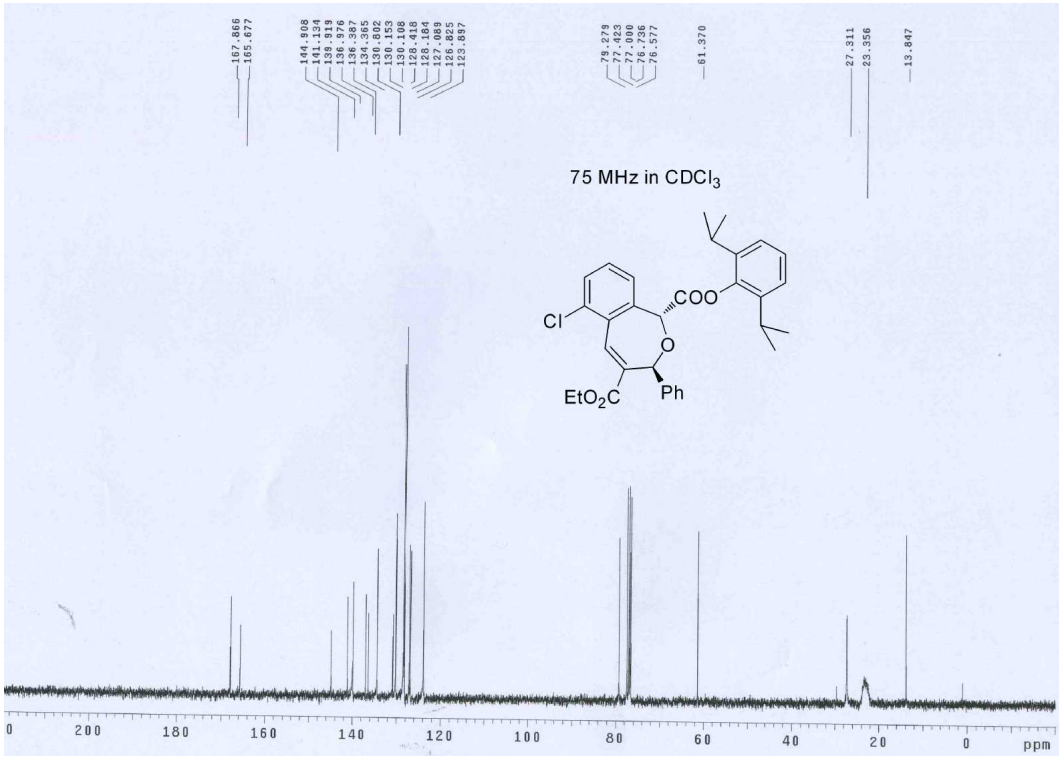


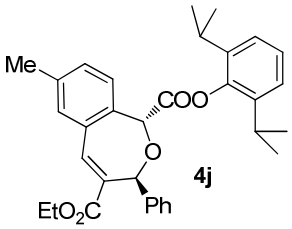


1-(2,6-diisopropylphenyl) 4-ethyl 6-chloro-3-phenyl-1,3-dihydrobenzo[c]oxepine-1,4-dicarboxylate (4i)

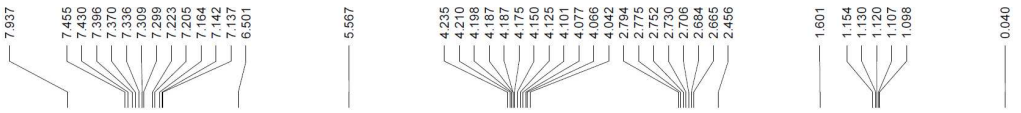


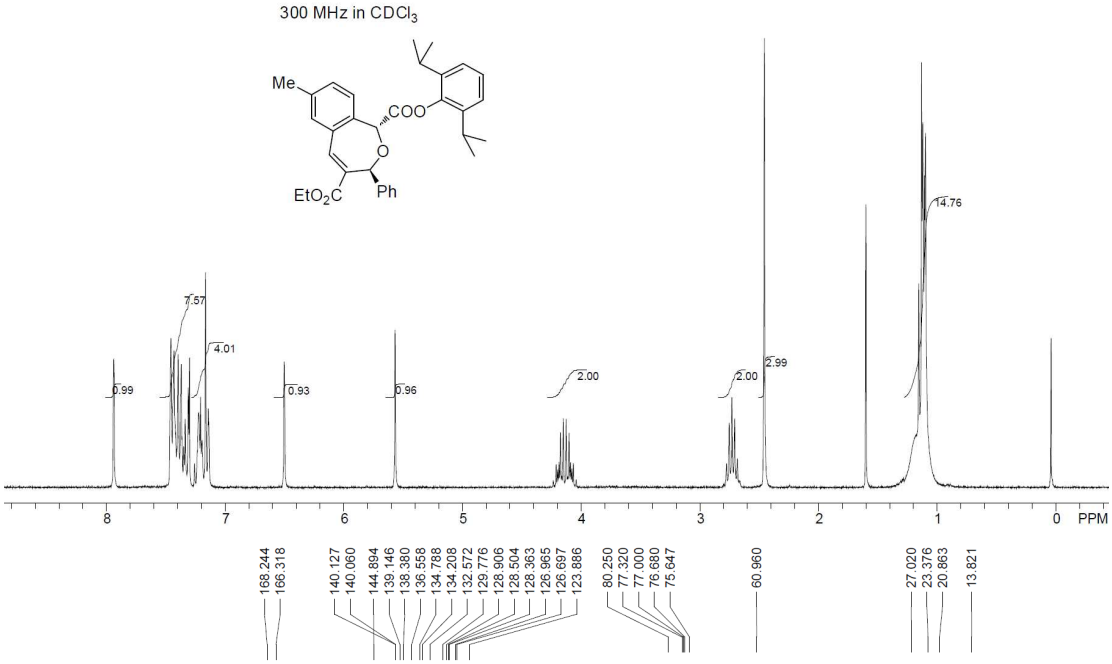


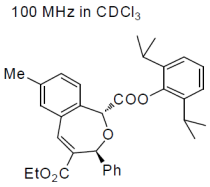


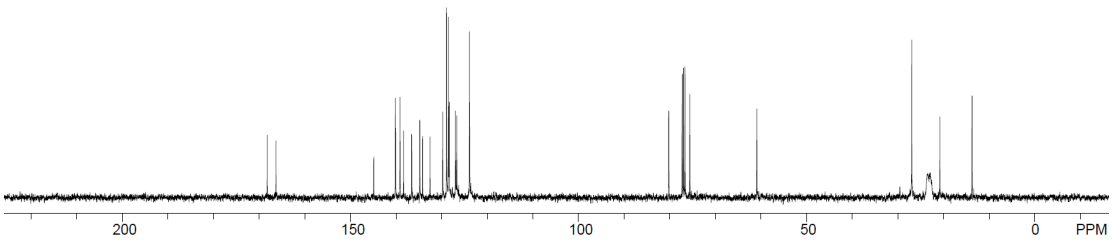


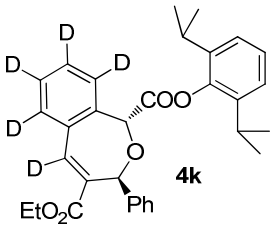
1-(2,6-diisopropylphenyl) 4-ethyl 7-methyl-3-phenyl-1,3-dihydrobenzo[c]oxepine-1,4-dicarboxylate (4j)



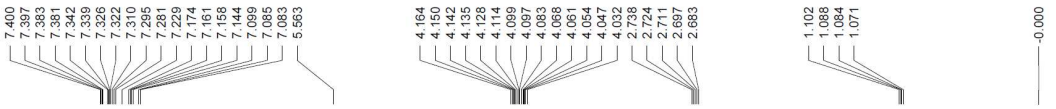




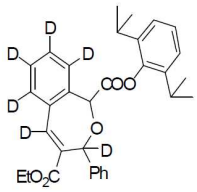


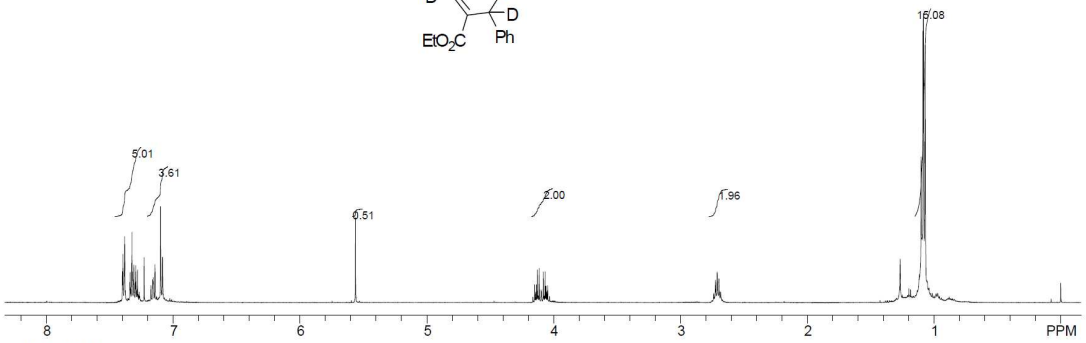


4k

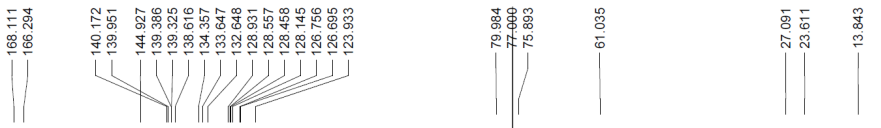


500 MHz in $CDCl_3$

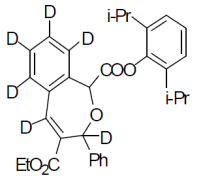


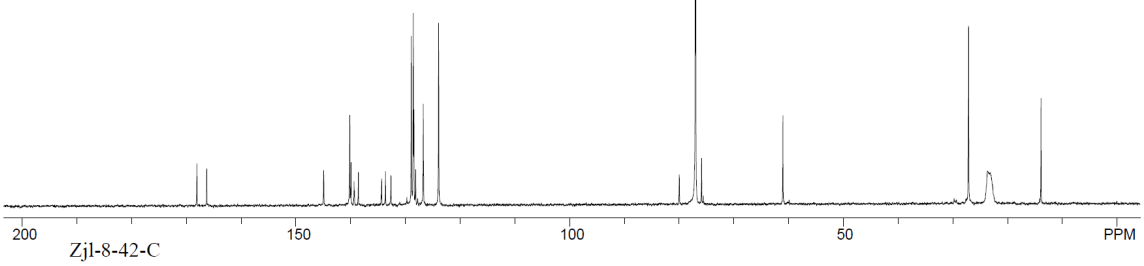


Zjl-8-42-H



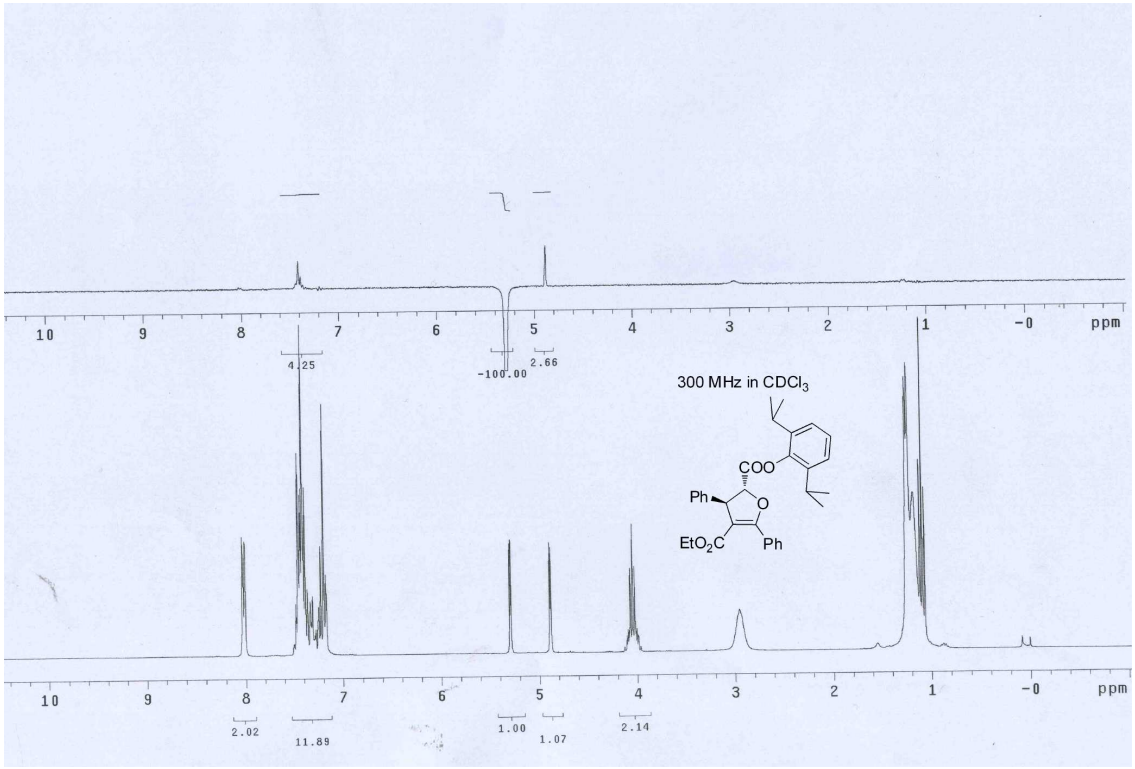
125 MHz in $CDCl_3$

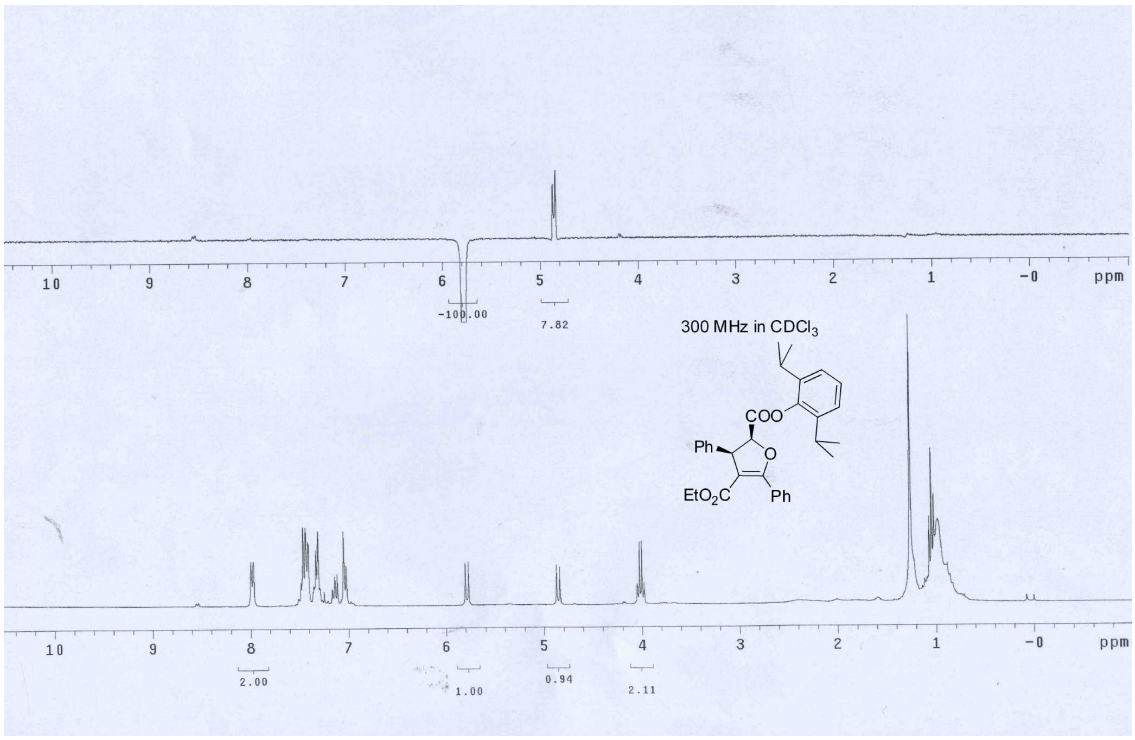


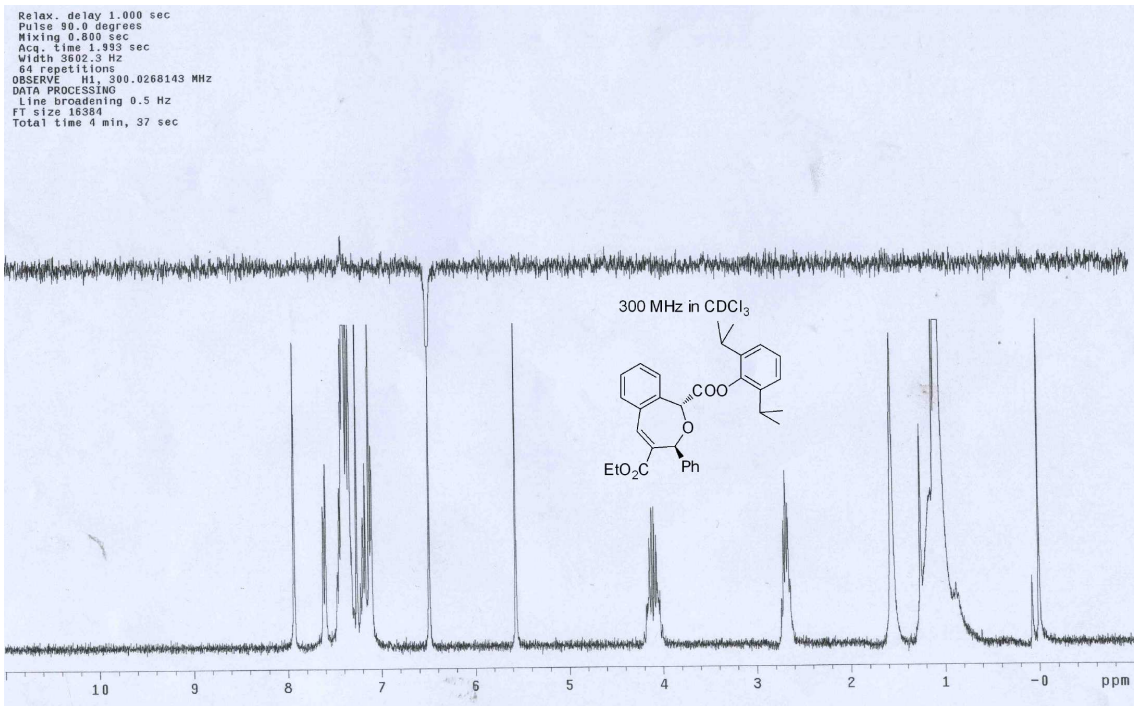


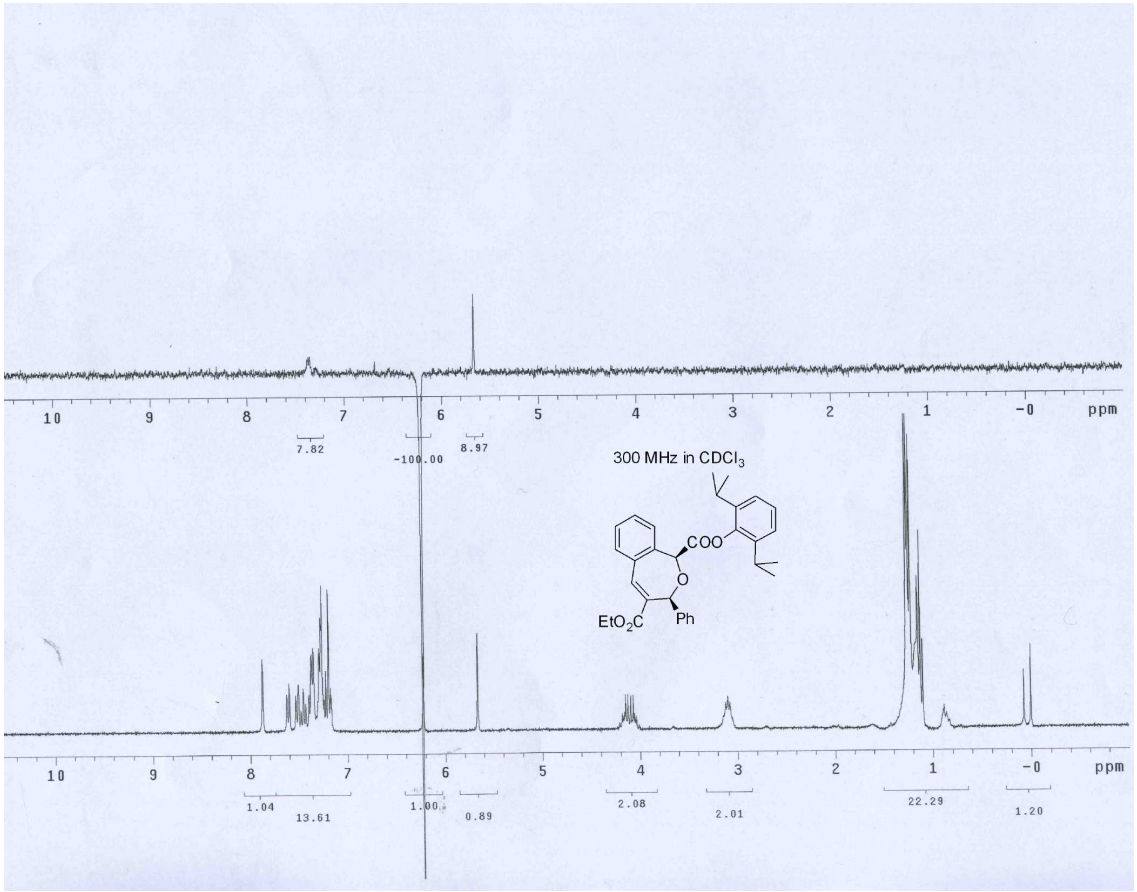
Zjl-8-42-C

9. NOESY-1D spectra





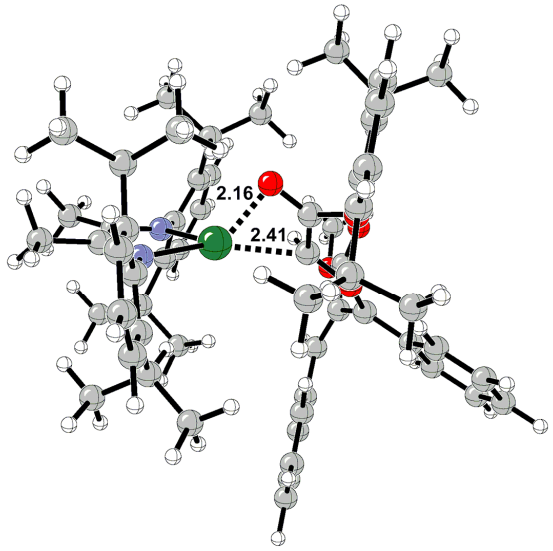

Relax. delay 1.000 sec
Pulse 90.0 degrees
Mixing 0.800 sec
Acq. time 1.993 sec
Width 3602.3 Hz
64 repetitions
OBSERVE H1, 300.0268143 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 16384
Total time 4 min, 37 sec
300 MHz in CDCl3
COO
O
EtO2C
Ph
10 9 8 7 6 5 4 3 2 1 -0 ppm


10 9 8 7 6 5 4 3 2 1 -0 ppm
7.82
-100.00
8.97
300 MHz in CDCl3
COO
O
EtO2C
Ph
10 9 8 7 6 5 4 3 2 1 -0 ppm
1.04
13.61
1.00
0.89
2.08
2.01
22.29
1.20

10. DFT study

10.1. Computational details

All DFT calculations were performed with the Gaussian 03 software package.[4] Geometry optimization of all the minima and transition states involved was carried out at the B3LYP level of theory.[5] The LANL2DZ basis set[6] was used for copper and the 6-31G(d) basis set[7] for the other atoms. The keyword "5D" in Gaussian 03 program was used to specify that five (instead of six) d-type STO orbitals were used as basis sets in all elements of the calculations. The vibrational frequencies were computed at the same level to check whether each optimized structure was an energy minimum or a transition state and to evaluate its zero-point vibrational energy (ZPVE). Solvent effects were computed at the same level using the gas-phase optimized structures. Solvation energies in dichloromethane (DCM) were evaluated by a self-consistent reaction field (SCRF) using the CPCM model,[8] where simple united atom topological model (UA0) was used to define the atom radii. In the paper and the Supporting Information, all discussed energies are Gibbs free energies in dichloromethane (ΔG_{DCM}) unless specified. The Gibbs free energies in gas phase (ΔG_{gas}) and the enthalpies in dichloromethane (ΔH_{DCM}) are also given for reference.



TS2 (L1)

Figure S2. DFT-computed structure of transition state **TS2 (L1)** (carbon, gray; hydrogen, white; oxygen, red; nitrogen, blue; copper, green; distances are given in Å).

DFT-computed overall free energy surface for the reaction of **1** and **2** in the presence of cationic **Cu(I)/La** complex is given in Figure S3. The calculations show that the nucleophilic attack of dicarbonyl compound **1** to copper carbenoid **S3** is the rate-determining step of the whole reaction, requiring an overall activation free energy of 23.4 kcal/mol. Formation of copper-associated carbonyl ylide **C (La)** with carbon anion as the coordinating atom is endergonic by 5.6 kcal/mol. The whole reaction for the generation of 5-membered dihydrofuran **3** is exergonic by 38.0 kcal/mol in CH_2Cl_2. In addition, the generation of 7-membered intermediate **S6** is exergonic by about 6 kcal/mol. The subsequent [1,5]-H shift process requires an activation free energy of 14.5 kcal/mol via transition state **TS-S3**. The whole reaction for the generation of 7-membered dihydrobenzoxepine **4** is exergonic by 24.3 kcal/mol in CH_2Cl_2.

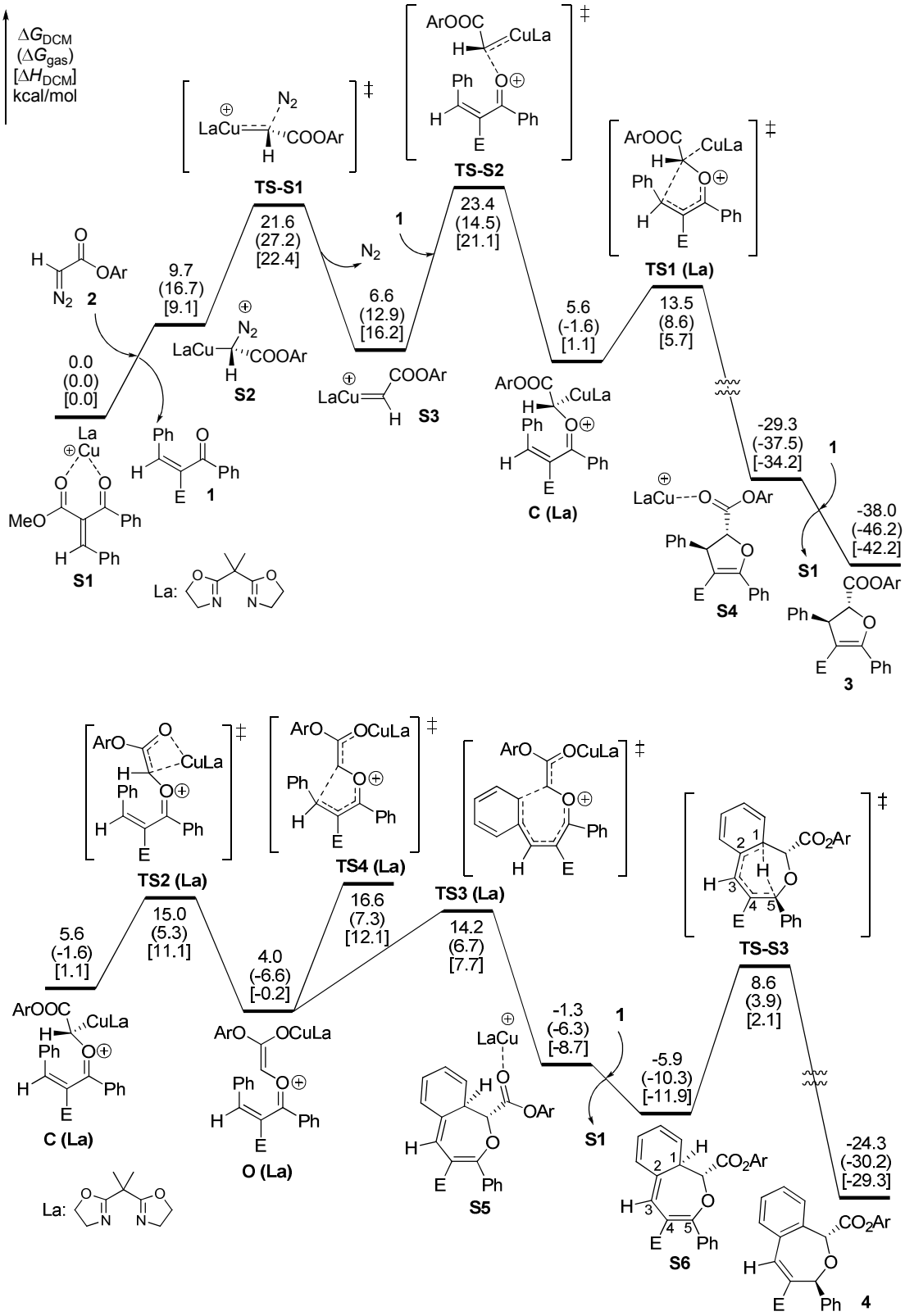


Figure S3. DFT-computed overall free energy surface for the reaction of **1** and **2** in the presence of cationic **Cu(I)/La** complex (Ar = 2,6-diisopropylphenyl; E = CO_2Me).

The 1,5- and 1,7-cyclizations may also take place via the free-ylide pathway. However, DFT calculations show that the free-ylide pathway is disfavored as compared with the copper-associated ylide pathway because the dissociation of free ylide **FY** from copper-associated ylide **O** is a remarkably endergonic and endothermic process (Figure S4). For instance, the formation of free ylide **FY** from **O (La)** is endergonic by 7.6 kcal/mol and endothermic by 19.7 kcal/mol in CH_2Cl_2. Similar conclusion was obtained in the Cu(I)-catalyzed O–H insertion reaction as well.[9] Further computational results indicate that the generation of 7-membered dihydrobenzoxepine **4** is much easier than that of 5-membered dihydrofuran **3** via the free-ylide pathway (Figure S5). This suggests that, if a free ylide is involved, only 7-membered dihydrobenzoxepine **4** will be generated. This is contradictory to experimental results. Therefore, we can rule out the possibility of free ylide in the present reaction.

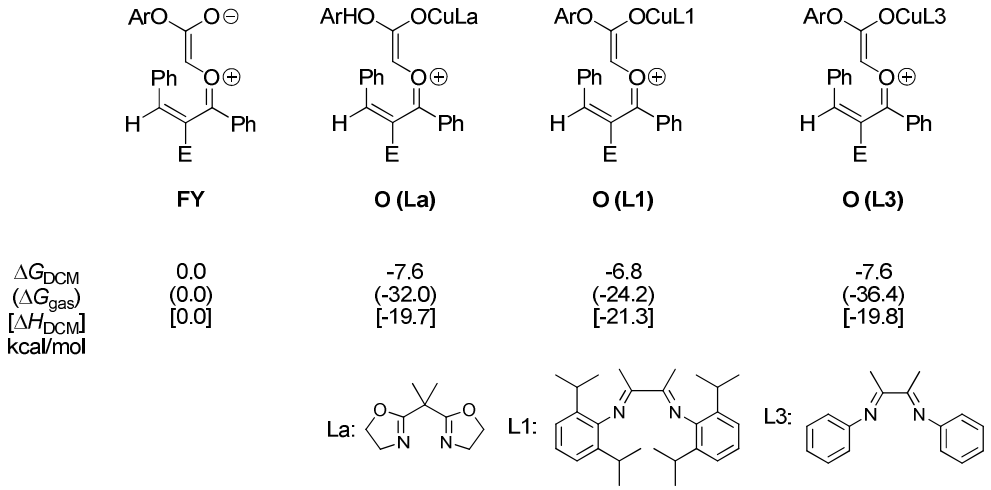


Figure S4. DFT-computed energy differences between free ylide **FY** and copper-associated ylide **O (Lx)** (Ar = 2,6-diisopropylphenyl; E = CO_2Me).

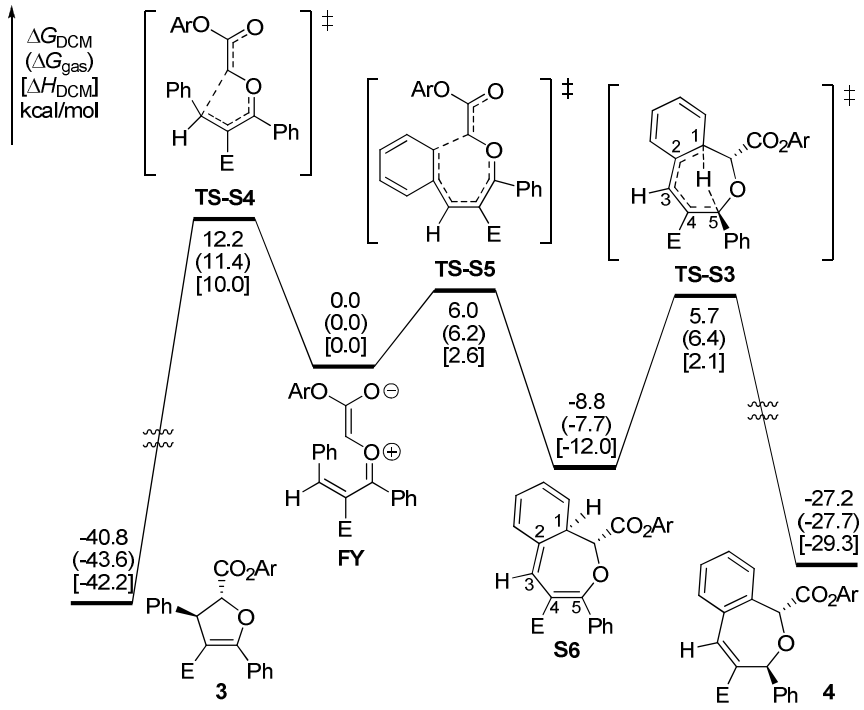
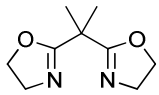
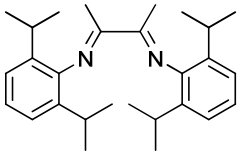


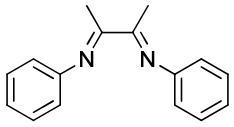
Figure S5. DFT-computed free energy surface for the free-ylide pathway (Ar = 2,6-diisopropylphenyl; E = CO_2Me).

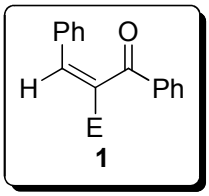
10.2. Coordinates of all stationary points

In this section, Ar is 2,6-diisopropylphenyl, and E is CO_2Me. The structures of La, L1, and L3 are shown as follows:

La: 

L1: 

L3: 

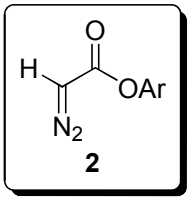


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.660826	1.216831	0.901453
2	6	0	4.700502	0.951111	0.006080
3	6	0	4.563864	-0.080446	-0.925419
4	6	0	3.392687	-0.832381	-0.960290
5	6	0	2.323687	-0.560821	-0.082205
6	6	0	2.484252	0.472473	0.863336
7	6	0	1.126038	-1.393963	-0.209949
8	6	0	-0.146591	-1.195251	0.200670
9	6	0	-0.662233	-0.003136	0.980458
10	6	0	-1.330449	1.104789	0.234248

11	8	0	-0.527091	0.035903	2.196051
12	6	0	-1.130404	-2.270641	-0.118025
13	8	0	-0.888579	-3.301445	-0.715455
14	8	0	-2.360482	-1.951124	0.345404
15	6	0	-3.387393	-2.923522	0.101167
16	6	0	-1.885357	2.163678	0.971628
17	6	0	-2.510705	3.221395	0.319612
18	6	0	-2.586083	3.234851	-1.077647
19	6	0	-2.034028	2.187795	-1.818637
20	6	0	-1.409223	1.125257	-1.166006
21	1	0	3.770135	2.004339	1.642129
22	1	0	5.615433	1.536237	0.042833
23	1	0	5.370597	-0.303013	-1.618374
24	1	0	3.289828	-1.638858	-1.682307
25	1	0	1.706248	0.669680	1.590163
26	1	0	1.274106	-2.322024	-0.761817
27	1	0	-4.294365	-2.505523	0.538474
28	1	0	-3.515460	-3.085020	-0.972654
29	1	0	-3.133396	-3.874989	0.575892
30	1	0	-1.812782	2.131025	2.053893
31	1	0	-2.940231	4.036817	0.895240
32	1	0	-3.073841	4.061822	-1.587068

33	1	0	-2.089156	2.199227	-2.903649
34	1	0	-0.974247	0.315497	-1.743613



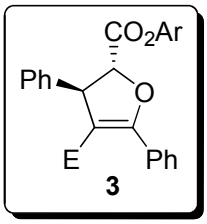
2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000350	3.115153	0.583691
2	7	0	0.000273	3.558843	-0.647615
3	7	0	0.000190	3.941237	-1.718818
4	6	0	0.000231	1.688310	0.873012
5	8	0	0.000299	1.228274	1.994402
6	8	0	0.000041	0.951073	-0.282490
7	1	0	0.000525	3.849908	1.375654
8	6	0	-0.000062	-0.455109	-0.175273
9	6	0	-1.235825	-1.118747	-0.163199
10	6	0	1.235592	-1.118929	-0.163139
11	6	0	-1.206967	-2.518444	-0.122455

12	6	0	1.206523	-2.518629	-0.122382
13	6	0	-0.000272	-3.213890	-0.100206
14	1	0	-2.142955	-3.069577	-0.104927
15	1	0	2.142431	-3.069899	-0.104794
16	1	0	-0.000361	-4.300124	-0.067447
17	6	0	2.557260	-0.359419	-0.158586
18	1	0	2.338163	0.685182	-0.402474
19	6	0	3.195417	-0.387764	1.245595
20	1	0	4.117575	0.206069	1.261946
21	1	0	2.508334	0.015707	1.995889
22	1	0	3.450745	-1.413507	1.538186
23	6	0	3.537273	-0.876245	-1.227446
24	1	0	3.855859	-1.905624	-1.026081
25	1	0	3.087562	-0.853039	-2.226187
26	1	0	4.439111	-0.253006	-1.245158
27	6	0	-2.557366	-0.359014	-0.158626
28	1	0	-2.338130	0.685472	-0.402889
29	6	0	-3.195226	-0.386828	1.245706
30	1	0	-2.507904	0.016689	1.995753
31	1	0	-4.117258	0.207199	1.262089
32	1	0	-3.450697	-1.412445	1.538617
33	6	0	-3.537724	-0.875997	-1.227090

34	1	0	-3.088202	-0.853344	-2.225928
35	1	0	-3.856596	-1.905191	-1.025231
36	1	0	-4.439376	-0.252491	-1.244890



3

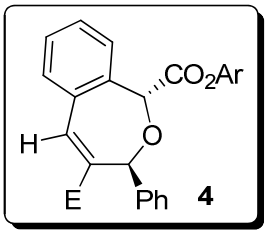
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.663422	-1.121447	0.235426
2	6	0	-1.993484	0.366352	0.307138
3	6	0	-1.369939	1.014435	-0.722469
4	8	0	-0.593767	0.162732	-1.467410
5	6	0	-0.479147	-1.083298	-0.769456
6	6	0	-1.317806	2.398351	-1.216818
7	6	0	0.870132	-1.223607	-0.055959
8	8	0	1.108870	-2.151784	0.681097
9	8	0	1.732234	-0.229996	-0.367776

10	6	0	-2.816550	-2.008754	-0.218811
11	6	0	-2.830378	0.914075	1.375223
12	8	0	-3.253934	2.053271	1.490512
13	8	0	-3.099211	-0.048643	2.298926
14	6	0	-3.929879	0.366578	3.389820
15	6	0	-2.363506	3.317430	-1.022177
16	6	0	-2.267389	4.604874	-1.547006
17	6	0	-1.135859	4.996386	-2.265378
18	6	0	-0.092412	4.088654	-2.463356
19	6	0	-0.182763	2.797761	-1.950867
20	6	0	-3.014496	-3.254555	0.389532
21	6	0	-4.038366	-4.102770	-0.035333
22	6	0	-4.880130	-3.715065	-1.079509
23	6	0	-4.690872	-2.474970	-1.693249
24	6	0	-3.667682	-1.627907	-1.265021
25	1	0	-1.305454	-1.498025	1.195790
26	1	0	-0.536306	-1.883959	-1.511620
27	1	0	-4.063973	-0.521746	4.008302
28	1	0	-4.894712	0.729659	3.025003
29	1	0	-3.447405	1.163836	3.962381
30	1	0	-3.231901	3.025469	-0.448265
31	1	0	-3.083419	5.305286	-1.392032

32	1	0	-1.066633	6.003336	-2.668610
33	1	0	0.792824	4.385928	-3.018932
34	1	0	0.623869	2.090106	-2.103001
35	1	0	-2.359700	-3.560205	1.202241
36	1	0	-4.179280	-5.064387	0.451339
37	1	0	-5.679222	-4.372804	-1.410997
38	1	0	-5.342986	-2.163600	-2.505201
39	1	0	-3.536192	-0.660103	-1.741590
40	6	0	3.022593	-0.260049	0.212202
41	6	0	4.057245	-0.855776	-0.523658
42	6	0	3.209716	0.370816	1.449982
43	6	0	5.338154	-0.822045	0.041560
44	6	0	4.511666	0.375381	1.967481
45	6	0	5.565405	-0.216352	1.275453
46	1	0	6.167603	-1.277861	-0.491396
47	1	0	4.699493	0.847720	2.927650
48	1	0	6.567025	-0.202605	1.696697
49	6	0	3.801835	-1.540228	-1.861684
50	1	0	2.808128	-1.233703	-2.204893
51	6	0	2.058659	1.004951	2.222925
52	1	0	1.179169	1.012682	1.571359
53	6	0	2.348236	2.470268	2.597690

54	1	0	3.197493	2.554773	3.285765
55	1	0	2.573297	3.070591	1.709543
56	1	0	1.476294	2.911814	3.093877
57	6	0	1.708232	0.166199	3.468703
58	1	0	1.474040	-0.866677	3.192014
59	1	0	2.544834	0.144940	4.177557
60	1	0	0.840453	0.592906	3.985895
61	6	0	4.803157	-1.108361	-2.948159
62	1	0	5.823863	-1.434530	-2.717655
63	1	0	4.528274	-1.554333	-3.911132
64	1	0	4.816860	-0.019597	-3.068522
65	6	0	3.788178	-3.074312	-1.695625
66	1	0	4.770128	-3.441484	-1.373236
67	1	0	3.052786	-3.383695	-0.946067
68	1	0	3.542430	-3.562474	-2.646664



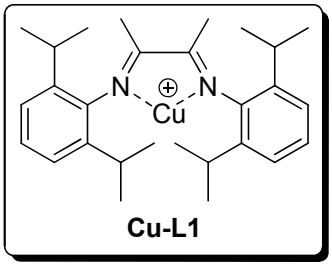
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.323803	5.119389	-0.311831
2	6	0	2.256917	4.184599	-0.750027
3	6	0	1.931194	2.819671	-0.813152
4	6	0	0.615959	2.399048	-0.486542
5	6	0	-0.308314	3.351307	-0.048539
6	6	0	0.042412	4.698393	0.049992
7	6	0	2.946627	1.840307	-1.215441
8	6	0	3.046682	0.610572	-0.663666
9	8	0	0.817565	0.015946	0.212337
10	6	0	0.253563	0.927301	-0.718452
11	6	0	4.018116	-0.332193	-1.297182
12	8	0	5.001183	0.011991	-1.925833
13	8	0	3.649615	-1.617807	-1.139898
14	6	0	4.531524	-2.589737	-1.721236
15	6	0	2.682612	-0.844138	1.446685
16	6	0	-1.255825	0.678858	-0.809280
17	8	0	-1.958413	1.235987	-1.620514
18	8	0	-1.685563	-0.248422	0.077071
19	6	0	3.916488	-0.691786	2.092397

20	6	0	4.402737	-1.688305	2.938212
21	6	0	3.651814	-2.845377	3.158979
22	6	0	2.415193	-2.993662	2.528897
23	6	0	1.931075	-1.999511	1.675720
24	1	0	1.591939	6.170583	-0.255047
25	1	0	3.259004	4.500503	-1.028848
26	1	0	-1.323826	3.052600	0.187347
27	1	0	-0.693976	5.420930	0.390319
28	1	0	3.648089	2.114062	-2.001273
29	1	0	0.623605	0.677337	-1.725702
30	1	0	4.086621	-3.558318	-1.492582
31	1	0	4.606730	-2.442625	-2.802084
32	1	0	5.529235	-2.511465	-1.281215
33	1	0	4.501696	0.212022	1.933290
34	1	0	5.362961	-1.557191	3.430332
35	1	0	4.025262	-3.620954	3.822490
36	1	0	1.820798	-3.887302	2.701917
37	1	0	0.968931	-2.108459	1.189068
38	6	0	-3.034794	-0.659600	0.012181
39	6	0	-3.968157	-0.010006	0.831509
40	6	0	-3.351296	-1.753867	-0.807209
41	6	0	-5.285635	-0.485043	0.797324

42	6	0	-4.683291	-2.186159	-0.804103
43	6	0	-5.643801	-1.558941	-0.013547
44	1	0	-6.039871	-0.003648	1.413704
45	1	0	-4.971024	-3.025745	-1.430457
46	1	0	-6.671913	-1.910642	-0.026673
47	6	0	-2.305821	-2.432075	-1.685668
48	1	0	-1.322012	-2.072224	-1.367313
49	6	0	-3.588436	1.175959	1.709913
50	1	0	-2.499374	1.281135	1.673320
51	6	0	-3.967512	0.950304	3.185387
52	1	0	-3.625873	1.792960	3.798079
53	1	0	-5.052475	0.865449	3.317648
54	1	0	-3.508446	0.036372	3.577397
55	6	0	-4.207245	2.479548	1.166114
56	1	0	-3.884032	3.340004	1.765167
57	1	0	-3.914022	2.648429	0.124457
58	1	0	-5.302664	2.441701	1.201720
59	6	0	-2.298565	-3.962135	-1.514447
60	1	0	-2.157204	-4.245118	-0.465608
61	1	0	-3.232846	-4.417799	-1.862778
62	1	0	-1.482413	-4.402316	-2.099244
63	6	0	-2.495893	-2.037384	-3.164818

64	1	0	-3.462597	-2.391075	-3.543529
65	1	0	-2.464522	-0.950321	-3.288961
66	1	0	-1.708662	-2.481523	-3.786221
67	6	0	2.178900	0.277557	0.555316
68	1	0	2.191615	1.193722	1.165055



Cu-L1

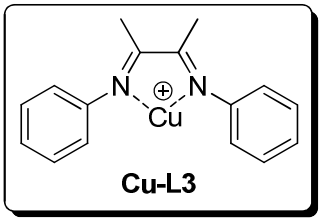
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	-0.022179	0.207197	-1.284491
2	1	0	6.503738	0.963133	-0.681309
3	6	0	5.456278	0.764272	-0.475874
4	6	0	5.086888	-0.382464	0.215304
5	6	0	4.477460	1.654081	-0.919522
6	6	0	3.745160	-0.666600	0.512155
7	1	0	5.854656	-1.082508	0.530204

8	6	0	3.125233	1.418692	-0.669444
9	1	0	4.777270	2.541559	-1.465952
10	6	0	2.774295	0.266763	0.084342
11	6	0	3.399741	-1.999851	1.173655
12	6	0	2.043591	2.358001	-1.206496
13	7	0	1.376444	0.030274	0.268699
14	1	0	2.330915	-2.008843	1.409310
15	1	0	1.232686	2.394338	-0.467769
16	6	0	0.760859	0.015401	1.398652
17	6	0	-0.739220	-0.249992	1.353994
18	7	0	-1.343182	-0.049397	0.231383
19	6	0	-2.752434	-0.224901	0.030836
20	6	0	-3.154870	-1.233497	-0.881242
21	6	0	-3.682145	0.658043	0.628855
22	6	0	-4.523001	-1.392178	-1.117507
23	6	0	-2.133996	-2.143107	-1.560709
24	6	0	-5.038615	0.455526	0.340483
25	6	0	-3.276788	1.868924	1.469115
26	6	0	-5.461226	-0.563962	-0.504685
27	1	0	-4.863438	-2.168316	-1.793808
28	1	0	-1.219600	-1.535474	-1.746420
29	1	0	-5.776070	1.119143	0.781230

30	1	0	-2.207556	1.801129	1.693518
31	1	0	-6.519811	-0.704091	-0.701703
32	6	0	-1.711977	-3.312482	-0.648022
33	1	0	-1.312387	-2.964436	0.310316
34	1	0	-2.574404	-3.953920	-0.435139
35	1	0	-0.945396	-3.926396	-1.134060
36	6	0	-2.581719	-2.666139	-2.935060
37	1	0	-2.926126	-1.855767	-3.586112
38	1	0	-1.746359	-3.172790	-3.429930
39	1	0	-3.391560	-3.398108	-2.845855
40	6	0	3.645513	-3.166152	0.192589
41	1	0	3.067537	-3.040876	-0.730047
42	1	0	4.703257	-3.235641	-0.083976
43	1	0	3.355634	-4.118262	0.651207
44	6	0	4.164359	-2.226272	2.492711
45	1	0	5.243024	-2.312268	2.324528
46	1	0	4.005796	-1.409013	3.204917
47	1	0	3.833895	-3.158387	2.964092
48	6	0	2.501549	3.812160	-1.408219
49	1	0	1.647655	4.439208	-1.686615
50	1	0	2.935992	4.219435	-0.489978
51	1	0	3.244874	3.902702	-2.207317

52	6	0	1.454927	1.821455	-2.538369
53	1	0	2.168705	1.948349	-3.360610
54	1	0	1.291064	0.712543	-2.551014
55	1	0	0.534394	2.345240	-2.822042
56	6	0	-3.477657	3.171218	0.664577
57	1	0	-3.139523	4.036771	1.245627
58	1	0	-2.916637	3.150851	-0.276895
59	1	0	-4.533851	3.324721	0.417794
60	6	0	-4.021891	1.938725	2.816272
61	1	0	-5.095288	2.105427	2.677953
62	1	0	-3.903621	1.017311	3.396859
63	1	0	-3.639530	2.772028	3.416078
64	6	0	-1.399676	-0.750869	2.608686
65	1	0	-0.812237	-1.564703	3.047869
66	1	0	-1.465612	0.040505	3.364754
67	1	0	-2.409113	-1.108439	2.401705
68	6	0	1.391598	0.273979	2.739415
69	1	0	0.807227	1.012245	3.300164
70	1	0	1.424829	-0.637532	3.347686
71	1	0	2.411920	0.641623	2.621474

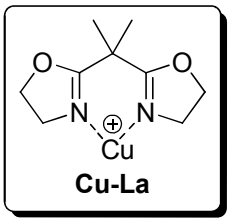


Cu-L3

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	-0.000043	1.351924	-0.000092
2	1	0	6.566602	0.826177	-0.013061
3	6	0	5.503728	0.606505	0.006786
4	6	0	4.951843	-0.263068	-0.936448
5	6	0	4.682260	1.207917	0.965479
6	6	0	3.588671	-0.556542	-0.913252
7	1	0	5.581693	-0.713543	-1.697463
8	6	0	3.314985	0.946458	0.977199
9	1	0	5.104997	1.890645	1.696077
10	6	0	2.766040	0.041130	0.055247
11	7	0	1.359300	-0.157612	0.090278
12	6	0	0.761201	-1.304450	0.018303
13	6	0	-0.761134	-1.304577	-0.018540
14	7	0	-1.359412	-0.157857	-0.090400

15	6	0	-2.766071	0.041001	-0.055237
16	6	0	-3.314889	0.947107	-0.976530
17	6	0	-3.588820	-0.557331	0.912762
18	6	0	-4.682122	1.208695	-0.964665
19	6	0	-4.951966	-0.263701	0.936148
20	6	0	-5.503697	0.606635	-0.006447
21	1	0	-5.104794	1.892016	-1.694747
22	1	0	-5.581881	-0.714674	1.696811
23	1	0	-6.566540	0.826457	0.013507
24	6	0	-1.463772	-2.636406	-0.033586
25	1	0	-0.962493	-3.324040	-0.720927
26	1	0	-1.452263	-3.107932	0.957250
27	1	0	-2.503886	-2.527556	-0.342565
28	6	0	1.463977	-2.636188	0.033306
29	1	0	0.962951	-3.323719	0.720944
30	1	0	1.452122	-3.107881	-0.957444
31	1	0	2.504194	-2.527249	0.341879
32	1	0	2.668794	1.416450	1.714598
33	1	0	-2.668606	1.417574	-1.713546
34	1	0	-3.159986	-1.210362	1.666018
35	1	0	3.159720	-1.208982	-1.666964

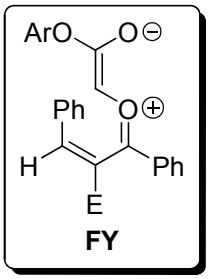


Cu-La

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.314481	0.506854	-0.000751
2	7	0	-1.560993	-0.762304	-0.000694
3	6	0	-3.027888	-0.957785	-0.002563
4	6	0	-3.583073	0.483427	-0.002076
5	8	0	-2.381201	1.312953	-0.001937
6	29	0	0.000177	-1.933870	0.001121
7	7	0	1.560880	-0.762050	0.000016
8	6	0	1.314483	0.507127	-0.000777
9	8	0	2.381185	1.313147	-0.002639
10	6	0	3.583050	0.483544	-0.002541
11	6	0	3.027784	-0.957653	-0.001798
12	6	0	-0.000050	1.291648	0.001460
13	1	0	-4.155714	0.740092	0.890603

14	1	0	-4.155946	0.740703	-0.894403
15	1	0	-3.319808	-1.527001	-0.889458
16	1	0	-3.321985	-1.528412	0.882684
17	1	0	3.319654	-1.527598	-0.888235
18	1	0	3.321877	-1.527536	0.883929
19	1	0	4.155618	0.740145	-0.895259
20	1	0	4.155977	0.740863	0.889759
21	6	0	-0.000160	2.186213	1.280335
22	6	0	-0.000159	2.194541	-1.271513
23	1	0	-0.888493	2.828190	-1.271534
24	1	0	0.887226	2.829531	-1.270649
25	1	0	0.000793	1.590320	-2.184843
26	1	0	0.887256	2.821214	1.283635
27	1	0	-0.888488	2.819895	1.284305
28	1	0	0.000797	1.575989	2.189672



FY

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.166439	-1.239486	1.503572
2	6	0	2.794220	-0.924529	1.593514
3	6	0	2.214283	-0.782303	2.876620
4	6	0	2.988125	-0.950949	4.017680
5	6	0	4.349809	-1.260144	3.916729
6	6	0	4.931339	-1.403105	2.654945
7	6	0	1.990018	-0.756229	0.398924
8	8	0	0.723373	-0.522738	0.609772
9	6	0	-0.275524	-0.314767	-0.239126
10	8	0	-2.495155	0.122823	-0.615355
11	6	0	-3.820263	0.351546	-0.221212
12	6	0	2.481412	-0.895576	-0.991059
13	6	0	2.051319	-2.168932	-1.650442
14	8	0	1.385789	-3.016881	-1.088352
15	6	0	3.268247	-0.008097	-1.652158
16	6	0	3.777472	1.303710	-1.253211
17	6	0	3.286982	2.055078	-0.165760
18	6	0	3.825494	3.302898	0.132178
19	6	0	4.863342	3.830015	-0.642721

20	6	0	5.353779	3.105172	-1.730789
21	6	0	4.809238	1.860896	-2.036181
22	8	0	2.472699	-2.283803	-2.930281
23	6	0	2.088381	-3.500944	-3.591278
24	1	0	6.153773	3.511177	-2.343341
25	1	0	5.187205	1.301081	-2.888234
26	1	0	5.280194	4.804499	-0.403845
27	1	0	3.430512	3.869617	0.970427
28	1	0	3.581166	-0.321417	-2.645394
29	1	0	2.471857	1.671809	0.436395
30	1	0	-0.090690	-0.325380	-1.303432
31	1	0	2.500097	-4.367974	-3.068079
32	1	0	0.999611	-3.590451	-3.624898
33	1	0	2.500206	-3.427389	-4.598138
34	1	0	1.157993	-0.547393	2.958311
35	1	0	2.526537	-0.841548	4.995271
36	1	0	4.949015	-1.390381	4.813479
37	1	0	5.986421	-1.647202	2.565530
38	1	0	4.627328	-1.359981	0.528789
39	6	0	-4.257284	1.679603	-0.090761
40	6	0	-5.604313	1.885975	0.231694
41	6	0	-6.473621	0.812570	0.413152

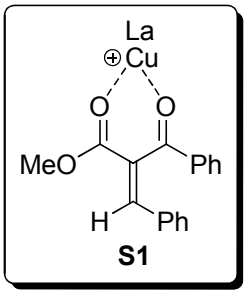
42	6	0	-6.007441	-0.492405	0.271282
43	6	0	-4.670013	-0.753424	-0.052188
44	6	0	-3.294566	2.850156	-0.251243
45	1	0	-5.976016	2.900565	0.346335
46	1	0	-7.515442	0.993418	0.664928
47	1	0	-6.691504	-1.323877	0.417480
48	6	0	-4.008259	-2.830819	1.213695
49	6	0	-5.030930	-3.045384	-1.105681
50	6	0	-3.849605	3.956660	-1.165392
51	6	0	-2.894213	3.412967	1.128386
52	1	0	-2.387568	2.462015	-0.725826
53	1	0	-3.582532	-3.838169	1.126802
54	1	0	-3.353412	-2.230304	1.852225
55	1	0	-4.982818	-2.917946	1.710212
56	1	0	-4.583907	-4.039122	-1.228714
57	1	0	-6.039464	-3.189310	-0.700223
58	1	0	-5.130133	-2.591136	-2.097998
59	1	0	-2.151960	4.213991	1.019402
60	1	0	-3.765741	3.830487	1.647717
61	1	0	-2.469702	2.626432	1.759943
62	1	0	-3.091837	4.734081	-1.321067
63	1	0	-4.135422	3.558919	-2.145563

64	1	0	-4.730507	4.443921	-0.730879
65	6	0	-4.155946	-2.182576	-0.178215
66	1	0	-3.159273	-2.135261	-0.627918
67	6	0	-1.544829	-0.069855	0.375916
68	8	0	-1.790773	-0.024913	1.571103

N_2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.000000	0.000000	0.552659
2	7	0	0.000000	0.000000	-0.552659



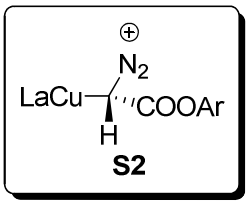
S1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.060639	3.345273	0.566346
2	6	0	-2.639128	2.755575	0.712721
3	7	0	-2.781661	1.358930	0.255540
4	6	0	-4.007832	1.173957	-0.070554
5	8	0	-4.843057	2.226264	0.064546
6	29	0	-1.283209	-0.057141	0.134168
7	7	0	-2.582117	-1.465074	-0.570139
8	6	0	-2.254060	-2.863465	-0.915064
9	6	0	-3.597297	-3.456583	-1.396774
10	8	0	-4.529717	-2.351762	-1.244466
11	6	0	-3.836675	-1.290446	-0.780944
12	6	0	-4.714417	-0.062417	-0.601036
13	6	0	-5.326812	0.293399	-1.988497
14	6	0	-5.853867	-0.428234	0.395922
15	1	0	-3.599921	-3.749905	-2.448884
16	1	0	-3.962403	-4.285410	-0.786780
17	1	0	-1.480435	-2.877139	-1.688598
18	1	0	-1.857093	-3.371880	-0.030939
19	1	0	-6.533845	0.418938	0.503358

20	1	0	-6.411916	-1.287501	0.019320
21	1	0	-5.447827	-0.678455	1.381880
22	1	0	-5.888366	-0.559791	-2.374030
23	1	0	-6.001020	1.145818	-1.885219
24	1	0	-4.543229	0.551949	-2.708759
25	1	0	-1.897958	3.267712	0.091980
26	1	0	-2.277839	2.764475	1.745655
27	1	0	-4.132644	4.153858	-0.164379
28	1	0	-4.508217	3.666211	1.509316
29	1	0	6.959542	-1.793781	-2.828391
30	6	0	6.165350	-1.704179	-2.092965
31	6	0	4.938945	-1.136996	-2.454509
32	6	0	6.360556	-2.175697	-0.792191
33	6	0	3.917751	-1.018961	-1.517557
34	1	0	4.777164	-0.795998	-3.472733
35	6	0	5.334532	-2.075015	0.142301
36	1	0	7.305697	-2.630738	-0.511843
37	6	0	4.105724	-1.469555	-0.194711
38	1	0	2.959950	-0.611844	-1.823342
39	1	0	5.482719	-2.452283	1.151047
40	6	0	3.084908	-1.390712	0.844119
41	6	0	1.999613	-0.575556	0.954411

42	1	0	3.200584	-2.123831	1.639443
43	6	0	1.665718	0.573995	0.051130
44	6	0	1.000605	-0.851382	2.025045
45	6	0	2.621390	1.694269	-0.108175
46	8	0	0.558849	0.622530	-0.513730
47	8	0	-0.186772	-0.534476	1.970004
48	8	0	1.516244	-1.483728	3.082032
49	6	0	2.384703	2.637494	-1.127288
50	6	0	3.720021	1.872168	0.752235
51	6	0	0.598142	-1.825491	4.143367
52	6	0	3.237719	3.722653	-1.290311
53	1	0	1.533200	2.495437	-1.784380
54	6	0	4.564790	2.967980	0.592382
55	1	0	3.904252	1.163734	1.552303
56	1	0	1.204957	-2.333978	4.891274
57	1	0	0.149475	-0.920579	4.558450
58	1	0	-0.187853	-2.484639	3.767584
59	6	0	4.329030	3.890370	-0.429902
60	1	0	3.056722	4.440000	-2.085351
61	1	0	5.406088	3.103467	1.265287
62	1	0	4.992727	4.740988	-0.556049



S2

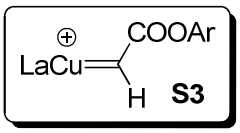
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.594744	1.636658	-1.320958
2	7	0	0.921252	2.837961	-0.756157
3	7	0	1.161826	3.815062	-0.258437
4	6	0	1.532719	0.507553	-0.978435
5	8	0	1.523548	-0.534073	-1.590502
6	8	0	2.305349	0.821501	0.076322
7	1	0	-2.883455	-3.084443	-3.445043
8	6	0	-2.430561	-2.811092	-2.491407
9	6	0	-1.535833	-1.556922	-2.542514
10	8	0	-3.507968	-2.420350	-1.587569
11	1	0	-1.938050	-3.683322	-2.054070
12	7	0	-2.086028	-0.693083	-1.472081
13	1	0	-1.611447	-1.025193	-3.497590

14	1	0	-0.480815	-1.759885	-2.351047
15	6	0	-3.166380	-1.240648	-1.042089
16	29	0	-1.263437	1.007627	-0.678249
17	6	0	-4.165022	-0.766153	0.000306
18	7	0	-2.829183	1.349601	0.532012
19	6	0	-3.847555	0.569188	0.654516
20	6	0	-4.237427	-1.839680	1.127616
21	6	0	-5.553975	-0.643951	-0.695971
22	6	0	-3.038752	2.516212	1.418954
23	8	0	-4.804310	0.960209	1.510543
24	1	0	-4.986898	-1.549062	1.866442
25	1	0	-4.518011	-2.802642	0.696764
26	1	0	-3.270787	-1.950305	1.630513
27	1	0	-5.827181	-1.604220	-1.136916
28	1	0	-6.311296	-0.360966	0.037185
29	1	0	-5.532846	0.111667	-1.488411
30	6	0	-4.391193	2.223719	2.104754
31	1	0	-3.057248	3.431765	0.819972
32	1	0	-2.210418	2.590960	2.129438
33	1	0	-5.168765	2.958807	1.889900
34	1	0	-4.318576	2.071843	3.183490
35	1	0	0.407790	1.765329	-2.388000

36	6	0	3.213112	-0.163127	0.571986
37	6	0	2.771760	-0.978113	1.622167
38	6	0	4.503538	-0.200594	0.029313
39	6	0	3.695751	-1.898918	2.132230
40	6	0	5.383277	-1.142828	0.578643
41	6	0	4.986126	-1.984683	1.614552
42	1	0	3.400502	-2.557073	2.944281
43	1	0	6.393684	-1.215809	0.187918
44	1	0	5.686456	-2.706858	2.023871
45	6	0	1.357543	-0.896484	2.186529
46	1	0	0.860349	-0.033848	1.726429
47	6	0	4.949424	0.712535	-1.107262
48	1	0	4.157638	1.451222	-1.276596
49	6	0	1.355253	-0.656728	3.707954
50	1	0	0.328186	-0.540469	4.074136
51	1	0	1.802846	-1.496291	4.250668
52	1	0	1.915943	0.246897	3.969557
53	6	0	0.544997	-2.153882	1.816426
54	1	0	0.517104	-2.299782	0.730996
55	1	0	0.983586	-3.053405	2.262569
56	1	0	-0.485292	-2.069066	2.185314
57	6	0	6.223813	1.500070	-0.747822

58	1	0	7.084867	0.837157	-0.609139
59	1	0	6.474773	2.198373	-1.554112
60	1	0	6.091772	2.076061	0.174361
61	6	0	5.133507	-0.082951	-2.415739
62	1	0	5.931660	-0.827239	-2.315141
63	1	0	4.215244	-0.611536	-2.692062
64	1	0	5.407140	0.589963	-3.236669



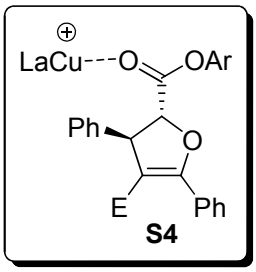
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.191481	2.448495	-2.284176
2	6	0	-2.794189	1.795875	-2.371684
3	7	0	-2.824169	0.761196	-1.312564
4	6	0	-3.972619	0.815935	-0.730427
5	8	0	-4.832677	1.734007	-1.184773
6	29	0	-1.332224	-0.506377	-0.914953

7	7	0	-2.410905	-1.398892	0.528693
8	6	0	-1.927155	-2.525470	1.358029
9	6	0	-3.033890	-2.687658	2.422333
10	8	0	-4.065852	-1.746836	1.988893
11	6	0	-3.580768	-1.063792	0.945397
12	6	0	-4.527421	-0.001905	0.421633
13	6	0	-5.825758	-0.712741	-0.064811
14	6	0	0.393699	-0.971561	-1.379730
15	6	0	1.571062	-0.731964	-0.549706
16	8	0	2.426575	0.213213	-0.894517
17	1	0	0.611116	-1.720307	-2.153020
18	8	0	1.605895	-1.480353	0.418139
19	6	0	-4.867108	0.973374	1.587353
20	1	0	-3.487376	-3.679050	2.452205
21	1	0	-2.727190	-2.391565	3.427762
22	1	0	-1.812514	-3.411517	0.725919
23	1	0	-0.948850	-2.282150	1.779121
24	1	0	-5.581369	1.723468	1.242490
25	1	0	-5.310413	0.414367	2.413559
26	1	0	-3.969472	1.483945	1.951686
27	1	0	-6.260050	-1.283416	0.758534
28	1	0	-6.549201	0.033211	-0.399451

29	1	0	-5.616138	-1.396561	-0.893971
30	1	0	-2.604562	1.324383	-3.339912
31	1	0	-1.981390	2.499618	-2.170962
32	1	0	-4.807785	2.301134	-3.172810
33	1	0	-4.173942	3.507050	-2.019803
34	6	0	3.569655	0.444098	-0.053548
35	6	0	4.726100	-0.304194	-0.301202
36	6	0	3.464814	1.458278	0.905736
37	6	0	5.837005	-0.010340	0.501105
38	6	0	4.607974	1.705862	1.676478
39	6	0	5.779932	0.978615	1.479947
40	1	0	6.758246	-0.565861	0.354366
41	1	0	4.578907	2.478139	2.439093
42	1	0	6.654271	1.187208	2.089503
43	6	0	2.175164	2.239241	1.133828
44	1	0	1.505666	2.031759	0.291066
45	6	0	4.794254	-1.396862	-1.362148
46	1	0	3.877746	-1.343926	-1.960796
47	6	0	2.407232	3.761104	1.158385
48	1	0	1.449565	4.287673	1.243196
49	1	0	3.022859	4.066209	2.011457
50	1	0	2.905247	4.103291	0.245156

51	6	0	1.470412	1.761246	2.420863
52	1	0	0.517513	2.287696	2.557346
53	1	0	1.273449	0.683686	2.388767
54	1	0	2.089369	1.958554	3.303475
55	6	0	4.848905	-2.793104	-0.708467
56	1	0	5.762112	-2.913023	-0.114525
57	1	0	3.993505	-2.954469	-0.044015
58	1	0	4.845327	-3.575318	-1.476445
59	6	0	5.971202	-1.188753	-2.334027
60	1	0	5.946313	-1.950162	-3.121528
61	1	0	5.927531	-0.203347	-2.809828
62	1	0	6.937859	-1.274829	-1.825811



S4

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

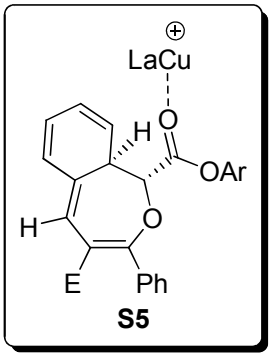
1	6	0	-1.069162	-1.555600	0.396635
2	6	0	-2.563574	-1.799990	0.587476
3	6	0	-3.251128	-1.323135	-0.491213
4	8	0	-2.411767	-0.708159	-1.399675
5	6	0	-1.104887	-0.609440	-0.848200
6	6	0	-4.653354	-1.300008	-0.918572
7	6	0	-0.764149	0.822867	-0.466246
8	8	0	0.396499	1.181568	-0.246542
9	8	0	-1.803796	1.623686	-0.365274
10	6	0	-0.247265	-2.818165	0.169347
11	6	0	-3.075453	-2.412245	1.817709
12	8	0	-4.214441	-2.772859	2.052090
13	8	0	-2.074136	-2.530470	2.732628
14	6	0	-2.454386	-3.149589	3.973229
15	6	0	-5.583926	-2.272089	-0.508403
16	6	0	-6.895339	-2.221368	-0.975464
17	6	0	-7.299223	-1.208188	-1.847247
18	6	0	-6.380773	-0.239312	-2.260660
19	6	0	-5.066334	-0.286529	-1.808159
20	6	0	0.828791	-3.122775	1.012071
21	6	0	1.586761	-4.280403	0.813225
22	6	0	1.277616	-5.147612	-0.236891

23	6	0	0.204615	-4.852053	-1.084236
24	6	0	-0.553890	-3.698552	-0.879441
25	1	0	-0.650023	-1.034489	1.262652
26	1	0	-0.387657	-0.914600	-1.615010
27	1	0	-1.541969	-3.192442	4.568721
28	1	0	-2.845807	-4.154342	3.795752
29	1	0	-3.219045	-2.556441	4.481240
30	1	0	-5.281379	-3.048376	0.180068
31	1	0	-7.604373	-2.979171	-0.655419
32	1	0	-8.324752	-1.173163	-2.204185
33	1	0	-6.689376	0.552054	-2.937631
34	1	0	-4.353010	0.463127	-2.130184
35	1	0	1.057660	-2.462740	1.845544
36	1	0	2.405075	-4.512665	1.489730
37	1	0	1.854354	-6.056696	-0.383717
38	1	0	-0.052160	-5.528560	-1.894696
39	1	0	-1.400121	-3.490739	-1.529823
40	6	0	-1.611738	2.987821	0.024402
41	6	0	-1.301098	3.919940	-0.972408
42	6	0	-1.834254	3.300439	1.371347
43	6	0	-1.169140	5.251464	-0.554556
44	6	0	-1.687214	4.647430	1.727239

45	6	0	-1.352145	5.611548	0.778465
46	1	0	-0.926837	6.015581	-1.287271
47	1	0	-1.845626	4.945230	2.759257
48	1	0	-1.247972	6.650657	1.077192
49	6	0	-1.115898	3.539602	-2.437694
50	1	0	-1.367538	2.479323	-2.550152
51	6	0	-2.199441	2.240022	2.405568
52	1	0	-2.500509	1.335374	1.866445
53	6	0	-3.396945	2.658137	3.278128
54	1	0	-3.160002	3.517964	3.914720
55	1	0	-4.264893	2.919871	2.664451
56	1	0	-3.684402	1.832230	3.937931
57	6	0	-0.978944	1.880824	3.279012
58	1	0	-0.132643	1.548610	2.665694
59	1	0	-0.647974	2.746790	3.864427
60	1	0	-1.232362	1.077013	3.979757
61	6	0	-2.076179	4.322576	-3.354053
62	1	0	-1.864964	5.397512	-3.337449
63	1	0	-1.971603	3.981350	-4.390066
64	1	0	-3.118816	4.180547	-3.051270
65	6	0	0.349314	3.722854	-2.881661
66	1	0	0.655481	4.772875	-2.811540

67	1	0	1.029419	3.132247	-2.257414
68	1	0	0.475419	3.407953	-3.924053
69	1	0	4.565758	-3.074741	-3.314138
70	6	0	4.210481	-2.958873	-2.289151
71	6	0	2.948399	-2.084688	-2.143452
72	8	0	5.224458	-2.215583	-1.552692
73	1	0	4.113863	-3.939437	-1.817416
74	7	0	3.363177	-1.022744	-1.199063
75	1	0	2.099872	-2.635257	-1.732411
76	1	0	2.640618	-1.622104	-3.087190
77	6	0	4.617485	-1.175759	-0.954575
78	29	0	2.180811	0.336253	-0.347251
79	6	0	5.575755	-0.354197	-0.106623
80	7	0	3.727305	1.177530	0.744468
81	6	0	4.951503	0.800296	0.659532
82	6	0	6.662353	0.227861	-1.060509
83	6	0	6.244407	-1.303451	0.931656
84	6	0	3.674100	2.350672	1.641816
85	8	0	5.858968	1.507856	1.358877
86	1	0	7.403199	0.780312	-0.479729
87	1	0	7.160704	-0.586036	-1.590762
88	1	0	6.217480	0.905724	-1.796826

89	1	0	6.750536	-2.120241	0.414104
90	1	0	6.976868	-0.746748	1.519408
91	1	0	5.499327	-1.728436	1.612795
92	6	0	5.147238	2.571053	2.055131
93	1	0	3.021167	2.130680	2.491797
94	1	0	3.249249	3.203559	1.104477
95	1	0	5.333118	2.447096	3.123902
96	1	0	5.565607	3.522312	1.719983



S5

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.855068	-3.233816	-2.643245
2	6	0	0.346659	-3.538381	-2.084759
3	6	0	1.254550	-2.538811	-1.577782

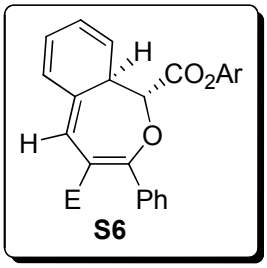
4	6	0	0.916522	-1.066066	-1.742277
5	6	0	-0.461559	-0.817460	-2.322750
6	6	0	-1.256002	-1.845883	-2.772306
7	6	0	2.381582	-2.946538	-0.916354
8	6	0	3.449123	-2.199986	-0.289447
9	6	0	3.598953	-0.825454	-0.196354
10	8	0	2.587846	0.070788	-0.346940
11	6	0	1.242097	-0.341931	-0.362651
12	6	0	4.505937	-3.113374	0.274666
13	8	0	4.757020	-4.212237	-0.180894
14	8	0	5.071193	-2.630027	1.396516
15	6	0	6.104781	-3.451137	1.970649
16	6	0	4.869064	-0.105873	0.008131
17	6	0	0.353908	0.856055	-0.058493
18	8	0	-0.853714	0.716543	0.091975
19	8	0	0.997149	2.013476	0.036204
20	6	0	6.061777	-0.574332	-0.573081
21	6	0	7.247511	0.137444	-0.418638
22	6	0	7.259997	1.329897	0.310844
23	6	0	6.077233	1.813262	0.875684
24	6	0	4.886974	1.107351	0.718975
25	1	0	-1.511654	-4.010787	-3.020781

26	1	0	0.657794	-4.576877	-1.996285
27	1	0	1.637852	-0.601293	-2.431625
28	1	0	-0.681600	0.198297	-2.644377
29	1	0	-2.143479	-1.614146	-3.357874
30	1	0	2.545748	-4.019473	-0.865396
31	1	0	1.060739	-1.063115	0.442650
32	1	0	6.440947	-2.913821	2.857179
33	1	0	5.707474	-4.433152	2.238248
34	1	0	6.928164	-3.579466	1.263142
35	1	0	6.051031	-1.482044	-1.169046
36	1	0	8.159770	-0.229818	-0.879455
37	1	0	8.186139	1.885001	0.429400
38	1	0	6.082661	2.742509	1.438022
39	1	0	3.966966	1.486886	1.150148
40	6	0	0.253513	3.199793	0.309414
41	6	0	-0.009106	4.047149	-0.775382
42	6	0	-0.087643	3.486313	1.637851
43	6	0	-0.696698	5.234729	-0.490512
44	6	0	-0.772356	4.688466	1.860301
45	6	0	-1.081461	5.550533	0.810492
46	1	0	-0.922645	5.924463	-1.298639
47	1	0	-1.059809	4.954547	2.873304

48	1	0	-1.609853	6.478502	1.009353
49	6	0	0.265483	2.568776	2.803641
50	1	0	0.857051	1.733141	2.414496
51	6	0	0.435102	3.723956	-2.198532
52	1	0	1.021447	2.799898	-2.167041
53	6	0	1.356154	4.820135	-2.768365
54	1	0	1.711950	4.535496	-3.764936
55	1	0	0.832941	5.778053	-2.864314
56	1	0	2.229352	4.976404	-2.126788
57	6	0	-0.773756	3.482678	-3.124159
58	1	0	-0.438767	3.212187	-4.132203
59	1	0	-1.411616	2.674357	-2.745590
60	1	0	-1.394968	4.381540	-3.210950
61	6	0	1.146426	3.289853	3.843015
62	1	0	2.059448	3.685687	3.385664
63	1	0	0.616240	4.127198	4.310238
64	1	0	1.436523	2.595991	4.640057
65	6	0	-0.998625	1.978734	3.459334
66	1	0	-1.621173	2.765972	3.899682
67	1	0	-1.605128	1.436517	2.726033
68	1	0	-0.723042	1.285709	4.262838
69	1	0	-5.549491	2.688234	-0.256697

70	6	0	-5.538653	1.762572	-0.835355
71	6	0	-4.141681	1.366998	-1.365209
72	8	0	-5.879924	0.673697	0.067041
73	1	0	-6.309529	1.805879	-1.608155
74	7	0	-3.881020	0.052612	-0.744545
75	1	0	-3.356181	2.066733	-1.063946
76	1	0	-4.114180	1.272458	-2.455263
77	6	0	-4.872075	-0.222385	0.020790
78	29	0	-2.032018	-0.951543	-0.789836
79	6	0	-5.133048	-1.439191	0.890650
80	7	0	-2.773503	-2.346060	0.543575
81	6	0	-3.968550	-2.407823	1.010309
82	6	0	-6.347190	-2.201159	0.281109
83	6	0	-5.488085	-0.953221	2.327042
84	6	0	-2.042606	-3.542627	1.012326
85	8	0	-4.275915	-3.488402	1.755639
86	1	0	-6.607152	-3.052290	0.913466
87	1	0	-7.206507	-1.529967	0.218681
88	1	0	-6.116850	-2.569109	-0.724467
89	1	0	-6.360296	-0.298484	2.289449
90	1	0	-5.714409	-1.813023	2.960480
91	1	0	-4.654772	-0.399023	2.771911

92	6	0	-3.108536	-4.355758	1.778341
93	1	0	-1.209983	-3.229073	1.650861
94	1	0	-1.626992	-4.076761	0.154062
95	1	0	-2.859143	-4.549245	2.823149
96	1	0	-3.383951	-5.293460	1.289556



S6

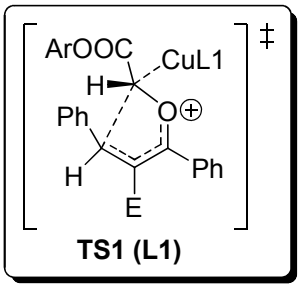
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.696242	5.199103	-0.566900
2	6	0	1.801711	4.414420	-0.570083
3	6	0	1.757300	3.009364	-0.231210
4	6	0	0.436273	2.393320	0.194437
5	6	0	-0.728798	3.347629	0.134600
6	6	0	-0.594822	4.640663	-0.211072
7	6	0	2.890678	2.259171	-0.366508

8	6	0	3.116568	0.845454	-0.153379
9	6	0	2.197109	-0.138441	0.154180
10	8	0	0.849672	-0.036128	0.022500
11	6	0	0.224190	1.053437	-0.633182
12	6	0	4.568141	0.486232	-0.290203
13	8	0	5.486511	1.223586	0.015055
14	8	0	4.760774	-0.712789	-0.884990
15	6	0	6.129536	-1.122750	-1.007226
16	6	0	2.527972	-1.452656	0.752467
17	6	0	-1.242920	0.678791	-0.842325
18	8	0	-1.888047	1.091506	-1.775920
19	8	0	-1.716266	-0.127277	0.139242
20	6	0	3.508620	-1.559010	1.753995
21	6	0	3.783561	-2.788012	2.349261
22	6	0	3.075975	-3.929315	1.963351
23	6	0	2.086635	-3.830834	0.982274
24	6	0	1.808444	-2.602088	0.386947
25	1	0	0.763566	6.248588	-0.837896
26	1	0	2.767809	4.824603	-0.855277
27	1	0	0.518786	2.027223	1.230172
28	1	0	-1.700195	2.961123	0.425823
29	1	0	-1.465198	5.292024	-0.213754

30	1	0	3.790547	2.794299	-0.656169
31	1	0	0.649020	1.194915	-1.629997
32	1	0	6.101014	-2.079482	-1.529791
33	1	0	6.703470	-0.387078	-1.576519
34	1	0	6.584981	-1.241417	-0.019523
35	1	0	4.039424	-0.669394	2.080287
36	1	0	4.540128	-2.851462	3.126639
37	1	0	3.287661	-4.887022	2.431140
38	1	0	1.528705	-4.713002	0.680103
39	1	0	1.038429	-2.528767	-0.373256
40	6	0	-3.018379	-0.660343	0.005109
41	6	0	-4.039051	-0.103358	0.788879
42	6	0	-3.207169	-1.769694	-0.834262
43	6	0	-5.308609	-0.688145	0.695216
44	6	0	-4.497232	-2.311662	-0.891980
45	6	0	-5.540485	-1.778131	-0.139321
46	1	0	-6.126095	-0.279847	1.282712
47	1	0	-4.685017	-3.165164	-1.537474
48	1	0	-6.533569	-2.214960	-0.200286
49	6	0	-2.079375	-2.372543	-1.664314
50	1	0	-1.148860	-1.869478	-1.383628
51	6	0	-3.802303	1.103995	1.687633

52	1	0	-2.722908	1.280626	1.725026
53	6	0	-4.266601	0.858142	3.134989
54	1	0	-4.014544	1.719864	3.764188
55	1	0	-5.351435	0.713345	3.196487
56	1	0	-3.784429	-0.027995	3.561719
57	6	0	-4.467252	2.362518	1.093846
58	1	0	-4.243434	3.244442	1.706509
59	1	0	-4.116154	2.549812	0.073156
60	1	0	-5.557316	2.249904	1.054418
61	6	0	-1.881700	-3.870281	-1.361670
62	1	0	-1.692815	-4.038157	-0.295545
63	1	0	-2.760506	-4.461428	-1.643774
64	1	0	-1.027762	-4.261696	-1.927759
65	6	0	-2.306775	-2.128883	-3.169387
66	1	0	-3.216343	-2.632971	-3.517512
67	1	0	-2.408934	-1.059952	-3.379414
68	1	0	-1.464086	-2.519239	-3.752871



TS1 (L1)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.683076	0.027684	2.567366
2	6	0	-1.595157	1.090209	2.739637
3	6	0	-2.556470	1.042034	3.749808
4	6	0	-2.615285	-0.058037	4.606616
5	6	0	-1.726434	-1.127861	4.436230
6	6	0	-0.785526	-1.099756	3.415022
7	6	0	0.471339	0.117159	1.626716
8	6	0	1.115497	1.443337	1.431853
9	6	0	1.570921	1.804150	0.198006
10	8	0	1.291034	0.955236	-0.839129
11	6	0	0.865606	-0.314163	-0.507345
12	29	0	-1.164444	-0.290483	0.261956
13	6	0	1.922998	-1.341114	-0.189740
14	8	0	3.165398	-0.825225	-0.251549

15	8	0	1.640996	-2.490229	0.073947
16	6	0	1.317691	2.293259	2.644581
17	8	0	1.735259	1.534131	3.680368
18	6	0	1.915684	2.233798	4.928965
19	8	0	1.130698	3.490146	2.732834
20	6	0	2.353873	2.968249	-0.263822
21	1	0	0.270393	-0.700625	-1.344227
22	1	0	-3.344212	-0.081619	5.411556
23	1	0	-3.238374	1.876384	3.883907
24	1	0	-1.766371	-1.978543	5.109114
25	1	0	-1.505136	1.972286	2.118394
26	1	0	-0.085049	-1.921529	3.293985
27	1	0	1.136778	-0.716168	1.822262
28	1	0	2.216215	1.470742	5.646270
29	1	0	0.980783	2.708925	5.236219
30	1	0	2.690889	2.996578	4.827364
31	6	0	3.457667	2.711903	-1.100866
32	6	0	4.234293	3.762809	-1.581256
33	6	0	3.909409	5.081028	-1.250866
34	6	0	2.805780	5.341220	-0.437175
35	6	0	2.028044	4.295071	0.058622
36	1	0	3.711005	1.686687	-1.349743

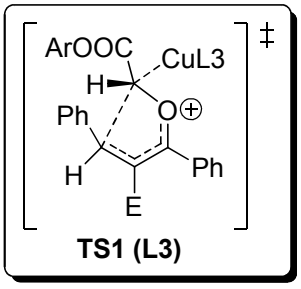
37	1	0	5.092905	3.552986	-2.212506
38	1	0	4.513522	5.901194	-1.628487
39	1	0	2.543880	6.364909	-0.185850
40	1	0	1.175047	4.502938	0.688846
41	1	0	-0.911238	6.078233	-2.668685
42	6	0	-1.202655	5.087506	-2.332730
43	6	0	-1.965273	4.934999	-1.181774
44	6	0	-0.815975	3.961855	-3.053669
45	6	0	-2.361916	3.670946	-0.721506
46	1	0	-2.267702	5.816633	-0.624945
47	6	0	-1.178271	2.673364	-2.647836
48	1	0	-0.220575	4.086084	-3.952146
49	6	0	-1.964410	2.541867	-1.474032
50	6	0	-3.212255	3.592969	0.546141
51	6	0	-0.776618	1.473244	-3.506840
52	7	0	-2.318156	1.197565	-1.069141
53	1	0	-3.296759	2.539770	0.838074
54	1	0	-0.818062	0.580457	-2.871760
55	6	0	-3.437159	0.681453	-1.436231
56	6	0	-3.647723	-0.799899	-1.170876
57	7	0	-2.785595	-1.424597	-0.443914
58	6	0	-2.865598	-2.867684	-0.314827

59	6	0	-3.475001	-3.430651	0.831970
60	6	0	-2.309575	-3.672872	-1.336527
61	6	0	-3.525354	-4.827286	0.918593
62	6	0	-4.099210	-2.569681	1.931395
63	6	0	-2.381384	-5.063628	-1.182415
64	6	0	-1.639443	-3.114807	-2.592671
65	6	0	-2.985246	-5.641087	-0.073144
66	1	0	-3.994267	-5.290000	1.779430
67	1	0	-3.496711	-1.656299	2.018977
68	1	0	-1.957525	-5.701868	-1.951916
69	1	0	-1.635161	-2.020391	-2.529824
70	1	0	-3.035146	-6.721760	0.021978
71	6	0	-5.544874	-2.144893	1.593108
72	1	0	-5.601729	-1.533778	0.688388
73	1	0	-6.182844	-3.023728	1.444121
74	1	0	-5.969452	-1.557531	2.415564
75	6	0	-4.095657	-3.259526	3.307094
76	1	0	-3.108149	-3.655334	3.563935
77	1	0	-4.390023	-2.542895	4.080343
78	1	0	-4.813528	-4.086086	3.348733
79	6	0	-2.567578	4.363953	1.718756
80	1	0	-1.519096	4.092529	1.880261

81	1	0	-2.597276	5.444947	1.545255
82	1	0	-3.121769	4.176676	2.646317
83	6	0	-4.642935	4.126685	0.315272
84	1	0	-4.622881	5.184890	0.031998
85	1	0	-5.167236	3.584137	-0.476729
86	1	0	-5.235273	4.039649	1.233545
87	6	0	-1.769615	1.261138	-4.669993
88	1	0	-1.487042	0.383115	-5.262865
89	1	0	-2.796432	1.116311	-4.319743
90	1	0	-1.771743	2.129807	-5.338237
91	6	0	0.655959	1.571442	-4.063960
92	1	0	0.740808	2.345740	-4.834239
93	1	0	1.380603	1.790785	-3.276281
94	1	0	0.933944	0.622226	-4.537012
95	6	0	-0.171372	-3.573047	-2.703255
96	1	0	0.312039	-3.089883	-3.561024
97	1	0	0.395613	-3.337240	-1.798453
98	1	0	-0.104813	-4.655206	-2.860967
99	6	0	-2.409950	-3.500058	-3.873300
100	1	0	-2.394281	-4.583987	-4.031193
101	1	0	-3.459631	-3.191158	-3.835276
102	1	0	-1.948494	-3.032645	-4.750806

103	6	0	4.279698	-1.693703	-0.059202
104	6	0	4.823778	-2.316628	-1.190257
105	6	0	4.817436	-1.802724	1.230764
106	6	0	5.960370	-3.110206	-0.986145
107	6	0	5.952117	-2.611283	1.374208
108	6	0	6.517792	-3.261933	0.280467
109	1	0	6.413859	-3.614386	-1.834560
110	1	0	6.399194	-2.729317	2.356759
111	1	0	7.398467	-3.883334	0.414823
112	6	0	4.202744	-1.099701	2.434545
113	1	0	3.471783	-0.374787	2.063472
114	6	0	3.454755	-2.106103	3.333726
115	1	0	2.942709	-1.582799	4.150417
116	1	0	2.714295	-2.675939	2.760685
117	1	0	4.149264	-2.827012	3.780548
118	6	0	5.239930	-0.299527	3.243081
119	1	0	5.982398	-0.951511	3.716356
120	1	0	5.774677	0.415252	2.608685
121	1	0	4.738968	0.261317	4.040378
122	6	0	4.240694	-2.152684	-2.589530
123	1	0	3.367201	-1.495846	-2.520787
124	6	0	3.764437	-3.502308	-3.160947

125	1	0	4.600473	-4.199313	-3.287347
126	1	0	3.031350	-3.975098	-2.499108
127	1	0	3.302044	-3.358951	-4.144754
128	6	0	5.244082	-1.467854	-3.538634
129	1	0	4.793272	-1.316650	-4.526349
130	1	0	5.555803	-0.491323	-3.151911
131	1	0	6.145710	-2.075527	-3.674636
132	6	0	-4.816401	-1.455645	-1.861359
133	1	0	-5.746090	-0.917940	-1.651632
134	1	0	-4.673053	-1.431168	-2.948356
135	1	0	-4.929582	-2.494186	-1.554990
136	6	0	-4.532439	1.411870	-2.173126
137	1	0	-4.804405	0.898961	-3.100229
138	1	0	-5.437191	1.448649	-1.553838
139	1	0	-4.234113	2.431241	-2.412758



TS1 (L3)

Standard orientation:

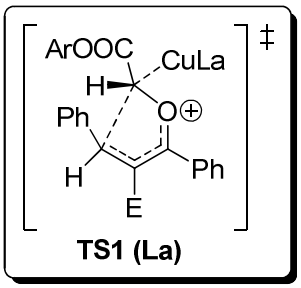
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.502521	-0.147793	2.071534
2	6	0	2.673388	-0.937709	1.981032
3	6	0	3.765417	-0.676655	2.805582
4	6	0	3.719311	0.377159	3.723270
5	6	0	2.576206	1.179278	3.813396
6	6	0	1.480388	0.926819	2.993437
7	6	0	0.286442	-0.437664	1.256754
8	6	0	0.008295	-1.859645	0.906770
9	6	0	-0.292588	-2.203402	-0.379281
10	8	0	-0.288912	-1.198016	-1.309801
11	6	0	-0.301429	0.098158	-0.827291
12	29	0	1.505492	0.834892	0.050174
13	6	0	-1.623571	0.694545	-0.419700
14	8	0	-2.645184	-0.171455	-0.554539
15	8	0	-1.703898	1.841137	-0.035159
16	6	0	-0.040855	-2.833756	2.035366
17	8	0	-0.375372	-2.192401	3.182114
18	6	0	-0.433786	-3.024368	4.357633

19	8	0	0.160492	-4.028813	1.985902
20	6	0	-0.611138	-3.495627	-1.016548
21	1	0	0.115195	0.738311	-1.615161
22	1	0	4.569630	0.570893	4.370606
23	1	0	4.651017	-1.301070	2.735801
24	1	0	2.536124	1.990163	4.534861
25	1	0	2.705972	-1.765042	1.278668
26	1	0	0.580484	1.530027	3.079120
27	1	0	-0.557747	0.144947	1.615766
28	1	0	-0.678937	-2.349258	5.177244
29	1	0	0.530270	-3.509297	4.529771
30	1	0	-1.204547	-3.790071	4.243400
31	6	0	-1.681288	-3.528506	-1.930604
32	6	0	-1.996891	-4.707417	-2.600293
33	6	0	-1.234789	-5.858853	-2.386462
34	6	0	-0.158848	-5.826787	-1.497203
35	6	0	0.154702	-4.654786	-0.810125
36	1	0	-2.268668	-2.631515	-2.095911
37	1	0	-2.835416	-4.727375	-3.290199
38	1	0	-1.478369	-6.777498	-2.912666
39	1	0	0.438714	-6.718685	-1.332822
40	1	0	0.980930	-4.637827	-0.113024

41	1	0	5.395428	-4.258688	-1.762284
42	6	0	4.968628	-3.265781	-1.658395
43	6	0	5.735895	-2.225468	-1.129510
44	6	0	3.646332	-3.025934	-2.042941
45	6	0	5.195277	-0.945698	-1.000461
46	1	0	6.759691	-2.407241	-0.815683
47	6	0	3.088841	-1.756553	-1.895658
48	1	0	3.038344	-3.830489	-2.445789
49	6	0	3.869342	-0.704307	-1.393679
50	7	0	3.250552	0.562165	-1.206450
51	6	0	3.746212	1.667382	-1.651579
52	6	0	3.007537	2.935209	-1.279925
53	7	0	2.028348	2.814151	-0.447166
54	6	0	1.210912	3.917463	-0.058340
55	6	0	1.130689	4.246417	1.300638
56	6	0	0.441206	4.617750	-0.996797
57	6	0	0.307349	5.293592	1.711009
58	6	0	-0.399038	5.646902	-0.572426
59	6	0	-0.463577	5.992379	0.778508
60	1	0	0.262664	5.559890	2.763039
61	1	0	-1.003847	6.177977	-1.301389
62	1	0	-1.115241	6.797296	1.104163

63	6	0	-3.966732	0.297779	-0.300411
64	6	0	-4.671883	0.871015	-1.367536
65	6	0	-4.506186	0.089494	0.975814
66	6	0	-5.987278	1.275664	-1.106518
67	6	0	-5.826438	0.512347	1.177708
68	6	0	-6.559376	1.103337	0.151492
69	1	0	-6.570449	1.731210	-1.901354
70	1	0	-6.285059	0.376051	2.152562
71	1	0	-7.581364	1.424671	0.330794
72	6	0	-3.702016	-0.537316	2.108493
73	1	0	-2.794993	-0.970985	1.675678
74	6	0	-3.268839	0.535784	3.128978
75	1	0	-2.621498	0.094616	3.896668
76	1	0	-2.727589	1.352918	2.638538
77	1	0	-4.138890	0.972924	3.632501
78	6	0	-4.455602	-1.687687	2.800497
79	1	0	-5.352503	-1.334407	3.321233
80	1	0	-4.763368	-2.453373	2.080635
81	1	0	-3.809033	-2.162227	3.547586
82	6	0	-4.053089	1.073075	-2.746610
83	1	0	-3.098312	0.536304	-2.768936
84	6	0	-3.758225	2.565560	-3.002907

85	1	0	-4.684536	3.151632	-3.014413
86	1	0	-3.109811	2.979493	-2.223386
87	1	0	-3.267443	2.698437	-3.974785
88	6	0	-4.924733	0.477364	-3.868186
89	1	0	-4.414787	0.572271	-4.833730
90	1	0	-5.129405	-0.584339	-3.693160
91	1	0	-5.886925	0.994142	-3.954014
92	6	0	3.490708	4.238797	-1.860587
93	1	0	4.578602	4.317822	-1.769515
94	1	0	3.253902	4.307544	-2.929828
95	1	0	3.030884	5.089595	-1.357891
96	6	0	4.959910	1.785039	-2.537775
97	1	0	4.755514	2.454414	-3.379129
98	1	0	5.811837	2.209917	-1.992051
99	1	0	5.260061	0.812109	-2.927536
100	1	0	2.056868	-1.571890	-2.176501
101	1	0	5.786551	-0.143816	-0.568522
102	1	0	1.728270	3.692492	2.017892
103	1	0	0.479325	4.337765	-2.045701



TS1 (La)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.489134	-3.383964	-1.172954
2	6	0	-4.852213	-3.727475	0.017074
3	6	0	-3.803839	-2.952252	0.529427
4	6	0	-3.429953	-1.828705	-0.220168
5	6	0	-4.052369	-1.434177	-1.411549
6	6	0	-5.094894	-2.247471	-1.874701
7	8	0	-2.400320	-0.994610	0.307590
8	6	0	-1.125275	-1.273170	-0.008171
9	8	0	-0.754947	-2.149390	-0.763976
10	6	0	-3.104268	-3.343607	1.826918
11	6	0	-4.099636	-3.579360	2.978388
12	6	0	-3.614775	-0.199990	-2.190406
13	6	0	-4.792331	0.737718	-2.513967

14	6	0	-0.139165	-0.386317	0.707350
15	29	0	1.769926	-0.036683	-0.165770
16	7	0	3.199021	0.341083	1.311450
17	6	0	3.162206	1.464459	2.271619
18	6	0	4.419675	1.252370	3.143076
19	8	0	5.050604	0.083273	2.548266
20	6	0	4.260713	-0.343727	1.545872
21	1	0	2.231260	1.427201	2.844958
22	6	0	4.802723	-1.590195	0.867646
23	6	0	4.997674	-2.685665	1.956916
24	8	0	-0.629289	0.550595	1.596905
25	6	0	-1.104366	1.715383	1.054352
26	6	0	-1.915839	2.455948	2.039387
27	6	0	-2.856474	1.727542	2.792655
28	6	0	-3.620944	2.363947	3.766211
29	6	0	-3.438950	3.726172	4.018868
30	6	0	-2.492015	4.448937	3.290999
31	6	0	-1.733905	3.823211	2.302699
32	6	0	-0.749385	1.984024	-0.236062
33	6	0	-1.257835	3.170187	-0.983843
34	8	0	-1.579790	4.246696	-0.526676
35	6	0	0.108458	1.028106	-0.996083

36	6	0	1.305570	1.596737	-1.683902
37	6	0	1.995706	2.720900	-1.173027
38	6	0	3.072146	3.267223	-1.867486
39	6	0	3.492729	2.698499	-3.074041
40	6	0	2.829606	1.579557	-3.588513
41	6	0	1.750051	1.030741	-2.901641
42	7	0	2.833454	-1.713560	-0.744200
43	6	0	3.922004	-2.161005	-0.230617
44	8	0	4.402193	-3.313374	-0.732878
45	6	0	3.439223	-3.798089	-1.714367
46	6	0	2.418916	-2.645782	-1.816295
47	1	0	2.469301	-2.122970	-2.777550
48	6	0	6.180434	-1.231990	0.233520
49	8	0	-1.338349	2.881742	-2.306513
50	6	0	-1.793218	3.963121	-3.143982
51	6	0	-2.200761	-4.575802	1.612780
52	6	0	-2.854523	-0.600333	-3.471515
53	1	0	4.200422	1.013916	4.186110
54	1	0	5.137317	2.073688	3.099506
55	1	0	3.183348	2.410344	1.721833
56	1	0	5.431660	-3.579515	1.505929
57	1	0	5.668038	-2.317150	2.735201

58	1	0	4.042168	-2.957520	2.418589
59	1	0	6.858652	-0.866217	1.007310
60	1	0	6.614377	-2.122258	-0.226483
61	1	0	6.071230	-0.458176	-0.533722
62	1	0	1.385484	-2.955106	-1.648154
63	1	0	3.983337	-4.003159	-2.637484
64	1	0	3.014707	-4.726931	-1.325299
65	1	0	0.536695	-1.043022	1.269400
66	1	0	4.327916	3.131638	-3.616539
67	1	0	3.578674	4.143950	-1.474435
68	1	0	3.144619	1.147289	-4.533756
69	1	0	1.652731	3.177603	-0.248929
70	1	0	1.209940	0.184341	-3.318411
71	1	0	-0.409138	0.326842	-1.646057
72	1	0	-1.765886	3.572199	-4.160877
73	1	0	-1.132278	4.827441	-3.042834
74	1	0	-2.809215	4.255448	-2.868869
75	1	0	-2.993178	0.669706	2.595157
76	1	0	-4.356663	1.797302	4.329412
77	1	0	-4.032168	4.221430	4.782374
78	1	0	-2.342085	5.505920	3.490190
79	1	0	-1.011917	4.391531	1.732862

80	1	0	-5.173745	-4.611537	0.559449
81	1	0	-5.603659	-1.984920	-2.797505
82	1	0	-6.299706	-4.000264	-1.551060
83	1	0	-2.462162	-2.508338	2.128000
84	1	0	-2.925340	0.367979	-1.558216
85	1	0	-2.794416	-5.452748	1.330016
86	1	0	-1.470182	-4.396810	0.816693
87	1	0	-1.660372	-4.821303	2.534966
88	1	0	-4.747506	-4.441448	2.785773
89	1	0	-3.558246	-3.778814	3.910193
90	1	0	-4.741509	-2.706094	3.136717
91	1	0	-2.012879	-1.263333	-3.240852
92	1	0	-3.511244	-1.131402	-4.170338
93	1	0	-2.469944	0.291060	-3.981548
94	1	0	-5.329379	1.031155	-1.605863
95	1	0	-4.423288	1.647850	-3.000704
96	1	0	-5.512379	0.270663	-3.195120

TS1-cis (La)

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)		

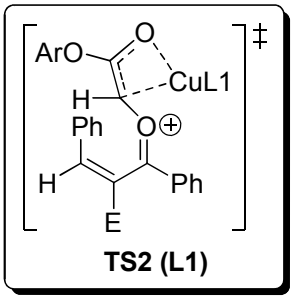
Number	Number	Type	X	Y	Z
1	6	0	-4.637787	4.143070	0.794045
2	6	0	-3.688216	4.450224	-0.176868
3	6	0	-2.793130	3.482910	-0.652344
4	6	0	-2.888224	2.204139	-0.083504
5	6	0	-3.845554	1.842254	0.875707
6	6	0	-4.719903	2.850066	1.303826
7	8	0	-2.045314	1.167693	-0.580526
8	6	0	-0.739982	1.155522	-0.262635
9	8	0	-0.178245	1.936446	0.478619
10	6	0	-1.800989	3.838354	-1.755404
11	6	0	-2.523932	4.316546	-3.030152
12	6	0	-3.987610	0.417327	1.397503
13	6	0	-5.222043	-0.275307	0.784704
14	6	0	0.016715	0.062409	-0.986251
15	29	0	1.900364	-0.224915	-0.089595
16	7	0	3.486772	-1.266451	-1.052856
17	6	0	3.378653	-2.568372	-1.746930
18	6	0	4.754376	-2.747321	-2.426953
19	8	0	5.461386	-1.521618	-2.087099
20	6	0	4.650032	-0.783294	-1.308038

21	1	0	2.552236	-2.534282	-2.463996
22	6	0	5.295839	0.515390	-0.860076
23	6	0	5.698625	1.325205	-2.128665
24	8	0	-0.757461	-0.790699	-1.761491
25	6	0	-1.459006	-1.734319	-1.048062
26	6	0	-2.605672	-2.266196	-1.796317
27	6	0	-3.345577	-1.398599	-2.620334
28	6	0	-4.425584	-1.881280	-3.355632
29	6	0	-4.767810	-3.234095	-3.293043
30	6	0	-4.023028	-4.105868	-2.494181
31	6	0	-2.947922	-3.627805	-1.750956
32	6	0	-0.954686	-2.059077	0.168583
33	6	0	-1.636148	-3.000216	1.098234
34	8	0	-2.833981	-3.077342	1.278833
35	6	0	0.407029	-1.564491	0.563543
36	7	0	3.177540	1.304820	0.320883
37	6	0	4.417854	1.408032	-0.000397
38	8	0	5.077798	2.481120	0.468235
39	6	0	4.112575	3.313849	1.177474
40	6	0	2.841943	2.443175	1.209137
41	1	0	2.613582	2.053160	2.206150
42	6	0	6.573160	0.152983	-0.045186

43	8	0	-0.731930	-3.755984	1.764142
44	6	0	-1.280012	-4.648753	2.754471
45	6	0	-0.772235	4.879281	-1.273733
46	6	0	-4.034735	0.351442	2.935382
47	1	0	4.707669	-2.811986	-3.515568
48	1	0	5.337109	-3.583843	-2.035578
49	1	0	3.161489	-3.358872	-1.021240
50	1	0	6.202067	2.246521	-1.828491
51	1	0	6.378111	0.733842	-2.745409
52	1	0	4.818894	1.585648	-2.726908
53	1	0	7.240873	-0.453360	-0.660113
54	1	0	7.092507	1.065661	0.251471
55	1	0	6.318173	-0.412089	0.857798
56	1	0	1.950077	2.947081	0.838257
57	1	0	4.531477	3.540020	2.158966
58	1	0	3.997911	4.238663	0.606170
59	1	0	0.727128	0.540955	-1.676322
60	1	0	-0.420443	-5.144553	3.204948
61	1	0	-1.943999	-5.378481	2.285042
62	1	0	-1.839796	-4.086072	3.505323
63	1	0	-3.075557	-0.349701	-2.666042
64	1	0	-4.998557	-1.202068	-3.980012

65	1	0	-5.607363	-3.610154	-3.870636
66	1	0	-4.276807	-5.160986	-2.455372
67	1	0	-2.364372	-4.315128	-1.148458
68	1	0	-3.644702	5.456778	-0.582909
69	1	0	-5.479491	2.612801	2.042551
70	1	0	-5.323953	4.909289	1.143267
71	1	0	-1.251213	2.931652	-2.029824
72	1	0	-3.116537	-0.155253	1.068339
73	1	0	-1.258108	5.827721	-1.018098
74	1	0	-0.243504	4.521336	-0.384687
75	1	0	-0.037560	5.085390	-2.061569
76	1	0	-3.074603	5.247490	-2.856195
77	1	0	-1.798952	4.505686	-3.830369
78	1	0	-3.238812	3.567364	-3.386881
79	1	0	-3.184739	0.874067	3.390425
80	1	0	-4.949124	0.804101	3.334615
81	1	0	-4.015563	-0.694182	3.261956
82	1	0	-5.179815	-0.264530	-0.309284
83	1	0	-5.263582	-1.320058	1.109778
84	1	0	-6.148632	0.223227	1.093237
85	6	0	0.682827	-1.091788	1.941214
86	6	0	-0.247319	-0.345442	2.693447

87	6	0	1.919935	-1.423763	2.540683
88	6	0	0.055822	0.060436	3.988528
89	1	0	-1.211565	-0.097993	2.266170
90	6	0	2.220575	-1.009765	3.837547
91	1	0	2.627333	-2.046406	1.997765
92	6	0	1.290519	-0.262576	4.563699
93	1	0	-0.676238	0.626746	4.556594
94	1	0	3.169122	-1.289064	4.287035
95	1	0	1.516700	0.051903	5.578365
96	1	0	1.166124	-2.296728	0.253688



TS2 (L1)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	5.186272	-0.281032	-4.741792

2	6	0	4.490564	-0.675575	-4.006845
3	6	0	3.142488	-0.820597	-4.327672
4	6	0	4.940890	-1.027651	-2.738438
5	6	0	2.227998	-1.324805	-3.397942
6	1	0	2.797115	-0.536085	-5.316683
7	6	0	4.076527	-1.559199	-1.770966
8	1	0	5.989413	-0.892397	-2.489756
9	6	0	2.718381	-1.718295	-2.130266
10	6	0	0.755642	-1.496127	-3.761232
11	6	0	4.625183	-1.893582	-0.384308
12	7	0	1.764551	-2.228509	-1.185493
13	1	0	0.188927	-1.531300	-2.822213
14	1	0	3.832076	-2.375159	0.197087
15	6	0	1.702154	-3.481487	-0.887440
16	6	0	0.651943	-3.895801	0.118954
17	7	0	-0.048081	-2.956054	0.656809
18	6	0	-1.146301	-3.233197	1.533667
19	6	0	-2.355038	-3.765637	1.018662
20	6	0	-1.009814	-2.886294	2.899393
21	6	0	-3.411083	-3.967273	1.916786
22	6	0	-2.578323	-4.073982	-0.462276
23	6	0	-2.091327	-3.137088	3.751388

24	6	0	0.293673	-2.314770	3.448772
25	6	0	-3.283325	-3.674426	3.270763
26	1	0	-4.348893	-4.371231	1.546709
27	1	0	-1.626702	-3.967103	-0.990950
28	1	0	-1.995358	-2.912680	4.809040
29	1	0	0.827636	-1.840547	2.617206
30	1	0	-4.109369	-3.865919	3.950005
31	6	0	0.195532	-0.321441	-4.582210
32	1	0	-0.889892	-0.428785	-4.690698
33	1	0	0.399970	0.639323	-4.096145
34	1	0	0.619049	-0.283747	-5.591997
35	6	0	0.513609	-2.831810	-4.494822
36	1	0	1.063899	-2.860565	-5.442395
37	1	0	0.843494	-3.688237	-3.896001
38	1	0	-0.551635	-2.964979	-4.718201
39	6	0	-3.073085	-5.514986	-0.697625
40	1	0	-3.135633	-5.722638	-1.771903
41	1	0	-2.404007	-6.255139	-0.245754
42	1	0	-4.071797	-5.674791	-0.276595
43	6	0	-3.549006	-3.056966	-1.094896
44	1	0	-4.537096	-3.107275	-0.622513
45	1	0	-3.175026	-2.033476	-0.987943

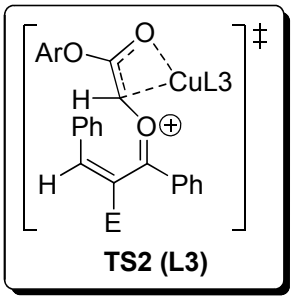
46	1	0	-3.678532	-3.261335	-2.164116
47	6	0	5.810234	-2.878289	-0.450497
48	1	0	5.553927	-3.795071	-0.993347
49	1	0	6.677466	-2.432269	-0.949801
50	1	0	6.124988	-3.158061	0.561260
51	6	0	5.020837	-0.613217	0.379645
52	1	0	5.808544	-0.063659	-0.148379
53	1	0	4.164641	0.054206	0.511486
54	1	0	5.404357	-0.871691	1.373804
55	6	0	0.072061	-1.226459	4.513970
56	1	0	1.027710	-0.753691	4.761856
57	1	0	-0.610284	-0.445693	4.159070
58	1	0	-0.336349	-1.636721	5.444852
59	6	0	1.202114	-3.436203	3.995587
60	1	0	0.725734	-3.949897	4.838983
61	1	0	1.422684	-4.189752	3.230568
62	1	0	2.154453	-3.022112	4.346126
63	1	0	-3.948795	7.124437	-1.605405
64	6	0	-3.650189	6.145028	-1.243343
65	6	0	-2.300444	5.772068	-1.265648
66	6	0	-4.611308	5.259727	-0.748565
67	6	0	-1.911737	4.523664	-0.801009

68	1	0	-1.551629	6.460891	-1.644894
69	6	0	-4.232904	4.005343	-0.282265
70	1	0	-5.657046	5.550130	-0.720547
71	6	0	-2.876295	3.615227	-0.306053
72	1	0	-0.866025	4.239271	-0.809141
73	1	0	-4.983078	3.330507	0.113506
74	6	0	-2.467905	2.317352	0.204532
75	6	0	-3.435957	1.281936	0.639152
76	8	0	-1.191941	2.135595	0.290192
77	6	0	-4.304395	0.646466	-0.191935
78	6	0	-3.456853	1.029725	2.113503
79	6	0	-0.468599	1.034936	0.704855
80	6	0	-4.430304	0.702473	-1.645210
81	1	0	-5.021084	-0.003789	0.303897
82	8	0	-4.507301	0.294495	2.507800
83	8	0	-2.606273	1.467659	2.868530
84	6	0	0.904248	1.331498	1.022346
85	1	0	-0.991736	0.367156	1.379607
86	6	0	-3.383624	1.074949	-2.513080
87	6	0	-5.673156	0.342167	-2.205984
88	6	0	-4.591089	0.028796	3.924040
89	8	0	1.278141	2.619053	0.941481

90	8	0	1.684589	0.400878	1.313168
91	6	0	-3.590828	1.124029	-3.888064
92	1	0	-2.397330	1.292382	-2.116256
93	6	0	-5.881233	0.403108	-3.580965
94	1	0	-6.481998	0.030854	-1.549877
95	1	0	-5.556520	-0.455503	4.067611
96	1	0	-4.535019	0.961921	4.488101
97	1	0	-3.778717	-0.635298	4.226974
98	29	0	0.625262	-1.012045	0.066961
99	6	0	-4.840747	0.798132	-4.425199
100	1	0	-2.774703	1.410286	-4.544668
101	1	0	-6.849363	0.136786	-3.994296
102	1	0	-4.997525	0.839023	-5.499179
103	6	0	2.570115	-4.552645	-1.494613
104	1	0	3.259120	-4.964030	-0.746531
105	1	0	1.963258	-5.386241	-1.863108
106	1	0	3.162437	-4.155438	-2.318909
107	6	0	0.503948	-5.364000	0.425194
108	1	0	0.099072	-5.909303	-0.435956
109	1	0	1.478590	-5.807694	0.654045
110	1	0	-0.163401	-5.522311	1.272747
111	6	0	2.648946	2.960698	1.083652

112	6	0	3.201473	3.045431	2.367904
113	6	0	3.339975	3.301215	-0.090242
114	6	0	4.539070	3.458280	2.450784
115	6	0	4.671041	3.710227	0.054022
116	6	0	5.269542	3.779499	1.310948
117	1	0	5.010003	3.534752	3.426571
118	1	0	5.245136	3.983339	-0.825587
119	1	0	6.304200	4.098063	1.401495
120	6	0	2.408907	2.749605	3.635899
121	1	0	1.395335	2.455316	3.347835
122	6	0	2.646718	3.307210	-1.448720
123	1	0	1.806456	2.605186	-1.400137
124	6	0	3.023609	1.580021	4.427115
125	1	0	3.076012	0.678252	3.808914
126	1	0	4.036820	1.816435	4.772312
127	1	0	2.416520	1.360929	5.313502
128	6	0	2.277232	4.010305	4.513544
129	1	0	3.254510	4.357019	4.868440
130	1	0	1.810688	4.832610	3.960431
131	1	0	1.659407	3.797703	5.393658
132	6	0	3.554540	2.853091	-2.602863
133	1	0	4.361900	3.569085	-2.793910

134	1	0	4.004358	1.876068	-2.401840
135	1	0	2.971059	2.772398	-3.527174
136	6	0	2.061723	4.707186	-1.734085
137	1	0	1.387087	5.028105	-0.932462
138	1	0	2.861515	5.453072	-1.809408
139	1	0	1.506831	4.711399	-2.680497



TS2 (L3)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.196828	-2.477070	-6.354246
2	6	0	0.898090	-2.619214	-5.320097
3	6	0	-0.023297	-1.750143	-4.728620
4	6	0	1.437445	-3.667501	-4.572023
5	6	0	-0.401269	-1.919650	-3.397424

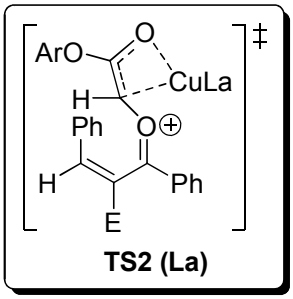
6	1	0	-0.447504	-0.933122	-5.305475
7	6	0	1.048660	-3.860512	-3.245882
8	1	0	2.163482	-4.340266	-5.018946
9	6	0	0.120112	-2.989989	-2.658105
10	7	0	-0.255485	-3.122783	-1.289502
11	6	0	-0.835492	-4.181268	-0.825083
12	6	0	-1.132647	-4.207883	0.656075
13	7	0	-0.877997	-3.123626	1.307913
14	6	0	-1.146482	-2.928634	2.683553
15	6	0	-2.393107	-3.223924	3.260912
16	6	0	-0.143514	-2.328858	3.464430
17	6	0	-2.617493	-2.949632	4.610009
18	6	0	-0.369960	-2.083807	4.817195
19	6	0	-1.605132	-2.392586	5.395581
20	1	0	-3.585419	-3.177361	5.047448
21	1	0	0.418182	-1.640498	5.418536
22	1	0	-1.778905	-2.195043	6.449251
23	1	0	-1.382626	7.477028	-1.712432
24	6	0	-1.374240	6.464617	-1.319473
25	6	0	-0.190620	5.715410	-1.342638
26	6	0	-2.541221	5.913762	-0.783325
27	6	0	-0.170292	4.423279	-0.837989

28	1	0	0.717706	6.147042	-1.751954
29	6	0	-2.533162	4.619595	-0.274645
30	1	0	-3.456948	6.496292	-0.756738
31	6	0	-1.348478	3.851728	-0.300258
32	1	0	0.748323	3.846913	-0.842672
33	1	0	-3.438746	4.200873	0.149479
34	6	0	-1.331039	2.508017	0.241567
35	6	0	-2.524476	1.839684	0.820001
36	8	0	-0.184539	1.909609	0.219745
37	6	0	-3.574611	1.366851	0.100503
38	6	0	-2.495240	1.745220	2.310979
39	6	0	0.136690	0.645307	0.658572
40	6	0	-3.785842	1.308322	-1.343323
41	1	0	-4.396487	0.975608	0.695876
42	8	0	-3.644596	1.299405	2.841897
43	8	0	-1.511818	2.048404	2.962620
44	6	0	1.538031	0.345776	0.680159
45	1	0	-0.469739	0.260220	1.469647
46	6	0	-2.751399	1.378960	-2.299369
47	6	0	-5.111450	1.159032	-1.799776
48	6	0	-3.661807	1.183671	4.280983
49	8	0	2.378548	1.323542	0.312091

50	8	0	1.916522	-0.811681	0.977310
51	6	0	-3.043306	1.339323	-3.659514
52	1	0	-1.715883	1.439255	-1.982014
53	6	0	-5.401688	1.128440	-3.161182
54	1	0	-5.917250	1.083647	-1.074032
55	1	0	-4.681300	0.892732	4.532375
56	1	0	-3.406063	2.140676	4.740488
57	1	0	-2.950193	0.420498	4.605123
58	29	0	0.198514	-1.695140	0.103904
59	6	0	-4.367684	1.222548	-4.095152
60	1	0	-2.236292	1.399388	-4.384179
61	1	0	-6.430576	1.027105	-3.493018
62	1	0	-4.589805	1.194796	-5.157933
63	6	0	-1.269054	-5.359981	-1.659013
64	1	0	-0.598203	-6.216427	-1.516119
65	1	0	-2.271638	-5.688210	-1.367729
66	1	0	-1.272146	-5.112346	-2.721052
67	6	0	-1.644273	-5.495349	1.253932
68	1	0	-2.708266	-5.650837	1.035219
69	1	0	-1.104622	-6.351504	0.837562
70	1	0	-1.521965	-5.497617	2.338064
71	6	0	3.772008	1.046006	0.256786

72	6	0	4.536039	1.300362	1.401240
73	6	0	4.305120	0.622143	-0.969353
74	6	0	5.919367	1.099279	1.290717
75	6	0	5.692025	0.441499	-1.022781
76	6	0	6.491935	0.674816	0.095727
77	1	0	6.552755	1.279112	2.154444
78	1	0	6.154561	0.112657	-1.947449
79	1	0	7.566236	0.526759	0.031943
80	6	0	3.912161	1.754324	2.715874
81	1	0	2.861912	1.996518	2.523082
82	6	0	3.413168	0.419949	-2.190252
83	1	0	2.437657	0.063977	-1.836186
84	6	0	3.945097	0.619165	3.759428
85	1	0	3.441885	-0.276439	3.379897
86	1	0	4.975859	0.343822	4.011736
87	1	0	3.446794	0.935078	4.683787
88	6	0	4.574226	3.032897	3.262971
89	1	0	5.624058	2.866672	3.529517
90	1	0	4.538681	3.845711	2.529557
91	1	0	4.054703	3.367506	4.168065
92	6	0	3.943607	-0.639929	-3.168596
93	1	0	4.856922	-0.308422	-3.675539

94	1	0	4.161816	-1.584125	-2.658053
95	1	0	3.195191	-0.838042	-3.943415
96	6	0	3.178355	1.761365	-2.916222
97	1	0	2.742211	2.507808	-2.243751
98	1	0	4.123558	2.165094	-3.297241
99	1	0	2.500284	1.626675	-3.767802
100	1	0	-1.113077	-1.244485	-2.931061
101	1	0	1.480311	-4.665685	-2.658597
102	1	0	0.805448	-2.072016	3.002935
103	1	0	-3.190316	-3.635167	2.649625



TS2 (La)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.484318	3.850049	-0.408146

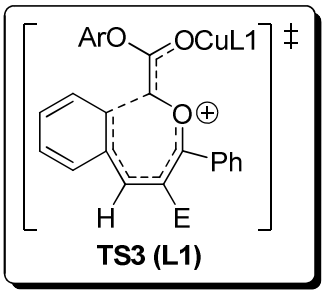
2	6	0	-0.851239	3.344633	-1.563123
3	6	0	-1.240717	3.775271	-2.828376
4	6	0	-2.269892	4.712812	-2.970964
5	6	0	-2.920183	5.208691	-1.839089
6	6	0	-2.537246	4.773415	-0.572963
7	6	0	-1.134113	3.473768	0.959731
8	6	0	-0.025804	2.870113	1.461179
9	6	0	1.177090	2.504660	0.669624
10	8	0	1.427832	1.268090	0.381180
11	6	0	0.711479	0.139734	0.694604
12	29	0	-1.189620	-1.181688	0.094440
13	7	0	-2.515580	-2.009901	1.472876
14	6	0	-3.678215	-2.449398	1.158989
15	8	0	-4.279574	-3.279907	2.036473
16	6	0	-3.356825	-3.483729	3.144546
17	6	0	-2.148588	-2.590923	2.779658
18	6	0	-4.538184	-2.159279	-0.059614
19	6	0	-5.784239	-1.362742	0.427617
20	6	0	1.348403	-1.101609	0.353739
21	8	0	2.581386	-1.017268	-0.179976
22	8	0	0.734886	-2.176911	0.504061
23	7	0	-2.634074	-0.995657	-1.306098

24	6	0	-2.515244	-0.299752	-2.604090
25	6	0	-3.945572	-0.347248	-3.185612
26	8	0	-4.704564	-1.051781	-2.165170
27	6	0	-3.857028	-1.365705	-1.164278
28	6	0	-4.992071	-3.514453	-0.679213
29	6	0	0.079067	2.528323	2.911612
30	8	0	-0.912103	3.043439	3.658576
31	6	0	-0.839677	2.757116	5.070910
32	8	0	0.983459	1.844594	3.357144
33	6	0	2.144772	3.470403	0.189893
34	1	0	-4.029821	-0.917600	-4.113156
35	1	0	-4.402816	0.635612	-3.318549
36	1	0	-2.157879	0.721204	-2.440424
37	1	0	-1.783447	-0.822340	-3.226945
38	1	0	-5.537603	-4.096507	0.065598
39	1	0	-5.645333	-3.327725	-1.534019
40	1	0	-4.130216	-4.099851	-1.016709
41	1	0	-6.464979	-1.188237	-0.407599
42	1	0	-6.305856	-1.936012	1.197098
43	1	0	-5.491566	-0.395303	0.849681
44	1	0	-1.983456	-1.785457	3.502685
45	1	0	-1.213702	-3.148664	2.676624

46	1	0	-3.870544	-3.186901	4.061157
47	1	0	-3.122349	-4.549656	3.186627
48	1	0	0.151126	0.181626	1.621414
49	1	0	-2.565140	5.049701	-3.960469
50	1	0	-0.737845	3.382811	-3.707709
51	1	0	-3.724346	5.930964	-1.942561
52	1	0	-0.063854	2.604258	-1.476368
53	1	0	-3.045459	5.160316	0.306635
54	1	0	-1.888197	3.727607	1.701279
55	1	0	-1.694420	3.268378	5.512433
56	1	0	0.096633	3.136262	5.486179
57	1	0	-0.899544	1.679863	5.243994
58	6	0	3.268358	3.047873	-0.560728
59	6	0	4.196361	3.976955	-1.008851
60	6	0	4.032286	5.337573	-0.718202
61	6	0	2.931834	5.764868	0.029449
62	6	0	1.994425	4.843415	0.483622
63	1	0	3.401976	1.992659	-0.772623
64	1	0	5.056103	3.643790	-1.582337
65	1	0	4.764538	6.059251	-1.068069
66	1	0	2.807348	6.817784	0.263176
67	1	0	1.147711	5.180555	1.071019

68	6	0	3.223421	-2.210094	-0.602683
69	6	0	4.055748	-2.864556	0.316023
70	6	0	3.059030	-2.615237	-1.933862
71	6	0	4.731347	-4.002273	-0.143927
72	6	0	3.758487	-3.759113	-2.339622
73	6	0	4.583548	-4.449394	-1.454882
74	1	0	5.382366	-4.544323	0.535559
75	1	0	3.655746	-4.112321	-3.361754
76	1	0	5.117312	-5.334368	-1.789502
77	6	0	4.208263	-2.388442	1.756416
78	1	0	3.750436	-1.396608	1.830447
79	6	0	5.683848	-2.234749	2.169177
80	1	0	6.207910	-3.196977	2.178051
81	1	0	6.221458	-1.565629	1.488655
82	1	0	5.749670	-1.817064	3.180242
83	6	0	3.454070	-3.324262	2.723428
84	1	0	2.396500	-3.400038	2.449461
85	1	0	3.880053	-4.334451	2.705616
86	1	0	3.522546	-2.948903	3.751445
87	6	0	2.150286	-1.868676	-2.903775
88	1	0	1.834211	-0.939619	-2.416527
89	6	0	0.881642	-2.690594	-3.208846

90	1	0	1.132826	-3.640698	-3.694248
91	1	0	0.332368	-2.918810	-2.288847
92	1	0	0.219085	-2.138057	-3.888249
93	6	0	2.883203	-1.473336	-4.199451
94	1	0	3.776676	-0.877380	-3.984559
95	1	0	3.198417	-2.351978	-4.772927
96	1	0	2.224436	-0.879990	-4.844939



TS3 (L1)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.443250	-0.298715	4.567511
2	6	0	-1.095853	0.681217	3.865312
3	6	0	-2.121692	0.352071	2.916077
4	6	0	-2.545946	-1.029535	2.821145

5	6	0	-1.848939	-2.013757	3.591031
6	6	0	-0.816666	-1.668086	4.425693
7	6	0	-3.550315	-1.438448	1.931766
8	6	0	-4.233881	-0.708323	0.940209
9	6	0	-5.304667	-1.480743	0.205646
10	8	0	-6.060232	-2.219494	1.043349
11	6	0	-7.047913	-3.056160	0.409783
12	6	0	-4.013643	0.606565	0.468153
13	6	0	-5.070056	1.434002	-0.132258
14	8	0	-2.831818	1.247545	0.482700
15	6	0	-1.662160	0.669520	0.877687
16	6	0	-0.492788	1.503892	0.679068
17	8	0	0.654044	1.038037	0.509233
18	29	0	1.330021	-0.657562	-0.166551
19	8	0	-0.712569	2.814838	0.796100
20	8	0	-5.436840	-1.486923	-1.001029
21	1	0	-1.538380	-0.374169	0.610557
22	1	0	-3.847780	-2.480272	2.010507
23	1	0	-2.883274	1.111150	2.753130
24	1	0	-2.156448	-3.052150	3.498460
25	1	0	-7.564491	-3.562713	1.224660
26	1	0	-6.567411	-3.780032	-0.253600

27	1	0	-7.743684	-2.446975	-0.171841
28	1	0	-0.862322	1.727415	4.036364
29	1	0	-0.302110	-2.428276	5.005566
30	1	0	0.334314	-0.031472	5.278058
31	6	0	-4.780256	2.350124	-1.159319
32	6	0	-5.784752	3.153900	-1.690789
33	6	0	-7.091183	3.062039	-1.203429
34	6	0	-7.388665	2.161726	-0.177255
35	6	0	-6.387636	1.356110	0.357871
36	1	0	-3.771742	2.410423	-1.552958
37	1	0	-5.551180	3.849126	-2.491994
38	1	0	-7.872714	3.691564	-1.618859
39	1	0	-8.399009	2.096997	0.215698
40	1	0	-6.618002	0.681090	1.176905
41	1	0	7.348644	2.077017	0.846271
42	6	0	6.538095	1.426332	0.531010
43	6	0	5.934505	1.615802	-0.707841
44	6	0	6.095425	0.406216	1.370587
45	6	0	4.897421	0.785591	-1.153773
46	1	0	6.273671	2.427304	-1.344677
47	6	0	5.050716	-0.441460	0.990342
48	1	0	6.567151	0.272160	2.338687

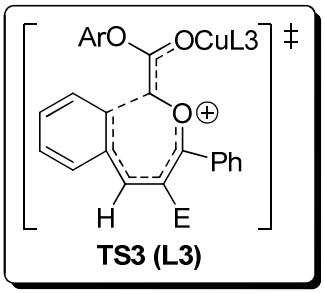
49	6	0	4.479317	-0.253534	-0.291044
50	6	0	4.215065	1.081809	-2.487644
51	6	0	4.575864	-1.568747	1.903208
52	7	0	3.379272	-1.100498	-0.642840
53	1	0	3.572432	0.233904	-2.747057
54	1	0	3.538558	-1.796897	1.624163
55	6	0	3.463061	-2.041856	-1.515409
56	6	0	2.202578	-2.851731	-1.746970
57	7	0	1.118511	-2.410097	-1.205231
58	6	0	-0.120546	-3.135088	-1.231693
59	6	0	-1.192680	-2.586397	-1.980522
60	6	0	-0.279440	-4.296750	-0.438538
61	6	0	-2.427347	-3.240825	-1.933961
62	6	0	-0.990948	-1.345716	-2.847175
63	6	0	-1.542350	-4.905378	-0.430562
64	6	0	0.823167	-4.875117	0.449079
65	6	0	-2.603207	-4.392498	-1.168260
66	1	0	-3.269722	-2.838798	-2.485228
67	1	0	-0.286286	-0.688703	-2.314396
68	1	0	-1.693592	-5.796921	0.171211
69	1	0	1.750392	-4.324115	0.264281
70	1	0	-3.570054	-4.887408	-1.148843

71	6	0	3.297209	2.315202	-2.360215
72	1	0	2.778348	2.506184	-3.307161
73	1	0	2.544178	2.176931	-1.576746
74	1	0	3.873819	3.211515	-2.106370
75	6	0	5.215765	1.256385	-3.645679
76	1	0	5.843877	2.143465	-3.511245
77	1	0	5.880431	0.390506	-3.741727
78	1	0	4.678144	1.380149	-4.592503
79	6	0	-0.341032	-1.704986	-4.201021
80	1	0	-0.178833	-0.801357	-4.800020
81	1	0	0.625742	-2.203548	-4.076145
82	1	0	-0.991651	-2.376379	-4.772846
83	6	0	-2.280261	-0.542516	-3.087890
84	1	0	-2.954216	-1.056037	-3.782393
85	1	0	-2.840238	-0.364439	-2.164588
86	1	0	-2.032457	0.425365	-3.537787
87	6	0	5.405257	-2.850883	1.678725
88	1	0	5.370450	-3.181527	0.634304
89	1	0	6.457371	-2.682050	1.935386
90	1	0	5.032080	-3.668881	2.306211
91	6	0	4.569152	-1.187687	3.393513
92	1	0	5.581896	-1.053839	3.789607

93	1	0	4.011989	-0.261160	3.568217
94	1	0	4.099126	-1.985966	3.979033
95	6	0	0.490136	-4.684251	1.942792
96	1	0	1.309781	-5.058794	2.567134
97	1	0	0.328052	-3.628767	2.186447
98	1	0	-0.416464	-5.234968	2.219388
99	6	0	1.102635	-6.360097	0.142554
100	1	0	0.241679	-6.991423	0.387779
101	1	0	1.337848	-6.522135	-0.914803
102	1	0	1.949722	-6.717092	0.739143
103	6	0	0.288970	3.755689	0.416518
104	6	0	0.103338	4.395168	-0.819016
105	6	0	1.321627	4.070896	1.310535
106	6	0	1.037632	5.377787	-1.170894
107	6	0	2.224270	5.063299	0.904380
108	6	0	2.091696	5.707477	-0.322756
109	1	0	0.928657	5.897445	-2.118406
110	1	0	3.039165	5.337825	1.567634
111	1	0	2.801906	6.476874	-0.612007
112	6	0	1.465858	3.422484	2.680757
113	1	0	0.697376	2.651684	2.773577
114	6	0	1.223759	4.449298	3.805721

115	1	0	1.976373	5.245660	3.788330
116	1	0	0.238912	4.919730	3.712053
117	1	0	1.279332	3.962583	4.786734
118	6	0	2.828841	2.725238	2.845246
119	1	0	2.878827	2.219826	3.817364
120	1	0	2.989272	1.980302	2.059548
121	1	0	3.657218	3.441462	2.805534
122	6	0	-1.070413	4.083272	-1.740952
123	1	0	-1.655517	3.283226	-1.279123
124	6	0	-2.002139	5.303793	-1.879678
125	1	0	-2.865807	5.056920	-2.508633
126	1	0	-2.374475	5.631211	-0.903496
127	1	0	-1.485524	6.151181	-2.344297
128	6	0	-0.601638	3.584250	-3.121389
129	1	0	-0.030855	4.352428	-3.655479
130	1	0	0.037281	2.698413	-3.030670
131	1	0	-1.464371	3.322695	-3.745610
132	6	0	4.707994	-2.412286	-2.276974
133	1	0	4.919595	-3.482952	-2.188632
134	1	0	4.585461	-2.196719	-3.346088
135	1	0	5.568280	-1.850362	-1.911860
136	6	0	2.299137	-4.098976	-2.582559

137	1	0	2.789656	-3.881501	-3.537371
138	1	0	2.905912	-4.861385	-2.078977
139	1	0	1.312523	-4.519748	-2.778554



TS3 (L3)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.899419	-0.820183	3.618761
2	6	0	0.121926	0.206775	3.143912
3	6	0	-1.115823	-0.056601	2.471050
4	6	0	-1.583195	-1.423672	2.404815
5	6	0	-0.752680	-2.456174	2.943158
6	6	0	0.460787	-2.172600	3.518730
7	6	0	-2.764910	-1.786380	1.735800
8	6	0	-3.624390	-1.034645	0.915569

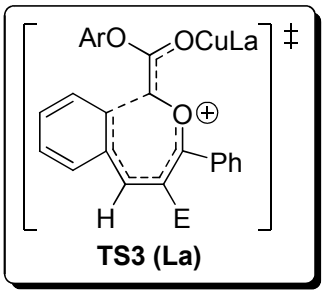
9	6	0	-4.824711	-1.794611	0.398425
10	8	0	-5.413781	-2.525568	1.367953
11	6	0	-6.515638	-3.349185	0.937813
12	6	0	-3.490168	0.288492	0.426997
13	6	0	-4.627540	1.139690	0.053412
14	8	0	-2.325840	0.923037	0.230659
15	6	0	-1.097368	0.361696	0.372793
16	6	0	-0.001718	1.235165	0.023242
17	8	0	1.168704	0.825681	-0.127757
18	29	0	1.953840	-0.932747	-0.325080
19	8	0	-0.305629	2.534766	-0.040773
20	8	0	-5.184722	-1.799798	-0.759905
21	1	0	-1.000411	-0.676162	0.080238
22	1	0	-3.059092	-2.825265	1.855174
23	1	0	-1.871244	0.724516	2.505966
24	1	0	-1.103459	-3.483195	2.879432
25	1	0	-6.875966	-3.844804	1.838909
26	1	0	-6.180245	-4.083081	0.200360
27	1	0	-7.300125	-2.731713	0.494212
28	1	0	0.433494	1.237174	3.283761
29	1	0	1.075000	-2.969767	3.926970
30	1	0	1.835563	-0.600884	4.126018

31	6	0	-4.487334	2.131426	-0.935976
32	6	0	-5.556976	2.961636	-1.257266
33	6	0	-6.780275	2.820997	-0.596369
34	6	0	-6.926717	1.848986	0.396893
35	6	0	-5.859566	1.018559	0.724829
36	1	0	-3.541129	2.239560	-1.454971
37	1	0	-5.439143	3.716834	-2.028877
38	1	0	-7.613556	3.469916	-0.849796
39	1	0	-7.869170	1.748593	0.927022
40	1	0	-5.970128	0.290796	1.523137
41	1	0	7.931866	1.052331	1.454506
42	6	0	7.100637	0.442836	1.113403
43	6	0	7.172305	-0.212759	-0.117144
44	6	0	5.948057	0.327105	1.896448
45	6	0	6.111321	-1.004054	-0.557589
46	1	0	8.055423	-0.108389	-0.740445
47	6	0	4.871141	-0.434680	1.450945
48	1	0	5.882362	0.844655	2.848878
49	6	0	4.958104	-1.128395	0.233640
50	7	0	3.817673	-1.859842	-0.188622
51	6	0	3.851186	-3.065524	-0.650644
52	6	0	2.530337	-3.640173	-1.118325

53	7	0	1.515884	-2.842124	-1.086007
54	6	0	0.183934	-3.217887	-1.398643
55	6	0	-0.558403	-2.364627	-2.232640
56	6	0	-0.438870	-4.336192	-0.821760
57	6	0	-1.893640	-2.646684	-2.510963
58	6	0	-1.783803	-4.597448	-1.089265
59	6	0	-2.513730	-3.760159	-1.935212
60	1	0	-2.460473	-1.988373	-3.162023
61	1	0	-2.260265	-5.459143	-0.630304
62	1	0	-3.563111	-3.954449	-2.131073
63	6	0	0.680929	3.463611	-0.473952
64	6	0	0.881723	3.620010	-1.853257
65	6	0	1.321333	4.236664	0.502568
66	6	0	1.807040	4.594342	-2.248619
67	6	0	2.233822	5.198093	0.048054
68	6	0	2.480350	5.373853	-1.310949
69	1	0	1.996495	4.747559	-3.307168
70	1	0	2.754757	5.819197	0.770997
71	1	0	3.191073	6.126100	-1.640803
72	6	0	1.057692	4.057973	1.992496
73	1	0	0.258344	3.317691	2.101765
74	6	0	0.558826	5.360346	2.647093

75	1	0	1.317122	6.150268	2.605630
76	1	0	-0.342571	5.734103	2.150276
77	1	0	0.319786	5.187437	3.702717
78	6	0	2.306704	3.513286	2.713923
79	1	0	2.094740	3.344689	3.776913
80	1	0	2.638513	2.567781	2.269973
81	1	0	3.140548	4.221931	2.652183
82	6	0	0.144247	2.786461	-2.895799
83	1	0	-0.594183	2.166603	-2.375866
84	6	0	-0.636772	3.671415	-3.886747
85	1	0	-1.209259	3.048367	-4.583537
86	1	0	-1.336436	4.331264	-3.362803
87	1	0	0.034104	4.300614	-4.481874
88	6	0	1.109210	1.839737	-3.637394
89	1	0	1.857953	2.402648	-4.206362
90	1	0	1.643719	1.191836	-2.933622
91	1	0	0.559702	1.208548	-4.346632
92	6	0	5.071039	-3.948879	-0.699304
93	1	0	4.830412	-4.952233	-0.334740
94	1	0	5.444198	-4.062585	-1.725036
95	1	0	5.878540	-3.538984	-0.091454
96	6	0	2.507960	-5.057782	-1.629124

97	1	0	3.360752	-5.237699	-2.290974
98	1	0	2.582915	-5.781901	-0.807929
99	1	0	1.588404	-5.264447	-2.177989
100	1	0	0.114246	-4.972345	-0.137803
101	1	0	-0.072612	-1.493667	-2.664190
102	1	0	6.160470	-1.490763	-1.526655
103	1	0	3.961149	-0.511840	2.039221



TS3 (La)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	0.729698	-1.812366	2.946792
2	6	0	-0.193588	-0.832042	2.672473
3	6	0	-1.372421	-1.121575	1.913347
4	6	0	-1.621170	-2.491699	1.526149

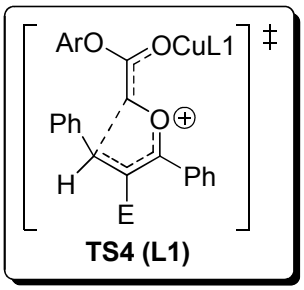
5	6	0	-0.652820	-3.485231	1.873060
6	6	0	0.497493	-3.161043	2.550309
7	6	0	-2.723919	-2.871563	0.739108
8	6	0	-3.689507	-2.097912	0.074295
9	6	0	-4.770575	-2.882143	-0.636220
10	8	0	-5.128940	-3.985773	0.054673
11	6	0	-6.086919	-4.837831	-0.604816
12	6	0	-3.758508	-0.689981	-0.093655
13	6	0	-5.011821	0.054084	-0.274383
14	8	0	-2.704512	0.134082	-0.116337
15	6	0	-1.398665	-0.229051	-0.046665
16	6	0	-0.476439	0.878789	-0.123514
17	8	0	0.756627	0.736409	-0.220083
18	29	0	2.128255	-0.643592	-0.231765
19	7	0	3.996988	0.249496	0.188750
20	6	0	5.126655	-0.301687	-0.058463
21	8	0	6.229877	0.462728	0.081199
22	6	0	5.785732	1.798339	0.457296
23	6	0	4.252500	1.647829	0.588560
24	6	0	5.446860	-1.724901	-0.481678
25	6	0	6.322472	-2.365757	0.635572
26	7	0	2.979133	-2.371803	-0.695115

27	6	0	2.258800	-3.613334	-1.053534
28	6	0	3.382772	-4.657639	-1.225907
29	8	0	4.598033	-3.882939	-1.026733
30	6	0	4.241887	-2.622583	-0.717854
31	6	0	6.255815	-1.669286	-1.812163
32	8	0	-1.032323	2.093160	0.001916
33	8	0	-5.228588	-2.589863	-1.719079
34	1	0	3.432789	-5.101046	-2.222000
35	1	0	3.370384	-5.449822	-0.473774
36	1	0	1.554864	-3.866409	-0.256511
37	1	0	1.689657	-3.446019	-1.973373
38	1	0	7.155840	-1.068832	-1.667812
39	1	0	6.545386	-2.678591	-2.111437
40	1	0	5.661663	-1.220918	-2.615679
41	1	0	6.619976	-3.374152	0.342244
42	1	0	7.218446	-1.760904	0.788338
43	1	0	5.773714	-2.422386	1.581744
44	1	0	3.896499	1.802465	1.612124
45	1	0	3.694041	2.325485	-0.062850
46	1	0	6.290609	2.064251	1.387912
47	1	0	6.096179	2.483725	-0.334800
48	1	0	-1.108725	-1.146997	-0.541701

49	1	0	-2.853596	-3.943102	0.617415
50	1	0	-2.239303	-0.487475	2.080843
51	1	0	-0.849732	-4.515811	1.586796
52	1	0	-6.263042	-5.663078	0.084764
53	1	0	-5.684871	-5.202791	-1.553313
54	1	0	-7.011661	-4.289028	-0.797412
55	1	0	-0.042914	0.177423	3.042719
56	1	0	1.214546	-3.931975	2.817243
57	1	0	1.619581	-1.572374	3.522944
58	6	0	-5.032796	1.253619	-1.010546
59	6	0	-6.213314	1.979452	-1.138198
60	6	0	-7.386972	1.526081	-0.530187
61	6	0	-7.373830	0.343849	0.215246
62	6	0	-6.196608	-0.385106	0.347048
63	1	0	-4.124440	1.603524	-1.488771
64	1	0	-6.220650	2.897350	-1.718625
65	1	0	-8.307151	2.093960	-0.632692
66	1	0	-8.279363	-0.002988	0.704072
67	1	0	-6.185667	-1.285056	0.954779
68	6	0	-0.195166	3.237279	-0.068686
69	6	0	0.194766	3.704811	-1.332835
70	6	0	0.117933	3.884057	1.134484

71	6	0	0.978407	4.865977	-1.360285
72	6	0	0.898420	5.044825	1.045241
73	6	0	1.333264	5.527942	-0.186431
74	1	0	1.305244	5.262839	-2.317177
75	1	0	1.161047	5.579191	1.953861
76	1	0	1.935162	6.431088	-0.233865
77	6	0	-0.213515	3.016229	-2.630997
78	1	0	-0.879435	2.183945	-2.380623
79	6	0	-0.372728	3.381706	2.487369
80	1	0	-0.956330	2.471682	2.315220
81	6	0	-1.314510	4.401904	3.157060
82	1	0	-1.701030	4.001798	4.101487
83	1	0	-0.795130	5.340529	3.381156
84	1	0	-2.167426	4.636236	2.511717
85	6	0	0.801399	3.018166	3.417174
86	1	0	0.429445	2.613220	4.365758
87	1	0	1.455741	2.268459	2.955865
88	1	0	1.413680	3.896071	3.653021
89	6	0	1.005914	2.428276	-3.368337
90	1	0	1.705965	3.215789	-3.670860
91	1	0	1.545916	1.719637	-2.730814
92	1	0	0.686387	1.902357	-4.275539

93	6	0	-1.012629	3.964362	-3.546559
94	1	0	-1.351423	3.430104	-4.441454
95	1	0	-1.893491	4.363764	-3.032825
96	1	0	-0.405207	4.813671	-3.878827



TS4 (L1)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.503230	4.998925	-2.434964
2	6	0	-1.105302	3.990560	-3.318464
3	6	0	-1.680891	2.727009	-3.236103
4	6	0	-2.666838	2.440040	-2.266061
5	6	0	-3.064986	3.475043	-1.390305
6	6	0	-2.483653	4.735660	-1.472186
7	6	0	-3.289702	1.126008	-2.288584

8	6	0	-4.325715	0.651935	-1.486148
9	6	0	-5.309382	-0.326287	-2.067696
10	8	0	-5.031240	-0.586077	-3.363909
11	6	0	-5.895872	-1.551629	-3.994843
12	6	0	-4.334157	0.804478	-0.068566
13	8	0	-3.183407	0.727084	0.593128
14	6	0	-1.928079	0.614627	-0.001115
15	6	0	-1.189207	-0.526691	0.337753
16	8	0	-1.943253	-1.514072	0.892064
17	8	0	0.033629	-0.721566	0.081042
18	29	0	1.665626	0.279697	0.136114
19	6	0	-5.494874	0.918033	0.796198
20	8	0	-6.236584	-0.835553	-1.474248
21	1	0	-1.474569	1.517494	-0.372257
22	1	0	-3.116109	0.569522	-3.205359
23	1	0	-1.381593	1.947405	-3.931971
24	1	0	-3.860967	3.301677	-0.672774
25	1	0	-5.548814	-1.617034	-5.025866
26	1	0	-6.933688	-1.213502	-3.955769
27	1	0	-5.813720	-2.520238	-3.495996
28	1	0	-0.357628	4.196046	-4.078701
29	1	0	-2.810905	5.523339	-0.800007

30	1	0	-1.065487	5.990178	-2.507641
31	6	0	-5.415237	0.545057	2.155714
32	6	0	-6.522060	0.687792	2.982058
33	6	0	-7.713228	1.220325	2.474430
34	6	0	-7.797285	1.609212	1.134121
35	6	0	-6.697891	1.458897	0.297785
36	1	0	-4.490217	0.132014	2.541164
37	1	0	-6.462045	0.384171	4.022734
38	1	0	-8.574999	1.334929	3.125754
39	1	0	-8.719304	2.029284	0.744565
40	1	0	-6.758736	1.767785	-0.739762
41	6	0	-1.437764	-2.820088	1.045965
42	6	0	-1.163892	-3.250153	2.354924
43	6	0	-1.368311	-3.659553	-0.075276
44	6	0	-0.788716	-4.588688	2.521144
45	6	0	-0.974563	-4.986249	0.147579
46	6	0	-0.688216	-5.449184	1.428502
47	1	0	-0.574749	-4.965435	3.516089
48	1	0	-0.906178	-5.667457	-0.696108
49	1	0	-0.397115	-6.484987	1.579548
50	6	0	-1.342402	-2.309373	3.541727
51	1	0	-1.150153	-1.290366	3.186347

52	6	0	-1.732011	-3.189234	-1.478905
53	1	0	-2.056956	-2.146218	-1.417898
54	6	0	-0.515783	-3.240387	-2.422695
55	1	0	0.305874	-2.631432	-2.033486
56	1	0	-0.146161	-4.264849	-2.546445
57	1	0	-0.787885	-2.864551	-3.417000
58	6	0	-2.919296	-3.990115	-2.049575
59	1	0	-2.671973	-5.050798	-2.170676
60	1	0	-3.794716	-3.923253	-1.394227
61	1	0	-3.197828	-3.600700	-3.036464
62	6	0	-2.801125	-2.352253	4.043952
63	1	0	-3.054536	-3.351796	4.416255
64	1	0	-2.949896	-1.638806	4.863814
65	1	0	-3.503197	-2.107937	3.239883
66	6	0	-0.363100	-2.583394	4.694536
67	1	0	-0.564587	-3.540652	5.188442
68	1	0	0.676183	-2.595915	4.346947
69	1	0	-0.458880	-1.804274	5.459689
70	1	0	6.075376	1.482752	1.861562
71	6	0	5.404921	2.111952	1.266739
72	6	0	4.258811	1.297921	0.729786
73	1	0	6.003685	2.531650	0.449051

74	1	0	5.047696	2.935178	1.885976
75	6	0	4.570430	-0.001953	0.017649
76	7	0	3.015283	1.628464	0.831730
77	7	0	3.572245	-0.603240	-0.524170
78	6	0	6.003338	-0.464546	-0.039693
79	6	0	2.602367	2.893567	1.376397
80	6	0	3.687935	-1.836957	-1.234622
81	1	0	6.662751	0.340716	-0.380177
82	1	0	6.355405	-0.769775	0.953674
83	1	0	6.107922	-1.315318	-0.714022
84	6	0	1.954902	2.898789	2.633948
85	6	0	2.770394	4.077797	0.619038
86	6	0	3.468848	-1.795592	-2.633062
87	6	0	3.908438	-3.053901	-0.548495
88	6	0	1.506865	4.124893	3.135960
89	6	0	1.794272	1.624216	3.457283
90	6	0	2.282191	5.271518	1.166447
91	6	0	3.401960	4.106966	-0.773011
92	6	0	3.531768	-2.997851	-3.342738
93	6	0	3.230182	-0.467165	-3.345405
94	6	0	3.937166	-4.229066	-1.311071
95	6	0	4.023192	-3.141616	0.971867

96	6	0	1.665252	5.304320	2.412713
97	1	0	1.028112	4.157989	4.109692
98	1	0	1.927963	0.770803	2.780666
99	6	0	2.888504	1.523191	4.540232
100	6	0	0.393201	1.487821	4.078683
101	1	0	2.392496	6.193815	0.603465
102	1	0	3.813523	3.117637	-0.994429
103	6	0	2.340550	4.394010	-1.853337
104	6	0	4.562745	5.117065	-0.869580
105	6	0	3.765348	-4.207471	-2.691283
106	1	0	3.390591	-2.991346	-4.418730
107	1	0	2.801773	0.223178	-2.606463
108	6	0	4.559476	0.148135	-3.831512
109	6	0	2.226230	-0.567941	-4.506391
110	1	0	4.094384	-5.179453	-0.809812
111	1	0	4.137307	-2.129150	1.372334
112	6	0	2.725579	-3.715182	1.575530
113	6	0	5.251544	-3.949768	1.431954
114	1	0	1.308747	6.245974	2.820151
115	1	0	3.893609	1.559734	4.104394
116	1	0	2.808820	2.349804	5.255802
117	1	0	2.794525	0.583999	5.097530

118	1	0	-0.390005	1.565228	3.316194
119	1	0	0.296902	0.513425	4.570004
120	1	0	0.202190	2.253752	4.838376
121	1	0	2.796762	4.379592	-2.850417
122	1	0	1.537207	3.650099	-1.832067
123	1	0	1.884584	5.379819	-1.706946
124	1	0	4.213759	6.147769	-0.743926
125	1	0	5.327192	4.934107	-0.106659
126	1	0	5.040767	5.051749	-1.853635
127	1	0	3.805833	-5.132463	-3.259285
128	1	0	4.387216	1.123418	-4.302355
129	1	0	5.266610	0.289759	-3.006239
130	1	0	5.041218	-0.502625	-4.570412
131	1	0	2.622851	-1.150543	-5.345360
132	1	0	1.288295	-1.033484	-4.185132
133	1	0	1.999721	0.433356	-4.890969
134	1	0	1.852473	-3.119552	1.290042
135	1	0	2.550546	-4.740694	1.232539
136	1	0	2.788131	-3.733990	2.670349
137	1	0	5.175405	-5.003991	1.144510
138	1	0	6.181394	-3.556850	1.005415
139	1	0	5.336932	-3.916864	2.524071

TS4-cis (L1)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.275336	-1.487690	1.166006
2	6	0	-4.303078	-0.805807	0.515257
3	6	0	-5.640342	-0.627494	1.208767
4	8	0	-6.194232	-1.822524	1.486092
5	6	0	-7.436056	-1.772900	2.218856
6	6	0	-4.135866	-0.077238	-0.688098
7	8	0	-2.958692	0.417228	-1.053131
8	6	0	-1.751005	0.055526	-0.486735
9	6	0	-0.832253	1.093617	-0.249518
10	8	0	-1.371267	2.333464	-0.254795
11	8	0	0.388847	0.928600	0.032969
12	29	0	1.667044	-0.441682	-0.358570
13	6	0	-5.226274	0.340934	-1.569843
14	8	0	-6.139969	0.439186	1.489100
15	1	0	-1.399420	-0.945633	-0.675440

16	1	0	-7.758409	-2.809569	2.310826
17	1	0	-8.175779	-1.179489	1.676808
18	1	0	-7.271761	-1.330940	3.204968
19	6	0	-5.121692	1.531000	-2.317707
20	6	0	-6.155796	1.916246	-3.162555
21	6	0	-7.295564	1.114889	-3.291417
22	6	0	-7.398469	-0.077319	-2.570424
23	6	0	-6.371846	-0.465029	-1.714418
24	1	0	-4.237185	2.149459	-2.214245
25	1	0	-6.076900	2.843427	-3.722206
26	1	0	-8.098950	1.417549	-3.956814
27	1	0	-8.274804	-0.708617	-2.682111
28	1	0	-6.445420	-1.403593	-1.173770
29	6	0	-0.558683	3.455588	0.025323
30	6	0	-0.120023	4.219828	-1.068146
31	6	0	-0.331242	3.806457	1.362213
32	6	0	0.602516	5.383588	-0.779029
33	6	0	0.404729	4.977228	1.593071
34	6	0	0.869455	5.756698	0.538030
35	1	0	0.959331	6.008515	-1.591299
36	1	0	0.606415	5.283449	2.615634
37	1	0	1.431098	6.664585	0.739893

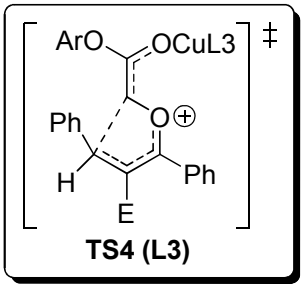
38	6	0	-0.481684	3.827993	-2.496983
39	1	0	-0.576599	2.736343	-2.529592
40	6	0	-0.860824	2.980075	2.528231
41	1	0	-1.476993	2.173040	2.119443
42	6	0	0.291127	2.331957	3.320600
43	1	0	0.912129	1.710915	2.667315
44	1	0	0.936623	3.090750	3.778174
45	1	0	-0.107371	1.703175	4.126341
46	6	0	-1.770483	3.816782	3.448727
47	1	0	-1.218966	4.632137	3.930665
48	1	0	-2.602809	4.258521	2.890624
49	1	0	-2.188298	3.186786	4.242781
50	6	0	-1.855604	4.418010	-2.880193
51	1	0	-1.822823	5.513820	-2.872284
52	1	0	-2.148899	4.095247	-3.886516
53	1	0	-2.631970	4.102696	-2.174916
54	6	0	0.584644	4.221396	-3.531975
55	1	0	0.660289	5.307924	-3.652947
56	1	0	1.574937	3.843141	-3.254385
57	1	0	0.322362	3.807870	-4.512565
58	1	0	5.409498	-2.790967	-2.496815
59	6	0	4.524440	-3.219756	-2.014140

60	6	0	3.739455	-2.151465	-1.303172
61	1	0	4.884406	-3.973540	-1.302521
62	1	0	3.917142	-3.720369	-2.768661
63	6	0	4.456074	-1.265434	-0.305228
64	7	0	2.481908	-1.926375	-1.478073
65	7	0	3.704630	-0.526471	0.430655
66	6	0	5.958969	-1.330263	-0.232836
67	6	0	1.661777	-2.739502	-2.335032
68	6	0	4.214784	0.376925	1.415530
69	1	0	6.304324	-2.364780	-0.134446
70	1	0	6.407858	-0.928402	-1.150192
71	1	0	6.331708	-0.750534	0.612376
72	6	0	1.264108	-2.205702	-3.580552
73	6	0	1.202404	-3.997895	-1.877620
74	6	0	4.008822	0.035559	2.773458
75	6	0	4.802021	1.604768	1.032660
76	6	0	0.420106	-2.980833	-4.384507
77	6	0	1.752112	-0.845040	-4.070039
78	6	0	0.343043	-4.717467	-2.717104
79	6	0	1.543471	-4.542201	-0.490743
80	6	0	4.460646	0.929403	3.748489
81	6	0	3.359479	-1.291410	3.156706

82	6	0	5.215068	2.469154	2.055039
83	6	0	4.913045	2.052284	-0.423358
84	6	0	-0.039760	-4.224698	-3.961926
85	1	0	0.119625	-2.602938	-5.357251
86	1	0	2.243313	-0.341418	-3.229547
87	6	0	2.800427	-0.998083	-5.191017
88	6	0	0.591265	0.061615	-4.520578
89	1	0	-0.029480	-5.684115	-2.392728
90	1	0	2.433707	-4.024119	-0.121057
91	6	0	0.405216	-4.226216	0.502161
92	6	0	1.872015	-6.046130	-0.488706
93	6	0	5.062005	2.136321	3.396987
94	1	0	4.335621	0.683137	4.798031
95	1	0	2.730221	-1.599182	2.311114
96	6	0	4.423016	-2.390248	3.364714
97	6	0	2.443215	-1.188997	4.388159
98	1	0	5.661569	3.423400	1.791733
99	1	0	4.698482	1.194006	-1.069014
100	6	0	3.849344	3.124547	-0.738896
101	6	0	6.324167	2.549238	-0.790286
102	1	0	-0.695246	-4.809709	-4.600514
103	1	0	3.657085	-1.598237	-4.862969

104	1	0	2.369177	-1.491613	-6.069533
105	1	0	3.173614	-0.017025	-5.506470
106	1	0	-0.152653	0.180079	-3.724523
107	1	0	0.970529	1.055485	-4.783576
108	1	0	0.079090	-0.337769	-5.402838
109	1	0	0.655183	-4.588281	1.506517
110	1	0	0.226927	-3.145520	0.566582
111	1	0	-0.528596	-4.708164	0.188075
112	1	0	0.997408	-6.660472	-0.727806
113	1	0	2.657336	-6.287595	-1.213199
114	1	0	2.219404	-6.352012	0.504424
115	1	0	5.402164	2.820097	4.169333
116	1	0	3.948740	-3.351141	3.597538
117	1	0	5.046954	-2.526828	2.473990
118	1	0	5.088642	-2.132686	4.196595
119	1	0	3.008529	-0.998818	5.307315
120	1	0	1.703980	-0.389485	4.272924
121	1	0	1.905237	-2.133090	4.531916
122	1	0	2.837658	2.761795	-0.528940
123	1	0	4.007050	4.026024	-0.136527
124	1	0	3.900648	3.414143	-1.795638
125	1	0	6.586953	3.464845	-0.249510

126	1	0	7.091064	1.799657	-0.564623
127	1	0	6.376394	2.778930	-1.860598
128	6	0	-3.205940	-1.814669	2.581611
129	6	0	-2.452490	-2.941470	2.976139
130	6	0	-3.818708	-1.029999	3.584122
131	6	0	-2.350236	-3.298496	4.316500
132	1	0	-1.966105	-3.547069	2.215692
133	6	0	-3.702525	-1.383057	4.924176
134	1	0	-4.356830	-0.127790	3.313038
135	6	0	-2.976778	-2.520509	5.294620
136	1	0	-1.781743	-4.178858	4.601676
137	1	0	-4.170368	-0.765523	5.685280
138	1	0	-2.891278	-2.792533	6.342724
139	1	0	-2.518761	-1.969103	0.566576



TS4 (L3)

Standard orientation:

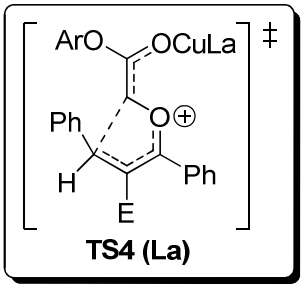
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.196224	-4.773540	-2.048680
2	6	0	-0.212955	-3.769816	-2.932581
3	6	0	0.485329	-2.567962	-2.991624
4	6	0	1.606929	-2.337728	-2.164241
5	6	0	2.013257	-3.368054	-1.287591
6	6	0	1.311540	-4.567819	-1.229831
7	6	0	2.324214	-1.079654	-2.307141
8	6	0	3.497695	-0.678119	-1.655866
9	6	0	4.519272	0.105416	-2.435751
10	8	0	4.126255	0.273168	-3.718211
11	6	0	5.019547	1.054700	-4.535284
12	6	0	3.640229	-0.702752	-0.244596
13	8	0	2.562502	-0.496772	0.514116
14	6	0	1.270689	-0.402614	0.031531
15	6	0	0.513000	0.683530	0.517706
16	8	0	1.239545	1.667378	1.094375
17	8	0	-0.732600	0.812488	0.374968
18	29	0	-2.234758	-0.341719	0.117471
19	6	0	4.871292	-0.789186	0.528178

20	8	0	5.563183	0.544667	-2.002974
21	1	0	0.782928	-1.311825	-0.272542
22	1	0	2.095675	-0.547057	-3.226185
23	1	0	0.175987	-1.793632	-3.689209
24	1	0	2.901368	-3.237754	-0.676771
25	1	0	4.553351	1.088159	-5.519822
26	1	0	6.000553	0.577053	-4.587438
27	1	0	5.132381	2.061110	-4.125006
28	1	0	-1.064424	-3.932732	-3.587257
29	1	0	1.645253	-5.353354	-0.558313
30	1	0	-0.337680	-5.718649	-2.012015
31	6	0	4.950720	-0.203799	1.809321
32	6	0	6.115057	-0.323213	2.557893
33	6	0	7.204248	-1.042042	2.052201
34	6	0	7.128922	-1.638941	0.790369
35	6	0	5.972385	-1.512331	0.029733
36	1	0	4.103845	0.354644	2.192288
37	1	0	6.178375	0.143749	3.536131
38	1	0	8.110661	-1.138098	2.643125
39	1	0	7.972113	-2.201501	0.401640
40	1	0	5.910799	-1.979058	-0.947257
41	6	0	0.582918	2.828924	1.563098

42	6	0	0.105254	2.839060	2.881197
43	6	0	0.531585	3.939628	0.709056
44	6	0	-0.477722	4.028694	3.336496
45	6	0	-0.061861	5.102955	1.215805
46	6	0	-0.566793	5.148842	2.513235
47	1	0	-0.862642	4.078224	4.351270
48	1	0	-0.125522	5.985214	0.585358
49	1	0	-1.020956	6.062233	2.886955
50	6	0	0.205181	1.621458	3.792564
51	1	0	0.775788	0.851790	3.262685
52	6	0	1.080858	3.895272	-0.712132
53	1	0	1.611387	2.945587	-0.834359
54	6	0	-0.062696	3.926973	-1.745902
55	1	0	-0.768258	3.106142	-1.579318
56	1	0	-0.623880	4.867028	-1.686198
57	1	0	0.337955	3.841179	-2.763570
58	6	0	2.099842	5.020210	-0.973526
59	1	0	1.637140	6.011559	-0.909464
60	1	0	2.923151	4.986863	-0.252136
61	1	0	2.524313	4.920723	-1.979374
62	6	0	0.969913	1.938377	5.091865
63	1	0	0.442549	2.680643	5.701597

64	1	0	1.082520	1.032376	5.698937
65	1	0	1.969031	2.332243	4.877156
66	6	0	-1.189818	1.040169	4.097836
67	1	0	-1.808976	1.757699	4.648669
68	1	0	-1.717554	0.785981	3.171271
69	1	0	-1.103742	0.135402	4.712480
70	1	0	-6.557952	-2.583393	0.753840
71	6	0	-5.612177	-3.034474	0.437757
72	6	0	-4.588972	-1.962687	0.165889
73	1	0	-5.825597	-3.620741	-0.465019
74	1	0	-5.273860	-3.721010	1.214180
75	6	0	-5.015102	-0.752308	-0.635841
76	7	0	-3.373339	-1.965708	0.607013
77	7	0	-4.087319	0.100440	-0.908927
78	6	0	-6.449974	-0.666087	-1.091494
79	6	0	-2.798531	-3.059645	1.313826
80	6	0	-4.307630	1.325092	-1.586993
81	1	0	-6.780561	-1.624840	-1.503177
82	1	0	-7.121532	-0.427774	-0.256960
83	1	0	-6.573907	0.104195	-1.853390
84	6	0	-2.160872	-2.797244	2.535390
85	6	0	-2.788876	-4.360180	0.787634

86	6	0	-3.457086	1.644339	-2.656614
87	6	0	-5.277040	2.250952	-1.168852
88	6	0	-1.562315	-3.837037	3.243522
89	6	0	-2.164115	-5.389570	1.492464
90	6	0	-3.614403	2.850678	-3.334708
91	6	0	-5.404568	3.470497	-1.833602
92	6	0	-1.559188	-5.135151	2.724671
93	1	0	-1.090254	-3.631051	4.199648
94	1	0	-2.155617	-6.393253	1.077191
95	6	0	-4.585576	3.768780	-2.924224
96	1	0	-2.967325	3.081468	-4.175718
97	1	0	-6.146828	4.187815	-1.496032
98	1	0	-1.082202	-5.940796	3.274580
99	1	0	-4.693916	4.716014	-3.443685
100	1	0	-2.691030	0.934273	-2.954034
101	1	0	-5.900034	2.030933	-0.307205
102	1	0	-2.155343	-1.784321	2.927074
103	1	0	-3.243013	-4.555734	-0.179058



TS4 (La)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.611196	-5.034401	-0.508681
2	6	0	0.916465	-4.508643	0.751679
3	6	0	0.057779	-3.591889	1.350496
4	6	0	-1.124657	-3.171914	0.701976
5	6	0	-1.421276	-3.719452	-0.565526
6	6	0	-0.560544	-4.636403	-1.162296
7	6	0	-2.007500	-2.247829	1.401894
8	6	0	-3.254543	-1.765445	0.984227
9	6	0	-4.340861	-1.599220	2.013615
10	8	0	-3.925623	-2.020680	3.229029
11	6	0	-4.880353	-1.851350	4.295086
12	6	0	-3.454953	-1.140083	-0.273291
13	8	0	-2.449717	-0.446056	-0.811352

14	6	0	-1.164969	-0.415196	-0.310236
15	6	0	-0.561999	0.862339	-0.239652
16	8	0	-1.421729	1.900904	-0.344258
17	8	0	0.659513	1.064027	-0.021785
18	29	0	2.289892	0.033089	-0.160608
19	7	0	3.856891	0.433797	1.169330
20	6	0	5.053637	-0.009916	1.053887
21	8	0	5.957542	0.413199	1.961521
22	6	0	5.267307	1.310578	2.877883
23	6	0	3.821315	1.344832	2.331254
24	6	0	5.652143	-0.957526	0.029070
25	6	0	6.251941	-2.176257	0.789946
26	7	0	3.432584	-1.234733	-1.205629
27	6	0	2.980949	-2.031252	-2.367227
28	6	0	4.263813	-2.742074	-2.850918
29	8	0	5.261069	-2.348577	-1.867462
30	6	0	4.679587	-1.484261	-1.013470
31	6	0	6.787426	-0.198182	-0.721136
32	6	0	-4.694778	-1.024845	-1.027896
33	8	0	-5.448000	-1.147123	1.814591
34	1	0	4.614230	-2.404716	-3.829069
35	1	0	4.202599	-3.831913	-2.841655

36	1	0	2.201973	-2.728822	-2.043983
37	1	0	2.552037	-1.366845	-3.122368
38	1	0	7.528601	0.156203	-0.002147
39	1	0	7.273327	-0.869491	-1.431979
40	1	0	6.389613	0.663924	-1.266997
41	1	0	6.739491	-2.851221	0.083973
42	1	0	6.989151	-1.828291	1.516042
43	1	0	5.471398	-2.729684	1.323120
44	1	0	3.082796	0.986944	3.054721
45	1	0	3.510926	2.340745	2.001772
46	1	0	5.353022	0.887323	3.881031
47	1	0	5.778874	2.274618	2.844249
48	1	0	-0.553375	-1.289353	-0.442606
49	1	0	-1.817930	-2.186892	2.469988
50	1	0	0.288235	-3.196243	2.336405
51	1	0	-2.347763	-3.451803	-1.064282
52	1	0	-4.386537	-2.236302	5.187108
53	1	0	-5.790403	-2.416549	4.081723
54	1	0	-5.134489	-0.795684	4.417362
55	1	0	1.812287	-4.831040	1.274887
56	1	0	-0.815945	-5.062174	-2.128428
57	1	0	1.266596	-5.770291	-0.966193

58	6	0	-4.911782	0.080177	-1.877606
59	6	0	-6.082119	0.166632	-2.621476
60	6	0	-7.039097	-0.851783	-2.546012
61	6	0	-6.825116	-1.958590	-1.719447
62	6	0	-5.662725	-2.045972	-0.962236
63	1	0	-4.167411	0.867111	-1.927535
64	1	0	-6.253010	1.027396	-3.260906
65	1	0	-7.950152	-0.783017	-3.133563
66	1	0	-7.564972	-2.751305	-1.666629
67	1	0	-5.493875	-2.906915	-0.324551
68	6	0	-0.917520	3.219372	-0.256080
69	6	0	-0.477666	3.845278	-1.431251
70	6	0	-0.970298	3.855789	0.992245
71	6	0	-0.043413	5.172459	-1.318143
72	6	0	-0.524704	5.182757	1.047330
73	6	0	-0.060928	5.835198	-0.092971
74	1	0	0.308891	5.694173	-2.203446
75	1	0	-0.545528	5.712498	1.995295
76	1	0	0.277325	6.865600	-0.028833
77	6	0	-0.456526	3.127202	-2.775888
78	1	0	-0.966669	2.166549	-2.649423
79	6	0	-1.466955	3.139092	2.242658

80	1	0	-1.930207	2.199841	1.923765
81	6	0	-0.289818	2.783637	3.174013
82	1	0	0.451410	2.172278	2.647066
83	1	0	0.212339	3.688509	3.536979
84	1	0	-0.644826	2.224071	4.047930
85	6	0	-2.544311	3.944351	2.992266
86	1	0	-2.148466	4.884511	3.392699
87	1	0	-3.387401	4.186884	2.336901
88	1	0	-2.927655	3.363936	3.839384
89	6	0	-1.223958	3.906338	-3.860681
90	1	0	-0.747800	4.867502	-4.084792
91	1	0	-1.253851	3.329552	-4.792405
92	1	0	-2.254945	4.108106	-3.550968
93	6	0	0.989182	2.831325	-3.224105
94	1	0	1.552366	3.758548	-3.382740
95	1	0	1.519478	2.240632	-2.468716
96	1	0	0.992399	2.273273	-4.168522

TS4-cis (La)

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)		

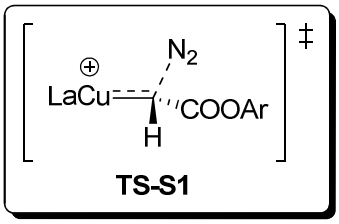
Number	Number	Type	X	Y	Z
1	6	0	-1.825975	-2.225465	-0.755127
2	6	0	-3.106903	-1.663146	-0.822186
3	6	0	-4.284053	-2.376183	-0.189999
4	8	0	-4.455875	-3.590372	-0.746024
5	6	0	-5.514570	-4.386960	-0.175179
6	6	0	-3.334952	-0.346994	-1.269525
7	8	0	-2.368037	0.567464	-1.220972
8	6	0	-1.049983	0.283369	-0.928022
9	6	0	-0.395025	1.226100	-0.095780
10	8	0	-1.219024	2.085031	0.542776
11	8	0	0.843127	1.259347	0.103847
12	29	0	2.419688	0.249579	-0.374894
13	7	0	3.395019	-1.324932	0.488064
14	6	0	4.587150	-1.713401	0.211539
15	8	0	5.082802	-2.729031	0.946214
16	6	0	4.078639	-3.084993	1.938475
17	6	0	2.885067	-2.168435	1.590135
18	6	0	5.573592	-1.210633	-0.828772
19	6	0	5.950807	-2.405560	-1.753344
20	7	0	3.945633	0.544915	-1.701767

21	6	0	3.987088	1.565068	-2.771019
22	6	0	5.407204	1.426568	-3.363856
23	8	0	5.979249	0.313998	-2.618876
24	6	0	5.069139	-0.077391	-1.706088
25	6	0	6.843691	-0.706203	-0.080656
26	6	0	-4.626893	0.206153	-1.673506
27	8	0	-4.972345	-1.929976	0.701016
28	1	0	6.043747	2.297986	-3.195282
29	1	0	5.425704	1.159825	-4.422161
30	1	0	3.199131	1.357626	-3.501763
31	1	0	3.796687	2.552855	-2.342150
32	1	0	7.258396	-1.513598	0.526069
33	1	0	7.593821	-0.384661	-0.805725
34	1	0	6.604546	0.137949	0.574803
35	1	0	6.696779	-2.085472	-2.483208
36	1	0	6.365754	-3.217990	-1.153739
37	1	0	5.073073	-2.779581	-2.291325
38	1	0	2.008159	-2.725168	1.245391
39	1	0	2.575551	-1.532792	2.424202
40	1	0	3.869741	-4.150923	1.829659
41	1	0	4.508707	-2.896477	2.924906
42	1	0	-0.469242	-0.217848	-1.684857

43	1	0	-5.535536	-5.303654	-0.763678
44	1	0	-6.467825	-3.857732	-0.242090
45	1	0	-5.297592	-4.605697	0.873535
46	6	0	-4.913538	1.569633	-1.461701
47	6	0	-6.140887	2.091690	-1.852999
48	6	0	-7.088839	1.271823	-2.475065
49	6	0	-6.805302	-0.076688	-2.705667
50	6	0	-5.581890	-0.609208	-2.309445
51	1	0	-4.176402	2.199402	-0.975818
52	1	0	-6.362930	3.139233	-1.672702
53	1	0	-8.044538	1.685537	-2.783672
54	1	0	-7.533913	-0.710158	-3.202479
55	1	0	-5.354257	-1.651408	-2.512413
56	6	0	-0.659844	3.061605	1.400450
57	6	0	-0.307466	4.302528	0.851011
58	6	0	-0.571774	2.762465	2.767233
59	6	0	0.183218	5.271490	1.735834
60	6	0	-0.074975	3.768244	3.606291
61	6	0	0.303796	5.008939	3.098539
62	1	0	0.471257	6.245742	1.351201
63	1	0	0.012721	3.576939	4.671961
64	1	0	0.684724	5.775623	3.767300

65	6	0	-0.433013	4.597437	-0.639440
66	1	0	-0.957800	3.756586	-1.104464
67	6	0	-0.977220	1.403493	3.326065
68	1	0	-1.472369	0.847759	2.523390
69	6	0	0.264028	0.595247	3.756234
70	1	0	0.965509	0.488759	2.920727
71	1	0	0.792952	1.090349	4.579220
72	1	0	-0.028382	-0.405096	4.098915
73	6	0	-1.988190	1.527425	4.481144
74	1	0	-1.556859	2.041212	5.347751
75	1	0	-2.878587	2.083782	4.170131
76	1	0	-2.308377	0.533224	4.813712
77	6	0	-1.273282	5.859614	-0.911066
78	1	0	-0.794614	6.760844	-0.511698
79	1	0	-1.400992	6.005418	-1.989991
80	1	0	-2.267064	5.780333	-0.457565
81	6	0	0.956707	4.702895	-1.299919
82	1	0	1.528627	5.540887	-0.884370
83	1	0	1.534991	3.786205	-1.136737
84	1	0	0.857959	4.866933	-2.379902
85	6	0	-1.395178	-3.295931	0.133506
86	6	0	-0.346406	-4.142135	-0.287190

87	6	0	-1.955046	-3.504655	1.412771
88	6	0	0.097615	-5.185986	0.520083
89	1	0	0.096038	-3.990486	-1.269105
90	6	0	-1.500918	-4.542065	2.221394
91	1	0	-2.729000	-2.838164	1.779311
92	6	0	-0.480576	-5.390051	1.777305
93	1	0	0.884829	-5.846687	0.167629
94	1	0	-1.939475	-4.688582	3.204166
95	1	0	-0.136471	-6.203889	2.409212
96	1	0	-1.142154	-2.032506	-1.567064



TS-S1

Standard orientation:

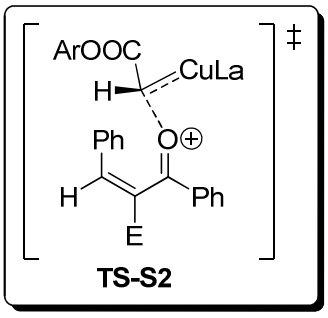
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-4.617541	2.587868	1.583045
2	6	0	-3.185345	2.673051	1.010657

3	7	0	-2.995279	1.371257	0.332466
4	6	0	-4.066233	0.675807	0.502481
5	8	0	-5.053465	1.250471	1.205033
6	29	0	-1.353517	0.810581	-0.697175
7	7	0	-2.216661	-0.962110	-1.211331
8	6	0	-1.596310	-2.005673	-2.058979
9	6	0	-2.562751	-3.201038	-1.926160
10	8	0	-3.690573	-2.646422	-1.182170
11	6	0	-3.352361	-1.404099	-0.803992
12	6	0	-4.410975	-0.732498	0.050593
13	6	0	-5.728268	-0.672576	-0.778429
14	6	0	0.417942	1.257357	-1.266188
15	7	0	0.943637	2.924849	-0.576319
16	7	0	0.945816	3.866524	0.006170
17	6	0	1.531079	0.351208	-0.873628
18	8	0	2.394762	0.810225	0.035724
19	8	0	1.514747	-0.753458	-1.380874
20	6	0	-4.631645	-1.600032	1.326006
21	1	0	-2.948365	-3.577427	-2.874464
22	1	0	-2.160673	-4.029225	-1.337804
23	1	0	-1.523287	-1.631552	-3.085430
24	1	0	-0.584514	-2.216696	-1.707676

25	1	0	-5.423898	-1.162769	1.936944
26	1	0	-4.924398	-2.610630	1.034778
27	1	0	-3.717455	-1.660073	1.926007
28	1	0	-6.018327	-1.682001	-1.075974
29	1	0	-6.525951	-0.236909	-0.174102
30	1	0	-5.599777	-0.065190	-1.680605
31	1	0	-3.066140	3.485807	0.288310
32	1	0	-2.424677	2.793681	1.788108
33	1	0	-5.316171	3.299043	1.137987
34	1	0	-4.668624	2.655932	2.671100
35	1	0	0.534200	1.584673	-2.303326
36	6	0	3.422322	-0.072269	0.496373
37	6	0	4.643377	-0.070387	-0.189791
38	6	0	3.160743	-0.824198	1.648456
39	6	0	5.646833	-0.902647	0.323442
40	6	0	4.202702	-1.635477	2.115699
41	6	0	5.430976	-1.678054	1.460196
42	1	0	6.610179	-0.942472	-0.175658
43	1	0	4.048720	-2.240929	3.003996
44	1	0	6.224771	-2.315098	1.839172
45	6	0	1.814522	-0.793119	2.363798
46	1	0	1.203157	-0.011148	1.898340

47	6	0	4.882143	0.763132	-1.443826
48	1	0	4.041353	1.458224	-1.549995
49	6	0	6.158467	1.619149	-1.340924
50	1	0	7.060507	0.999644	-1.290223
51	1	0	6.252731	2.260772	-2.224169
52	1	0	6.140613	2.260231	-0.453066
53	6	0	1.068665	-2.131830	2.189574
54	1	0	1.620069	-2.955713	2.656402
55	1	0	0.079240	-2.085145	2.661379
56	1	0	0.940247	-2.376070	1.129253
57	6	0	1.959630	-0.424123	3.852227
58	1	0	2.467791	0.538019	3.976371
59	1	0	0.972690	-0.354181	4.324495
60	1	0	2.533096	-1.178376	4.401874
61	6	0	4.910594	-0.133400	-2.699043
62	1	0	5.749007	-0.838064	-2.657764
63	1	0	3.987977	-0.715920	-2.791660
64	1	0	5.030150	0.475648	-3.602651



TS-S2

Standard orientation:

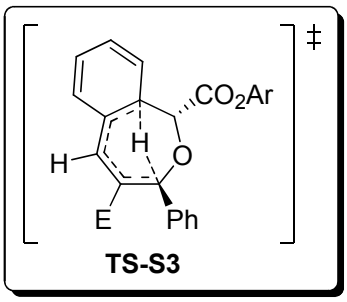
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.583278	-0.185966	-2.283568
2	6	0	-7.148963	-0.231042	-1.006311
3	6	0	-6.329100	-0.350491	0.112018
4	6	0	-4.931173	-0.462363	-0.026911
5	6	0	-4.373324	-0.392771	-1.319067
6	6	0	-5.195596	-0.255360	-2.434425
7	6	0	-4.126327	-0.598462	1.186830
8	6	0	-2.907129	-1.172187	1.344978
9	6	0	-2.194390	-1.052963	2.650077
10	8	0	-3.029619	-0.820915	3.679762
11	6	0	-2.407284	-0.650335	4.967189
12	6	0	-2.166097	-1.918802	0.261394
13	8	0	-1.081671	-1.519811	-0.159372

14	6	0	0.727445	0.534792	0.649755
15	29	0	2.306339	-0.370598	0.357548
16	7	0	4.172677	-0.500269	1.104355
17	6	0	5.085064	-1.349485	0.785157
18	8	0	6.254322	-1.251516	1.434282
19	6	0	6.155394	-0.135014	2.367315
20	6	0	4.713031	0.379685	2.163458
21	6	0	5.053635	-2.488312	-0.217279
22	6	0	5.253858	-3.820781	0.564021
23	6	0	0.230831	1.690229	-0.099317
24	8	0	0.467649	2.865516	0.507366
25	8	0	-0.298236	1.514906	-1.179766
26	7	0	2.708759	-1.853380	-0.942688
27	6	0	1.741151	-2.345274	-1.947395
28	6	0	2.417819	-3.617942	-2.499286
29	8	0	3.744652	-3.595736	-1.887011
30	6	0	3.760871	-2.586353	-1.002623
31	6	0	6.221190	-2.289001	-1.227276
32	6	0	-2.770567	-3.182842	-0.252937
33	8	0	-0.985190	-1.154150	2.787235
34	1	0	2.557139	-3.623069	-3.581198
35	1	0	1.932248	-4.545402	-2.185861

36	1	0	0.777539	-2.524113	-1.465616
37	1	0	1.598572	-1.571967	-2.709155
38	1	0	7.171888	-2.261026	-0.691434
39	1	0	6.236598	-3.118933	-1.936419
40	1	0	6.105165	-1.354024	-1.785489
41	1	0	5.271567	-4.656530	-0.138383
42	1	0	6.201437	-3.791731	1.105861
43	1	0	4.442755	-3.983048	1.281752
44	1	0	4.095651	0.286928	3.061667
45	1	0	4.673929	1.420652	1.830853
46	1	0	6.352515	-0.524951	3.367492
47	1	0	6.927769	0.587532	2.096586
48	1	0	0.009399	0.113632	1.361803
49	1	0	-4.566317	-0.159970	2.079980
50	1	0	-6.768828	-0.375170	1.106055
51	1	0	-3.295734	-0.394796	-1.445765
52	1	0	-3.227565	-0.474416	5.662556
53	1	0	-1.724574	0.203118	4.952059
54	1	0	-1.852999	-1.550329	5.243620
55	1	0	-8.225774	-0.161887	-0.883176
56	1	0	-4.752244	-0.188587	-3.423695
57	1	0	-7.220487	-0.078560	-3.156693

58	6	0	-2.319302	-3.698867	-1.480269
59	6	0	-2.834680	-4.891760	-1.975555
60	6	0	-3.796212	-5.595719	-1.241789
61	6	0	-4.245334	-5.096258	-0.017979
62	6	0	-3.742969	-3.890956	0.471472
63	1	0	-1.582590	-3.136304	-2.044616
64	1	0	-2.496208	-5.274818	-2.934202
65	1	0	-4.196372	-6.529326	-1.627040
66	1	0	-4.989264	-5.642938	0.553888
67	1	0	-4.096086	-3.505946	1.422210
68	6	0	0.152708	4.069968	-0.189214
69	6	0	-1.094157	4.660825	0.050988
70	6	0	1.141553	4.626038	-1.011566
71	6	0	-1.347894	5.876860	-0.597045
72	6	0	0.832590	5.842489	-1.633695
73	6	0	-0.398689	6.461591	-1.431908
74	1	0	-2.303307	6.370658	-0.446321
75	1	0	1.565712	6.309089	-2.285237
76	1	0	-0.618222	7.404404	-1.924682
77	6	0	2.483786	3.944114	-1.251164
78	1	0	2.558278	3.099165	-0.557033
79	6	0	-2.145145	4.010508	0.942761

80	1	0	-1.660267	3.190410	1.483447
81	6	0	-2.699556	4.982290	2.000452
82	1	0	-3.252826	5.810485	1.543533
83	1	0	-3.392357	4.456888	2.667836
84	1	0	-1.896800	5.410339	2.610423
85	6	0	-3.279391	3.404231	0.091336
86	1	0	-3.813545	4.184292	-0.463675
87	1	0	-2.887609	2.684571	-0.634677
88	1	0	-4.007933	2.890077	0.729571
89	6	0	3.671970	4.876588	-0.950368
90	1	0	4.618495	4.335143	-1.067861
91	1	0	3.700780	5.733065	-1.632978
92	1	0	3.624079	5.266296	0.072293
93	6	0	2.563386	3.378333	-2.683882
94	1	0	3.507818	2.840132	-2.833984
95	1	0	1.734432	2.690448	-2.880891
96	1	0	2.516689	4.181642	-3.428146



TS-S3

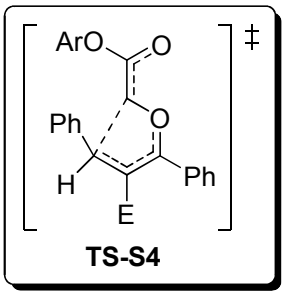
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.827948	4.794109	0.047898
2	6	0	1.739703	4.117598	-0.729377
3	6	0	1.809984	2.699341	-0.715557
4	6	0	0.798763	1.924080	0.031648
5	6	0	-0.093792	2.701144	0.876576
6	6	0	-0.060696	4.071082	0.889861
7	6	0	2.973282	2.044201	-1.166737
8	6	0	3.310133	0.758709	-0.752328
9	6	0	2.293600	-0.053302	-0.124212
10	8	0	1.147328	-0.246279	-0.920194
11	6	0	0.152449	0.757249	-0.763079
12	6	0	4.732374	0.359542	-0.979160
13	8	0	5.615651	1.136191	-1.296046

14	8	0	4.927566	-0.970874	-0.879171
15	6	0	6.271032	-1.414456	-1.112558
16	6	0	2.573525	-1.146276	0.831664
17	6	0	-1.063279	0.132217	-0.060553
18	8	0	-1.040220	-0.383128	1.030671
19	8	0	-2.157191	0.207665	-0.866427
20	6	0	3.532027	-0.962888	1.845126
21	6	0	3.783223	-1.967261	2.774820
22	6	0	3.075350	-3.171807	2.716346
23	6	0	2.112716	-3.357697	1.722438
24	6	0	1.858533	-2.353151	0.789710
25	1	0	0.808536	5.879926	0.049444
26	1	0	2.470853	4.662888	-1.321429
27	1	0	1.601906	1.068644	0.619034
28	1	0	-0.801197	2.167972	1.502976
29	1	0	-0.741613	4.617030	1.537857
30	1	0	3.735935	2.623122	-1.679288
31	1	0	-0.150670	1.095992	-1.757518
32	1	0	6.251736	-2.493140	-0.954909
33	1	0	6.581066	-1.179186	-2.134530
34	1	0	6.963238	-0.935234	-0.414659
35	1	0	4.066705	-0.018770	1.912120

36	1	0	4.523381	-1.806735	3.554364
37	1	0	3.267323	-3.953995	3.445955
38	1	0	1.554295	-4.288749	1.672451
39	1	0	1.112922	-2.497827	0.017244
40	6	0	-3.361092	-0.395632	-0.437560
41	6	0	-3.574900	-1.745011	-0.756502
42	6	0	-4.310164	0.406544	0.211670
43	6	0	-4.806327	-2.298905	-0.384149
44	6	0	-5.524832	-0.198258	0.559488
45	6	0	-5.773050	-1.537222	0.268080
46	1	0	-5.008234	-3.342498	-0.609023
47	1	0	-6.284137	0.389547	1.067966
48	1	0	-6.721704	-1.987336	0.547852
49	6	0	-2.518821	-2.593528	-1.456025
50	1	0	-1.705260	-1.930617	-1.766227
51	6	0	-3.064756	-3.261826	-2.731695
52	1	0	-2.263963	-3.806118	-3.245769
53	1	0	-3.859360	-3.981955	-2.504808
54	1	0	-3.472652	-2.519530	-3.426483
55	6	0	-1.925005	-3.636416	-0.487541
56	1	0	-1.133367	-4.211842	-0.983089
57	1	0	-1.500705	-3.150898	0.397061

58	1	0	-2.692034	-4.343969	-0.150141
59	6	0	-4.040584	1.866743	0.553933
60	1	0	-3.087791	2.148109	0.095290
61	6	0	-5.115051	2.806114	-0.024697
62	1	0	-6.102052	2.611735	0.410937
63	1	0	-4.860481	3.851061	0.188785
64	1	0	-5.199429	2.691403	-1.110832
65	6	0	-3.897044	2.052898	2.077958
66	1	0	-4.833821	1.815475	2.596296
67	1	0	-3.118134	1.397562	2.482553
68	1	0	-3.637861	3.091730	2.316928



TS-S4

Standard orientation:

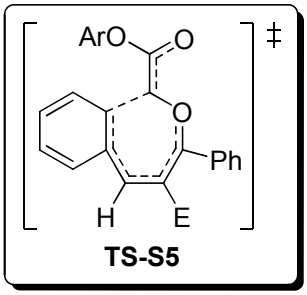
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	3.445909	4.302565	-2.105840
2	6	0	3.230232	4.633989	-0.764289
3	6	0	2.955564	3.637688	0.165814
4	6	0	2.881799	2.280091	-0.218490
5	6	0	3.107772	1.964434	-1.577020
6	6	0	3.385677	2.964420	-2.504685
7	6	0	2.621437	1.279363	0.805912
8	6	0	2.605672	-0.118146	0.656919
9	6	0	3.206074	-0.958533	1.744283
10	8	0	3.846223	-0.188366	2.661654
11	6	0	4.383159	-0.903626	3.784009
12	6	0	1.802596	-0.784056	-0.298293
13	8	0	0.642267	-0.232864	-0.666220
14	6	0	0.214983	1.015994	-0.352788
15	6	0	-1.207134	1.171496	-0.144152
16	8	0	-1.855236	-0.038235	-0.008493
17	8	0	-1.761796	2.254089	-0.049868
18	6	0	1.984599	-2.123775	-0.862430
19	8	0	3.147207	-2.167426	1.842290
20	1	0	0.771425	1.869022	-0.688663
21	1	0	2.775399	1.641008	1.818357
22	1	0	2.786726	3.899377	1.207280

23	1	0	3.091448	0.926730	-1.897223
24	1	0	4.848256	-0.145708	4.415366
25	1	0	5.123412	-1.636589	3.452852
26	1	0	3.589763	-1.423758	4.327691
27	1	0	3.277838	5.671257	-0.444697
28	1	0	3.563374	2.697751	-3.542910
29	1	0	3.663080	5.080047	-2.832717
30	6	0	0.868284	-2.896220	-1.237414
31	6	0	1.046477	-4.152553	-1.807880
32	6	0	2.334313	-4.650719	-2.027774
33	6	0	3.447170	-3.884315	-1.671963
34	6	0	3.275451	-2.629607	-1.095568
35	1	0	-0.128943	-2.505491	-1.065295
36	1	0	0.178757	-4.746161	-2.081707
37	1	0	2.469614	-5.630055	-2.478700
38	1	0	4.449869	-4.263219	-1.848344
39	1	0	4.140493	-2.031124	-0.828746
40	6	0	-3.241009	-0.020247	0.216853
41	6	0	-4.099233	-0.076179	-0.892431
42	6	0	-3.699711	-0.029176	1.543425
43	6	0	-5.475196	-0.131099	-0.637339
44	6	0	-5.084750	-0.086014	1.743148

45	6	0	-5.966790	-0.135024	0.666034
46	1	0	-6.170366	-0.167712	-1.471552
47	1	0	-5.476575	-0.088696	2.756437
48	1	0	-7.038410	-0.177357	0.842482
49	6	0	-3.563164	-0.041868	-2.318742
50	1	0	-2.482143	-0.205972	-2.266685
51	6	0	-2.736465	0.056972	2.721264
52	1	0	-1.728899	-0.126512	2.334784
53	6	0	-2.751208	1.474052	3.330993
54	1	0	-2.515224	2.226040	2.571835
55	1	0	-3.737941	1.710771	3.747997
56	1	0	-2.016102	1.552736	4.141846
57	6	0	-3.012234	-1.013844	3.792311
58	1	0	-3.985269	-0.868615	4.276178
59	1	0	-2.997713	-2.021615	3.362671
60	1	0	-2.247728	-0.967314	4.576951
61	6	0	-4.149598	-1.161835	-3.197380
62	1	0	-5.228911	-1.041388	-3.347475
63	1	0	-3.679125	-1.150813	-4.187860
64	1	0	-3.981526	-2.148540	-2.751370
65	6	0	-3.794093	1.344872	-2.953994
66	1	0	-4.865920	1.558951	-3.047982

67	1	0	-3.344024	2.133309	-2.342775
68	1	0	-3.353467	1.387455	-3.957902



TS-S5

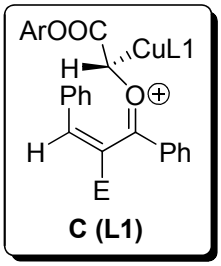
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.111193	4.633378	0.279641
2	6	0	0.020252	3.391060	0.864791
3	6	0	0.983687	2.383617	0.584569
4	6	0	2.119483	2.708229	-0.233539
5	6	0	2.192708	4.019638	-0.792940
6	6	0	1.211386	4.953460	-0.557957
7	6	0	3.109478	1.761567	-0.583637
8	6	0	3.153357	0.376910	-0.373128
9	6	0	4.425625	-0.312288	-0.793181

10	8	0	5.512294	0.486905	-0.645871
11	6	0	6.744497	-0.072401	-1.126786
12	6	0	2.126869	-0.486906	0.106488
13	6	0	2.370520	-1.720530	0.869206
14	8	0	0.816830	-0.287565	-0.080130
15	6	0	0.228207	0.718786	-0.745806
16	6	0	-1.227561	0.659686	-0.839436
17	8	0	-1.871627	1.394899	-1.563277
18	8	0	-1.776443	-0.268958	0.008305
19	8	0	4.494196	-1.433180	-1.251992
20	1	0	0.751279	1.156300	-1.583849
21	1	0	3.971542	2.168551	-1.103422
22	1	0	1.078029	1.558155	1.283395
23	1	0	3.040011	4.263438	-1.429440
24	1	0	7.502153	0.690112	-0.942836
25	1	0	6.675903	-0.298797	-2.194386
26	1	0	6.983550	-0.992164	-0.586495
27	1	0	-0.798755	3.162796	1.539918
28	1	0	1.279428	5.941239	-1.004614
29	1	0	-0.648083	5.385121	0.477205
30	6	0	1.448438	-2.783191	0.832234
31	6	0	1.657839	-3.928114	1.596386

32	6	0	2.788121	-4.036678	2.410226
33	6	0	3.704440	-2.983174	2.463955
34	6	0	3.494793	-1.833290	1.708832
35	1	0	0.571647	-2.704874	0.198780
36	1	0	0.938971	-4.741627	1.551214
37	1	0	2.950406	-4.932414	3.003451
38	1	0	4.576816	-3.051151	3.108128
39	1	0	4.191994	-1.004183	1.786035
40	6	0	-3.165829	-0.479876	-0.057233
41	6	0	-3.656271	-1.406953	-0.990892
42	6	0	-3.985336	0.184055	0.867663
43	6	0	-5.035262	-1.650774	-0.987905
44	6	0	-5.356638	-0.098828	0.830139
45	6	0	-5.880454	-1.004473	-0.089007
46	1	0	-5.451919	-2.356092	-1.701612
47	1	0	-6.022676	0.401592	1.527587
48	1	0	-6.947859	-1.208206	-0.103785
49	6	0	-2.742345	-2.105185	-1.991292
50	1	0	-1.708529	-1.900610	-1.694726
51	6	0	-3.422171	1.200836	1.852403
52	1	0	-2.331308	1.110505	1.825997
53	6	0	-3.864528	0.926762	3.301429

54	1	0	-3.378334	1.632121	3.985995
55	1	0	-4.947219	1.043169	3.427641
56	1	0	-3.597688	-0.088869	3.613634
57	6	0	-3.787121	2.634107	1.415070
58	1	0	-3.351057	3.372097	2.100764
59	1	0	-3.420800	2.836945	0.403659
60	1	0	-4.874145	2.779749	1.417406
61	6	0	-2.942643	-1.532081	-3.409287
62	1	0	-3.960571	-1.724624	-3.769493
63	1	0	-2.779175	-0.450071	-3.419358
64	1	0	-2.243195	-1.997117	-4.114862
65	6	0	-2.919709	-3.634847	-1.977651
66	1	0	-2.194495	-4.105763	-2.651805
67	1	0	-2.768185	-4.044970	-0.972913
68	1	0	-3.919887	-3.932163	-2.313627



C (L1)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.564561	5.174440	0.382095
2	6	0	-0.882554	4.086920	-0.204628
3	6	0	-0.443744	4.187983	-1.546021
4	6	0	-0.697439	5.340884	-2.275138
5	6	0	-1.384815	6.409611	-1.685450
6	6	0	-1.813898	6.324533	-0.357902
7	6	0	-0.584887	2.892624	0.567975
8	8	0	0.100365	1.995901	-0.038356
9	6	0	0.581778	0.730654	0.470347
10	6	0	-0.992593	2.728228	1.989571
11	6	0	0.150832	2.865746	2.941769
12	8	0	1.285739	3.100965	2.568533
13	6	0	-2.268919	2.571040	2.426002
14	6	0	-3.513405	2.451510	1.675118
15	6	0	-3.587629	2.046982	0.326562
16	6	0	-4.811682	2.010248	-0.333473
17	6	0	-5.984288	2.370341	0.339267
18	6	0	-5.932662	2.745379	1.684212
19	6	0	-4.710255	2.772413	2.349106

20	29	0	-0.393157	-0.931414	-0.092418
21	8	0	2.444110	1.470249	-0.837781
22	6	0	3.809224	1.444901	-1.215993
23	8	0	-0.206713	2.721987	4.226407
24	6	0	0.855108	2.891200	5.191818
25	1	0	0.508609	0.717938	1.557560
26	1	0	-6.937832	2.343234	-0.180315
27	1	0	-4.853025	1.681819	-1.366845
28	1	0	-6.842660	3.011314	2.213579
29	1	0	-2.695528	1.722197	-0.199840
30	1	0	-4.669665	3.064215	3.395434
31	1	0	-2.381788	2.557439	3.507676
32	1	0	0.376733	2.785801	6.164742
33	1	0	1.309633	3.878509	5.085997
34	1	0	1.617674	2.122382	5.048536
35	1	0	0.105321	3.365656	-1.989997
36	1	0	-0.355715	5.415168	-3.302866
37	1	0	-1.578017	7.310994	-2.259818
38	1	0	-2.336886	7.157833	0.100700
39	1	0	-1.888320	5.117170	1.414603
40	6	0	4.768237	1.977706	-0.339233
41	6	0	6.098148	1.979239	-0.779073

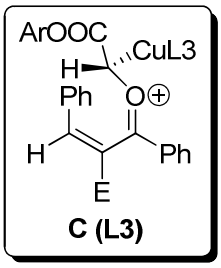
42	6	0	6.448056	1.493205	-2.036172
43	6	0	5.462984	1.004665	-2.889652
44	6	0	4.117844	0.969303	-2.499052
45	6	0	4.410806	2.552449	1.026650
46	1	0	6.870238	2.373942	-0.124754
47	1	0	7.486498	1.506642	-2.355068
48	1	0	5.739922	0.647207	-3.877405
49	6	0	3.049051	0.478869	-3.469273
50	6	0	2.903988	1.455520	-4.654108
51	6	0	3.323383	-0.952424	-3.966660
52	6	0	4.991206	1.694998	2.167939
53	6	0	4.853109	4.023128	1.154841
54	1	0	3.323527	2.546389	1.131392
55	1	0	4.677461	2.097488	3.138646
56	1	0	4.644998	0.659913	2.092538
57	1	0	6.087610	1.691799	2.146609
58	1	0	4.513967	4.433280	2.112980
59	1	0	5.943672	4.126419	1.116106
60	1	0	4.429689	4.637964	0.352831
61	1	0	2.112793	1.125370	-5.338722
62	1	0	2.659623	2.466125	-4.308208
63	1	0	3.833582	1.519267	-5.231120

64	1	0	2.511250	-1.292578	-4.621309
65	1	0	4.252802	-1.009630	-4.544357
66	1	0	3.407560	-1.653032	-3.129699
67	1	0	2.093452	0.465533	-2.934360
68	6	0	2.013698	0.562992	0.080981
69	8	0	2.701419	-0.318913	0.552442
70	1	0	-2.838749	-5.093398	-1.156188
71	6	0	-2.174400	-4.500459	-1.796342
72	6	0	-1.449650	-3.448427	-0.998303
73	1	0	-1.459663	-5.197473	-2.245832
74	1	0	-2.779614	-4.051053	-2.584059
75	7	0	-1.719326	-2.186736	-1.042333
76	6	0	-0.364266	-3.900675	-0.042097
77	6	0	-2.873603	-1.704306	-1.753015
78	7	0	0.277594	-2.976673	0.576047
79	6	0	-0.195558	-5.382537	0.179198
80	6	0	-2.685937	-0.973997	-2.948064
81	6	0	-4.163511	-1.915943	-1.203855
82	6	0	1.264861	-3.248454	1.576073
83	1	0	-1.165623	-5.869562	0.322744
84	1	0	0.280270	-5.859516	-0.685758
85	1	0	0.426949	-5.570636	1.054374

86	6	0	-3.821944	-0.496740	-3.612897
87	6	0	-1.300032	-0.753742	-3.545675
88	6	0	-5.260077	-1.401354	-1.907330
89	6	0	-4.407282	-2.621263	0.131730
90	6	0	0.927815	-2.891000	2.905325
91	6	0	2.536448	-3.775642	1.250768
92	6	0	-5.100911	-0.710717	-3.105269
93	1	0	-3.703613	0.040963	-4.548439
94	1	0	-0.561213	-0.936878	-2.754812
95	6	0	-1.018060	-1.760688	-4.679992
96	6	0	-1.089276	0.690951	-4.032528
97	1	0	-6.259288	-1.550380	-1.508936
98	1	0	-3.473964	-3.088532	0.458292
99	6	0	-4.795915	-1.607819	1.227700
100	6	0	-5.462892	-3.739540	0.027647
101	6	0	1.870674	-3.118314	3.910521
102	6	0	-0.455886	-2.344299	3.246029
103	6	0	3.446102	-3.963568	2.300284
104	6	0	2.989939	-4.093098	-0.173514
105	1	0	-5.970222	-0.342499	-3.642952
106	1	0	-0.004883	-1.623675	-5.074945
107	1	0	-1.107606	-2.796473	-4.333630

108	1	0	-1.724377	-1.625502	-5.507378
109	1	0	-1.725656	0.933499	-4.890705
110	1	0	-1.304242	1.414900	-3.238213
111	1	0	-0.050867	0.832648	-4.349121
112	1	0	-4.021633	-0.844351	1.358218
113	1	0	-5.730323	-1.092020	0.979810
114	1	0	-4.938532	-2.119887	2.186797
115	1	0	-6.458995	-3.339831	-0.190816
116	1	0	-5.217583	-4.460628	-0.759818
117	1	0	-5.532137	-4.281430	0.977527
118	6	0	3.123387	-3.651583	3.615491
119	1	0	1.624644	-2.876907	4.939910
120	1	0	-0.867136	-1.896351	2.331251
121	6	0	-1.413036	-3.480297	3.664123
122	6	0	-0.432181	-1.239252	4.315768
123	1	0	4.431902	-4.359541	2.075178
124	1	0	2.156152	-3.898562	-0.857609
125	6	0	4.151762	-3.173276	-0.603344
126	6	0	3.396893	-5.572397	-0.338773
127	1	0	3.846608	-3.817383	4.408745
128	1	0	-1.493631	-4.247653	2.885596
129	1	0	-1.055184	-3.972895	4.575561

130	1	0	-2.418599	-3.089964	3.862757
131	1	0	0.261621	-0.434585	4.047466
132	1	0	-1.432415	-0.805158	4.429061
133	1	0	-0.135422	-1.622969	5.298067
134	1	0	4.419787	-3.368822	-1.648598
135	1	0	3.887861	-2.118512	-0.493313
136	1	0	5.045382	-3.358709	0.003810
137	1	0	4.278043	-5.810333	0.267226
138	1	0	2.599586	-6.261519	-0.040917
139	1	0	3.653973	-5.779909	-1.383950



C (L3)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.553267	4.859855	-0.839248
2	6	0	-0.081295	3.551232	-1.078427

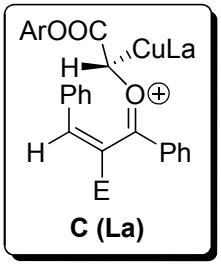
3	6	0	0.394291	3.208473	-2.366386
4	6	0	0.386972	4.153675	-3.381602
5	6	0	-0.091392	5.447538	-3.135339
6	6	0	-0.559105	5.797690	-1.865472
7	6	0	-0.053476	2.572817	-0.009631
8	8	0	0.377344	1.406203	-0.319505
9	6	0	0.456004	0.255220	0.551388
10	6	0	-0.437397	2.898188	1.393015
11	6	0	0.763308	3.169812	2.239874
12	8	0	1.895893	3.091528	1.798576
13	6	0	-1.701735	2.989416	1.872565
14	6	0	-2.979313	2.739189	1.212159
15	6	0	-3.121593	1.977457	0.034033
16	6	0	-4.374124	1.798972	-0.545792
17	6	0	-5.508324	2.373454	0.037878
18	6	0	-5.387912	3.114622	1.215732
19	6	0	-4.137105	3.285599	1.802558
20	29	0	-0.939068	-1.123636	0.164663
21	8	0	2.369860	-0.123129	-0.811320
22	6	0	3.637532	-0.692909	-1.077569
23	8	0	0.461471	3.503232	3.502243
24	6	0	1.590699	3.786555	4.358263

25	1	0	0.346325	0.560219	1.591167
26	1	0	-6.483972	2.234279	-0.418844
27	1	0	-4.465832	1.203859	-1.449592
28	1	0	-6.266915	3.553447	1.678064
29	1	0	-2.260701	1.494882	-0.418368
30	1	0	-4.044592	3.859493	2.721102
31	1	0	-1.774981	3.313144	2.908462
32	1	0	1.160320	4.026967	5.329634
33	1	0	2.158940	4.632447	3.965064
34	1	0	2.241030	2.911723	4.425291
35	1	0	0.780032	2.210610	-2.542435
36	1	0	0.759580	3.890747	-4.366778
37	1	0	-0.092617	6.183910	-3.933764
38	1	0	-0.922968	6.802661	-1.676264
39	1	0	-0.909894	5.134108	0.147093
40	6	0	4.773979	0.034980	-0.694818
41	6	0	6.018977	-0.509453	-1.035015
42	6	0	6.115790	-1.715884	-1.724873
43	6	0	4.962302	-2.405340	-2.091132
44	6	0	3.691831	-1.907315	-1.775258
45	6	0	4.670496	1.338364	0.088562
46	1	0	6.924982	0.018577	-0.752421

47	1	0	7.092221	-2.119310	-1.978053
48	1	0	5.048637	-3.346359	-2.627360
49	6	0	2.434115	-2.678420	-2.156592
50	6	0	2.375868	-2.990428	-3.663615
51	6	0	2.301284	-3.961782	-1.312153
52	6	0	5.046088	1.117030	1.568303
53	6	0	5.510521	2.468417	-0.533851
54	1	0	3.626713	1.664306	0.064614
55	1	0	4.892737	2.040304	2.138938
56	1	0	4.432416	0.328199	2.015508
57	1	0	6.098035	0.823632	1.668795
58	1	0	5.336916	3.405200	0.007893
59	1	0	6.584728	2.255999	-0.484956
60	1	0	5.248672	2.629199	-1.585674
61	1	0	1.426767	-3.478277	-3.918506
62	1	0	2.464741	-2.077763	-4.263454
63	1	0	3.181740	-3.667283	-3.968233
64	1	0	1.367149	-4.487346	-1.551404
65	1	0	3.129657	-4.651814	-1.510396
66	1	0	2.308993	-3.723393	-0.243679
67	1	0	1.573168	-2.040927	-1.923387
68	6	0	1.753520	-0.450386	0.357543

69	8	0	2.172810	-1.262974	1.155716
70	1	0	-4.487864	-4.435528	-0.669532
71	6	0	-3.480922	-4.411928	-1.105093
72	6	0	-2.616343	-3.381755	-0.426240
73	1	0	-3.053859	-5.410638	-0.969769
74	1	0	-3.577338	-4.212892	-2.172595
75	7	0	-2.210297	-2.278851	-0.966551
76	6	0	-2.137532	-3.663619	0.981320
77	6	0	-2.652711	-1.824436	-2.240492
78	7	0	-1.521985	-2.695124	1.567367
79	6	0	-2.464781	-5.000431	1.597357
80	6	0	-1.687918	-1.451413	-3.188056
81	6	0	-4.015755	-1.662582	-2.534994
82	6	0	-0.959987	-2.773261	2.864971
83	1	0	-3.511789	-5.263380	1.417134
84	1	0	-1.853079	-5.800294	1.160786
85	1	0	-2.285867	-4.989091	2.673037
86	6	0	-2.086233	-0.965928	-4.432182
87	6	0	-4.403835	-1.150218	-3.774221
88	6	0	-1.271555	-1.747931	3.771538
89	6	0	-0.048140	-3.774942	3.232112
90	6	0	-3.443258	-0.809277	-4.728696

91	1	0	-1.333388	-0.703276	-5.169601
92	1	0	-5.460203	-1.024079	-3.993626
93	6	0	-0.718531	-1.758625	5.049527
94	6	0	0.525831	-3.757573	4.502958
95	1	0	-3.749348	-0.420137	-5.695009
96	6	0	0.184455	-2.760387	5.418203
97	1	0	-0.983574	-0.977441	5.756234
98	1	0	1.244163	-4.525178	4.774938
99	1	0	0.628387	-2.756039	6.409095
100	1	0	-0.634864	-1.562338	-2.947027
101	1	0	-4.763238	-1.913987	-1.788323
102	1	0	-1.962749	-0.966386	3.468777
103	1	0	0.240543	-4.534355	2.512128



C (La)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

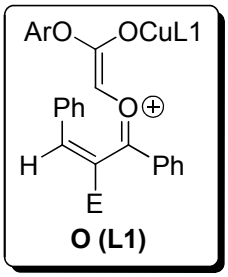
1	6	0	4.624752	-2.776822	0.004140
2	6	0	3.310029	-2.616251	-0.483648
3	6	0	2.887158	-3.366693	-1.607531
4	6	0	3.771282	-4.235649	-2.230154
5	6	0	5.077339	-4.380864	-1.743406
6	6	0	5.499694	-3.654055	-0.626341
7	6	0	2.375647	-1.720775	0.174750
8	8	0	1.188351	-1.722031	-0.298937
9	6	0	0.023440	-1.021978	0.187817
10	6	0	2.754787	-0.859491	1.328302
11	6	0	2.203803	-1.319657	2.635200
12	8	0	1.459992	-2.280307	2.727633
13	6	0	3.574334	0.220898	1.241268
14	6	0	4.210475	0.840269	0.082586
15	6	0	3.777769	0.663609	-1.248269
16	6	0	4.468865	1.258632	-2.300158
17	6	0	5.596656	2.047761	-2.047498
18	6	0	6.021141	2.255857	-0.733074
19	6	0	5.327988	1.666865	0.321148
20	29	0	-0.109466	0.974806	0.007675
21	7	0	0.082429	2.775158	-0.890954

22	6	0	0.820103	2.984683	-2.156493
23	6	0	0.712134	4.504011	-2.405661
24	8	0	-0.150145	4.962088	-1.328527
25	6	0	-0.420583	3.905654	-0.537849
26	6	0	-1.291378	4.284052	0.648671
27	6	0	-2.565950	4.993189	0.105789
28	7	0	-1.337924	1.897306	1.496187
29	6	0	-1.721508	3.118371	1.518675
30	8	0	-2.620763	3.468145	2.463272
31	6	0	-2.962960	2.259326	3.200197
32	6	0	-2.042069	1.183812	2.579861
33	6	0	-0.483445	5.271660	1.542796
34	8	0	-2.287963	-1.278508	0.045492
35	6	0	-3.498109	-1.748853	-0.516763
36	8	0	2.616935	-0.584226	3.679644
37	6	0	2.160411	-1.030112	4.974834
38	1	0	0.233169	4.770751	-3.349533
39	1	0	1.663095	5.034919	-2.316406
40	1	0	1.852185	2.645368	-2.040998
41	1	0	0.351436	2.388598	-2.946007
42	1	0	-3.190844	5.312992	0.941244
43	1	0	-2.282933	5.866964	-0.483475

44	1	0	-3.152178	4.318350	-0.526855
45	1	0	-0.201803	6.152604	0.961687
46	1	0	-1.099731	5.587145	2.387805
47	1	0	0.425506	4.798202	1.928969
48	1	0	-1.307505	0.794983	3.293469
49	1	0	-2.586509	0.334246	2.160039
50	1	0	-2.777229	2.453203	4.258406
51	1	0	-4.027754	2.069602	3.045916
52	1	0	-0.063662	-1.218842	1.256357
53	1	0	6.134955	2.505664	-2.872251
54	1	0	4.128692	1.107529	-3.320715
55	1	0	6.888448	2.876841	-0.530452
56	1	0	2.885459	0.084774	-1.461864
57	1	0	5.660705	1.828418	1.343322
58	1	0	3.801841	0.695346	2.193099
59	1	0	2.600439	-0.335396	5.689267
60	1	0	2.500939	-2.050376	5.164702
61	1	0	1.069443	-0.999801	5.023765
62	1	0	1.868917	-3.259075	-1.966563
63	1	0	3.445241	-4.809280	-3.092185
64	1	0	5.762235	-5.068492	-2.231093
65	1	0	6.508353	-3.777736	-0.244776

66	1	0	4.950459	-2.223306	0.877543
67	6	0	-4.153997	-0.949918	-1.465125
68	6	0	-5.383658	-1.414359	-1.949750
69	6	0	-5.926908	-2.615758	-1.501639
70	6	0	-5.247986	-3.377887	-0.554093
71	6	0	-4.014889	-2.961608	-0.036064
72	6	0	-3.552981	0.350633	-1.985078
73	1	0	-5.920324	-0.829792	-2.691549
74	1	0	-6.881082	-2.958747	-1.891623
75	1	0	-5.679721	-4.314313	-0.213481
76	6	0	-3.256893	-3.819840	0.970555
77	6	0	-4.143231	-4.287384	2.139197
78	6	0	-2.590205	-5.018345	0.263168
79	6	0	-3.013223	0.168877	-3.418594
80	6	0	-4.543446	1.527144	-1.908637
81	1	0	-2.702412	0.605088	-1.341904
82	1	0	-2.529308	1.090073	-3.769269
83	1	0	-2.285529	-0.647192	-3.459029
84	1	0	-3.824790	-0.066268	-4.116952
85	1	0	-4.053327	2.457480	-2.223110
86	1	0	-5.405499	1.379555	-2.568266
87	1	0	-4.925075	1.665252	-0.890466

88	1	0	-3.538526	-4.826745	2.877206
89	1	0	-4.622052	-3.440681	2.643897
90	1	0	-4.933792	-4.969085	1.806232
91	1	0	-1.993097	-5.601702	0.974311
92	1	0	-3.344820	-5.685415	-0.170047
93	1	0	-1.935770	-4.681172	-0.547069
94	1	0	-2.459004	-3.203436	1.398177
95	6	0	-1.111218	-1.597988	-0.585730
96	8	0	-1.041818	-2.217639	-1.623962



O (L1)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.108311	1.175619	-1.072743
2	6	0	-4.018420	0.791415	-0.260916
3	6	0	-3.625320	1.639665	0.799241

4	6	0	-4.307413	2.825981	1.037055
5	6	0	-5.388712	3.193639	0.228139
6	6	0	-5.782331	2.366639	-0.828247
7	6	0	-3.337646	-0.463760	-0.498124
8	8	0	-2.175573	-0.608765	0.085854
9	6	0	-1.524873	-1.786814	0.225823
10	8	0	0.111433	-3.041267	1.150454
11	6	0	1.402054	-3.359588	1.614598
12	6	0	-3.857174	-1.545702	-1.354796
13	6	0	-3.006548	-1.794503	-2.564919
14	8	0	-2.058056	-1.092717	-2.866799
15	6	0	-5.023643	-2.223612	-1.172132
16	6	0	-5.962107	-2.198805	-0.056297
17	6	0	-5.617601	-1.801074	1.251824
18	6	0	-6.567270	-1.814217	2.267622
19	6	0	-7.878714	-2.221716	2.001140
20	6	0	-8.232744	-2.636937	0.715143
21	6	0	-7.279763	-2.639336	-0.299082
22	8	0	-3.412708	-2.856553	-3.281274
23	6	0	-2.678868	-3.114131	-4.494273
24	1	0	-9.245637	-2.968343	0.507227
25	1	0	-7.552558	-2.972933	-1.297062

26	1	0	-8.616547	-2.231158	2.798126
27	1	0	-6.284358	-1.517477	3.273228
28	1	0	-5.299678	-2.893616	-1.982998
29	1	0	-4.596121	-1.518098	1.484127
30	1	0	-2.068677	-2.697016	0.022983
31	1	0	-2.734594	-2.252500	-5.164020
32	1	0	-1.632284	-3.327312	-4.264952
33	1	0	-3.159755	-3.982988	-4.942603
34	1	0	-2.798451	1.351045	1.439230
35	1	0	-3.996929	3.465109	1.856833
36	1	0	-5.924675	4.117976	0.423517
37	1	0	-6.617655	2.650769	-1.461255
38	1	0	-5.415284	0.539736	-1.895579
39	6	0	1.772447	-3.028569	2.924856
40	6	0	3.034691	-3.465260	3.354521
41	6	0	3.863914	-4.209308	2.521246
42	6	0	3.442088	-4.550892	1.236032
43	6	0	2.194572	-4.140631	0.753866
44	6	0	0.846149	-2.291747	3.885241
45	1	0	3.362738	-3.229634	4.363200
46	1	0	4.834628	-4.541827	2.878602
47	1	0	4.090333	-5.149788	0.605461

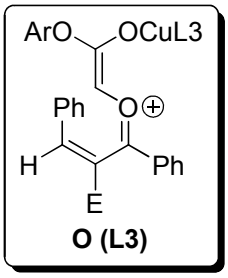
48	6	0	2.759328	-4.944855	-1.615823
49	6	0	0.671846	-5.752125	-0.444178
50	6	0	0.468187	-3.186114	5.083344
51	6	0	1.453514	-0.958754	4.358311
52	1	0	-0.081889	-2.059642	3.354712
53	1	0	2.311155	-5.134844	-2.597795
54	1	0	3.494570	-4.141852	-1.727444
55	1	0	3.289050	-5.859305	-1.324170
56	1	0	0.250187	-6.037089	-1.415729
57	1	0	1.182590	-6.628952	-0.029227
58	1	0	-0.153717	-5.493058	0.225289
59	1	0	0.753863	-0.435332	5.020723
60	1	0	2.382961	-1.117145	4.917565
61	1	0	1.674069	-0.308460	3.505631
62	1	0	-0.243129	-2.667561	5.737045
63	1	0	0.005897	-4.121333	4.749815
64	1	0	1.346359	-3.443999	5.686170
65	6	0	1.660894	-4.576723	-0.607734
66	1	0	1.098833	-3.732233	-1.027642
67	6	0	-0.237068	-1.778824	0.778905
68	8	0	0.536642	-0.804936	0.962932
69	1	0	5.031864	2.112866	-2.235623

70	6	0	4.495070	2.910276	-1.721477
71	6	0	3.237561	2.382951	-1.078262
72	1	0	4.263269	3.703129	-2.439888
73	1	0	5.166514	3.343609	-0.969725
74	6	0	2.244680	3.383063	-0.525890
75	7	0	2.918272	1.142209	-0.979429
76	7	0	1.194019	2.915223	0.060036
77	6	0	2.549006	4.848306	-0.692923
78	6	0	3.780160	0.100736	-1.446084
79	29	0	1.058267	0.886656	0.199739
80	6	0	0.164776	3.796136	0.543959
81	1	0	3.574446	5.066224	-0.377545
82	1	0	2.470428	5.142804	-1.746925
83	1	0	1.861007	5.465380	-0.115586
84	6	0	3.372315	-0.609592	-2.599650
85	6	0	4.955801	-0.237028	-0.735633
86	6	0	0.047055	3.973976	1.942238
87	6	0	-0.715960	4.422493	-0.369557
88	6	0	4.214666	-1.617187	-3.079082
89	6	0	2.075519	-0.253904	-3.320719
90	6	0	5.743796	-1.275750	-1.247877
91	6	0	5.347797	0.419080	0.587506

92	6	0	-0.944501	4.844537	2.408493
93	6	0	1.008560	3.293800	2.913310
94	6	0	-1.698613	5.269083	0.159385
95	6	0	-0.672862	4.174720	-1.877656
96	6	0	5.395828	-1.946260	-2.416312
97	1	0	3.940331	-2.157551	-3.979461
98	1	0	1.404466	0.195763	-2.576882
99	6	0	2.312947	0.800385	-4.421932
100	6	0	1.345982	-1.478951	-3.898748
101	1	0	6.648613	-1.562245	-0.720215
102	1	0	4.710872	1.295641	0.745430
103	6	0	5.080610	-0.541866	1.764232
104	6	0	6.808316	0.910063	0.600371
105	6	0	-1.805918	5.495487	1.528250
106	1	0	-1.038934	5.022418	3.474835
107	1	0	1.382279	2.384437	2.423511
108	6	0	2.230122	4.189286	3.209247
109	6	0	0.336092	2.853300	4.224758
110	1	0	-2.389316	5.763364	-0.517026
111	1	0	0.257865	3.652843	-2.120016
112	6	0	-1.824991	3.246509	-2.314041
113	6	0	-0.685291	5.481225	-2.695075

114	1	0	6.036967	-2.732715	-2.804211
115	1	0	2.766016	1.714763	-4.021785
116	1	0	2.985492	0.409814	-5.194675
117	1	0	1.366942	1.073934	-4.903715
118	1	0	1.247961	-2.272050	-3.149374
119	1	0	0.338269	-1.193755	-4.216582
120	1	0	1.868986	-1.894732	-4.767905
121	1	0	5.326588	-0.057451	2.716931
122	1	0	4.032156	-0.855096	1.796841
123	1	0	5.690661	-1.447946	1.679777
124	1	0	7.517051	0.077430	0.535674
125	1	0	7.018725	1.587996	-0.234461
126	1	0	7.018944	1.443530	1.534243
127	1	0	-2.560938	6.177224	1.910081
128	1	0	2.932086	3.674928	3.875739
129	1	0	2.769847	4.459395	2.294725
130	1	0	1.920207	5.120184	3.698229
131	1	0	0.037246	3.707382	4.842666
132	1	0	-0.554064	2.243447	4.034905
133	1	0	1.035393	2.254765	4.817825
134	1	0	-1.770579	2.276123	-1.810249
135	1	0	-2.799812	3.689695	-2.081447

136	1	0	-1.782019	3.068866	-3.394923
137	1	0	-1.636617	6.014985	-2.595864
138	1	0	0.111660	6.165813	-2.383919
139	1	0	-0.547919	5.259471	-3.759322



O (L3)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.015543	1.556759	-1.705845
2	6	0	-2.948466	1.208228	-0.850284
3	6	0	-2.262284	2.237774	-0.164549
4	6	0	-2.634185	3.564927	-0.338030
5	6	0	-3.691724	3.897873	-1.192722
6	6	0	-4.377934	2.889149	-1.874184
7	6	0	-2.567105	-0.180654	-0.684688
8	8	0	-1.417691	-0.382969	-0.100821

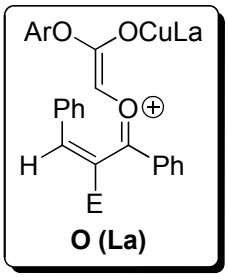
9	6	0	-0.878475	-1.558353	0.280905
10	8	0	0.820158	-2.708246	1.287947
11	6	0	2.106041	-2.824243	1.866286
12	6	0	-3.354848	-1.332498	-1.170171
13	6	0	-2.705749	-2.058522	-2.305984
14	8	0	-1.669507	-1.680946	-2.827133
15	6	0	-4.584402	-1.701528	-0.717338
16	6	0	-5.379386	-1.187605	0.390988
17	6	0	-4.846157	-0.464297	1.477850
18	6	0	-5.673939	-0.013140	2.499962
19	6	0	-7.048359	-0.271466	2.460213
20	6	0	-7.591044	-1.002192	1.400525
21	6	0	-6.762128	-1.467164	0.384064
22	8	0	-3.379232	-3.153698	-2.691086
23	6	0	-2.825060	-3.875243	-3.809398
24	1	0	-8.654890	-1.217578	1.372989
25	1	0	-7.182720	-2.044463	-0.435350
26	1	0	-7.690334	0.082536	3.261595
27	1	0	-5.247758	0.532300	3.336712
28	1	0	-5.052732	-2.511585	-1.271568
29	1	0	-3.778176	-0.285820	1.542395
30	1	0	-1.459804	-2.462729	0.188980

31	1	0	-2.777937	-3.232125	-4.691507
32	1	0	-1.822514	-4.235406	-3.566911
33	1	0	-3.503811	-4.710665	-3.977219
34	1	0	-1.456049	1.986346	0.516443
35	1	0	-2.107541	4.341666	0.209011
36	1	0	-3.983221	4.936256	-1.320564
37	1	0	-5.197978	3.141828	-2.539545
38	1	0	-4.548685	0.780185	-2.243014
39	6	0	2.224778	-2.669552	3.252369
40	6	0	3.498524	-2.867081	3.804804
41	6	0	4.583505	-3.209926	3.004084
42	6	0	4.418359	-3.368252	1.627763
43	6	0	3.170831	-3.178715	1.022364
44	6	0	1.038161	-2.295403	4.132987
45	1	0	3.637601	-2.753020	4.876132
46	1	0	5.561521	-3.362387	3.451952
47	1	0	5.272864	-3.643906	1.018887
48	6	0	4.207148	-3.164381	-1.321877
49	6	0	2.366480	-4.800818	-0.731853
50	6	0	0.839859	-3.293042	5.289470
51	6	0	1.173013	-0.852000	4.658659
52	1	0	0.136508	-2.338833	3.513421

53	1	0	3.945879	-3.195461	-2.385117
54	1	0	4.662394	-2.189321	-1.114810
55	1	0	4.965776	-3.936778	-1.150220
56	1	0	2.167947	-4.942796	-1.801028
57	1	0	3.072600	-5.576407	-0.413062
58	1	0	1.430031	-4.951764	-0.185665
59	1	0	0.297707	-0.578192	5.260117
60	1	0	2.061394	-0.744258	5.292453
61	1	0	1.258946	-0.141524	3.829196
62	1	0	-0.061416	-3.038760	5.859386
63	1	0	0.729520	-4.316795	4.916467
64	1	0	1.684201	-3.280006	5.988005
65	6	0	2.948064	-3.394750	-0.471457
66	1	0	2.201029	-2.665267	-0.807699
67	6	0	0.408065	-1.498024	0.838896
68	8	0	1.139086	-0.481684	0.959672
69	1	0	2.886269	2.894954	-4.213723
70	6	0	3.085190	3.510850	-3.335717
71	6	0	2.555600	2.855976	-2.085087
72	1	0	2.620873	4.491350	-3.479667
73	1	0	4.168611	3.675181	-3.278741
74	6	0	2.372960	3.714927	-0.852462

75	7	0	2.190935	1.621737	-1.982677
76	7	0	1.845231	3.139138	0.176228
77	6	0	2.870259	5.137522	-0.899379
78	6	0	2.345861	0.649593	-3.004365
79	29	0	1.476965	1.090362	-0.087493
80	6	0	1.533054	3.796706	1.393042
81	1	0	3.841053	5.183223	-1.402071
82	1	0	2.188352	5.786284	-1.463503
83	1	0	2.974834	5.551701	0.104304
84	6	0	1.260496	-0.201649	-3.263240
85	6	0	3.559502	0.456688	-3.685381
86	6	0	1.880413	3.152372	2.591300
87	6	0	0.819479	5.006365	1.438741
88	6	0	1.370562	-1.195126	-4.232796
89	6	0	3.668561	-0.559463	-4.634490
90	6	0	1.566741	3.738716	3.815097
91	6	0	0.483789	5.570655	2.669949
92	6	0	2.573866	-1.378756	-4.920705
93	1	0	0.512430	-1.830006	-4.427493
94	1	0	4.613602	-0.711102	-5.147858
95	6	0	0.865801	4.947559	3.859638
96	1	0	1.858768	3.243008	4.736058

97	1	0	-0.075696	6.501298	2.696901
98	1	0	2.663204	-2.163515	-5.666169
99	1	0	0.609637	5.394653	4.815347
100	1	0	0.504265	5.485353	0.516881
101	1	0	2.405696	2.202393	2.550458
102	1	0	4.421954	1.070395	-3.445021
103	1	0	0.329080	-0.079478	-2.720455



O (La)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.900252	2.061276	0.133781
2	6	0	2.760106	1.348594	-0.296206
3	6	0	1.948491	1.913198	-1.307881
4	6	0	2.270867	3.147709	-1.859082
5	6	0	3.402598	3.846095	-1.421139

6	6	0	4.213006	3.296784	-0.423908
7	6	0	2.433175	0.064342	0.292044
8	8	0	1.240585	-0.393144	0.020063
9	6	0	0.732498	-1.603054	0.322958
10	8	0	-0.991627	-3.098266	0.209426
11	6	0	-2.330037	-3.473394	-0.049292
12	6	0	3.311530	-0.696729	1.202617
13	6	0	2.795646	-0.746860	2.606691
14	8	0	1.818135	-0.118152	2.978993
15	6	0	4.510356	-1.255781	0.880666
16	6	0	5.188398	-1.375964	-0.403915
17	6	0	4.543406	-1.269844	-1.653691
18	6	0	5.264489	-1.408148	-2.834459
19	6	0	6.641768	-1.651724	-2.795702
20	6	0	7.294454	-1.775063	-1.566890
21	6	0	6.571895	-1.651768	-0.384021
22	8	0	3.516831	-1.542452	3.410728
23	6	0	3.095327	-1.594864	4.788990
24	29	0	-1.610805	0.957931	-0.256086
25	7	0	-2.397640	2.389305	-1.495104
26	6	0	-2.966060	2.171957	-2.841881
27	6	0	-3.487767	3.566436	-3.256594

28	8	0	-3.155742	4.407287	-2.115914
29	6	0	-2.556792	3.627219	-1.193382
30	6	0	-2.155004	4.399303	0.052380
31	6	0	-3.415215	5.134478	0.596391
32	7	0	-1.358914	2.296903	1.252255
33	6	0	-1.583221	3.558348	1.181461
34	8	0	-1.279869	4.292928	2.270845
35	6	0	-0.673980	3.394955	3.245787
36	6	0	-0.843548	2.000454	2.607621
37	6	0	-1.077173	5.443692	-0.364542
38	1	0	-4.569841	3.611536	-3.396341
39	1	0	-2.989810	3.986157	-4.133247
40	1	0	-2.188036	1.790714	-3.510257
41	1	0	-3.757742	1.419197	-2.785976
42	1	0	-3.144269	5.730507	1.469645
43	1	0	-3.820608	5.793238	-0.173603
44	1	0	-4.191622	4.419459	0.888732
45	1	0	-1.472892	6.088010	-1.152807
46	1	0	-0.810717	6.059888	0.496759
47	1	0	-0.172909	4.947027	-0.732237
48	1	0	0.090236	1.438295	2.544143
49	1	0	-1.576922	1.379922	3.133499

50	1	0	0.369864	3.696696	3.365548
51	1	0	-1.203632	3.527688	4.190481
52	1	0	8.360607	-1.977489	-1.531788
53	1	0	7.077832	-1.758588	0.572136
54	1	0	7.199812	-1.759701	-3.721208
55	1	0	4.752548	-1.336643	-3.789510
56	1	0	5.055309	-1.684619	1.718450
57	1	0	3.471210	-1.113119	-1.702120
58	1	0	1.379529	-2.357573	0.743974
59	1	0	3.139927	-0.599886	5.238232
60	1	0	2.074842	-1.978583	4.857207
61	1	0	3.795381	-2.271257	5.277968
62	1	0	1.082167	1.366967	-1.665814
63	1	0	1.649878	3.561627	-2.648793
64	1	0	3.654792	4.806424	-1.861064
65	1	0	5.092502	3.832907	-0.080200
66	1	0	4.531767	1.644209	0.910513
67	6	0	-2.638230	-3.976302	-1.321556
68	6	0	-3.956208	-4.400195	-1.534200
69	6	0	-4.908684	-4.330620	-0.519732
70	6	0	-4.556442	-3.841291	0.736022
71	6	0	-3.253041	-3.402828	1.003542

72	6	0	-1.599958	-4.049360	-2.435160
73	1	0	-4.238257	-4.794007	-2.506512
74	1	0	-5.924661	-4.667642	-0.705289
75	1	0	-5.303213	-3.801915	1.524029
76	6	0	-3.551948	-1.506951	2.649549
77	6	0	-3.192498	-3.875798	3.499330
78	6	0	-1.505248	-5.457465	-3.051653
79	6	0	-1.875414	-2.985299	-3.517180
80	1	0	-0.623554	-3.825990	-1.992967
81	1	0	-3.237615	-1.108262	3.622317
82	1	0	-3.291462	-0.777853	1.873636
83	1	0	-4.643962	-1.602669	2.666312
84	1	0	-2.855396	-3.487839	4.467719
85	1	0	-4.267993	-4.070212	3.579129
86	1	0	-2.691754	-4.833599	3.322630
87	1	0	-1.096498	-3.011483	-4.288858
88	1	0	-2.839244	-3.162476	-4.009071
89	1	0	-1.898387	-1.981431	-3.079227
90	1	0	-0.702322	-5.490578	-3.797216
91	1	0	-1.292041	-6.212700	-2.287733
92	1	0	-2.433969	-5.744690	-3.557439
93	6	0	-2.875575	-2.866350	2.379756

94	1	0	-1.792806	-2.704572	2.389565
95	6	0	-0.619368	-1.812066	-0.007328
96	8	0	-1.433055	-0.969610	-0.456399

10.3. Computed energies of all stationary points

Table S3. Sum of electronic and thermal enthalpies (*H*, in Hartree), sum of electronic and thermal free energies (*G*, in Hartree), thermal correction to Enthalpy (*TCH*, in Hartree), thermal correction to Gibbs free energy (*TCGFE*, in Hartree), and total free energy in solution (E_S, in Hartree, solvent = dichloromethane).

Structure	*H*	*G*	*TCH*	*TCGFE*	E_S
S1	-1688.71922	-1688.827854	0.53694	0.428306	-1689.277024
1	-881.601112	-881.668757	0.287139	0.219493	-881.889304
2	-803.914578	-803.982256	0.319125	0.251447	-804.225299
S2	-1611.007098	-1611.114698	0.568919	0.46132	-1611.598588
TS-S1	-1610.988132	-1611.097941	0.566602	0.456793	-1611.575068
N_2	-109.511814	-109.533568	0.008905	-0.01285	-109.518183
S3	-1501.48505	-1501.587242	0.556666	0.454473	-1502.065698
TS-S2	-2383.102727	-2383.25349	0.844619	0.693857	-2383.948051
C (La)	-2383.131847	-2383.279113	0.847549	0.700282	-2383.982824
TS1 (La)	-2383.120777	-2383.262835	0.846453	0.704394	-2383.974397
TS1-cis (La)	-2383.107401	-2383.249158	0.845558	0.703801	-2383.960000
S4	-2383.18962	-2383.33634	0.849707	0.702987	-2384.041147
3	-1576.084169	-1576.191035	0.599511	0.492646	-1576.665754
TS2 (La)	-2383.119811	-2383.268088	0.845863	0.697586	-2383.965197
O (La)	-2383.139171	-2383.286987	0.847288	0.699472	-2383.984592
TS3 (La)	-2383.12173	-2383.265891	0.846377	0.702216	-2383.971125
TS4 (La)	-2383.117506	-2383.264831	0.845832	0.698506	-2383.963519
TS4-cis (La)	-2383.118311	-2383.265423	0.846095	0.698982	-2383.968637
S5	-2383.143787	-2383.286548	0.848356	0.705595	-2383.999126
S6	-1576.029814	-1576.133793	0.598345	0.494366	-1576.616425
TS-S3	-1576.007961	-1576.111309	0.593386	0.490037	-1576.589035
4	-1576.059987	-1576.165647	0.599154	0.493494	-1576.644857
C (L1)	-2971.966344	-2972.154909	1.25854	1.069975	-2973.20227
TS1 (L1)	-2971.940043	-2972.121466	1.258171	1.076748	-2973.181515
TS2 (L1)	-2971.959562	-2972.146612	1.257085	1.070035	-2973.193566
O (L1)	-2971.970314	-2972.159272	1.258301	1.069343	-2973.203999
TS3 (L1)	-2971.958684	-2972.144332	1.257399	1.071751	-2973.194026
TS4 (L1)	-2971.953895	-2972.144344	1.256438	1.065989	-2973.186332
TS4-cis (L1)	-2971.958013	-2972.148469	1.256929	1.066474	-2973.186970
C (L3)	-2500.57169	-2500.72847	0.901386	0.744605	-2501.469976
TS1 (L3)	-2500.557828	-2500.708667	0.900288	0.74945	-2501.462291
TS2 (L3)	-2500.561545	-2500.715473	0.900027	0.746099	-2501.460338
O (L3)	-2500.577819	-2500.733184	0.901366	0.746001	-2501.474834
TS3 (L3)	-2500.56123	-2500.713793	0.900317	0.747754	-2501.459917
TS4 (L3)	-2500.555969	-2500.711188	0.899691	0.744473	-2501.453945

FY	-1576.012403	-1576.121504	0.597118	0.488017	-1576.596063
Cu-La	-807.056525	-807.114491	0.248202	0.190236	-807.355216
Cu-L1	-1395.896371	-1395.999194	0.657591	0.554768	-1396.570468
Cu-L3	-924.487936	-924.553652	0.301871	0.236155	-924.844857
TS-S4	-1575.997908	-1576.103367	0.595505	0.490045	-1576.578572
TS-S5	-1576.007822	-1576.111579	0.596031	0.492274	-1576.590814

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