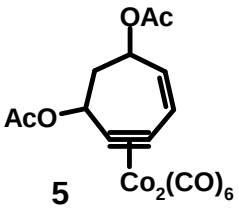
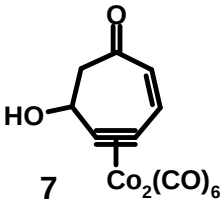
Supplementary Information

Hexacarbonyl[μ-η^4-(5,7-diacetoxycyclohept-1-en-3-yne)]dicobalt (5): To a solution of **4** (1.419 g, mmol) in CH_3CO_2H (20 mL) was added H_2SO_4 (10 drops). Following stirring for 1.5 h, water was added, and the mixture was subjected to a conventional extractive workup (hexanes). The organic layers were dried over $MgSO_4$, and concentrated under reduced pressure. Flash chromatography (10:1 petroleum ether : Et_2O) afforded **5** (1.356 g, 96% yield) as a single diastereomer; (**5**), (R_f = 0.37, 4:1 petroleum ether : Et_2O); IR (neat, NaCl) ν_{max} 3030, 2928, 2095, 2056, 2029, 1741 cm^{-1}; ^{1}H NMR ($CDCl_3$) δ 6.77 (d, J = 10.0, 1H, vinyl-C*H*), 6.27 (dd, J = 10.3, 3.7, 1H, C*H*-OAc), 6.14 (dd, J = 10.0, 6.3, 1H, vinyl-C*H*), 5.57 (apparent t, J = 6.8, 1H, C*H*-OAc), 2.40 (m, 1H, CH*H*), 2.16 (s, 3H, C(O)-C*H*$_3$), 2.05 (m, 1H, C*H*H), 2.03 (s, 3H, C(O)-CH$_3$); ^{13}C NMR ($CDCl_3$) 198.9 (br), 170.2, 170.0, 130.6, 130.3, 93.9, 81.4, 71.0, 67.3, 35.0, 21.0, 20.8; MS (EI, 20 eV) m/e 466 (M – CO$^+$), 438 (M$^+$-2CO), 354 (M$^+$-5CO), 326 (M$^+$-6CO) ; HRMS (TOF) m/e for $C_{17}H_{12}Co_2O_{10}$ calcd. 465.9145 (M – CO$^+$), found 465.9159.



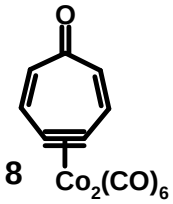
5

Hexacarbonyl[μ-η^4-(6-hydroxycyclohept-2-en-4-ynone)]dicobalt (7): Compound **5** (0.3572 g, 0.723 mmol) was dissolved in Et_2O and cooled to -78 ^{o}C. DIBAL-H (3.0 mL of a 1 M solution in Et_2O, 4 equiv) was added and the solution stirrer for 1.5 h. Saturated $NH_4Cl_{(aq)}$ was added and the reaction mixture was subjected to a conventional extractive workup (Et_2O). Removal of the volatiles under reduced pressure afforded crude **6**, which was dissolved in CH_2Cl_2. Addition of MnO_2 (excess), and the mixture stirred 12 h. Filtration through silica gel and concentration under reduced pressure gave a residue, which was subjected to flash chromatography (4:1 petroleum ether : Et_2O) to afford **7** (0.1829 g, 62%); (**7**), (R_f = 0.30, 2:1 petroleum ether : Et_2O); IR (neat, NaCl) ν_{max} 3417, 3027, 2925, 2099, 2059, 2030, 1651cm^{-1}; ^{1}H NMR ($CDCl_3$) δ 7.36 (d, J = 10.4, 1H, vinyl-C*H*), 6.26 (d, J = 10.4, 1H, vinyl-C*H*), 5.17 (m, 1H, C*H*-OH), 3.02 (m, 2H, C*H*$_2$), 2.20 (d, J = 5.0, 1H, O*H*); ^{13}C NMR ($CDCl_3$) 198.3 (br, obscured), 198.3, 139.5, 132.2, 97.8, 78.4, 68.7, 52.3; MS (EI, 20 eV) m/e 408 (M$^+$), 380 (M-CO$^+$), 352 (M-2CO$^+$), 324 (M-3CO$^+$), 296 (M-4CO$^+$); HRMS (TOF) m/e for $C_{13}H_6Co_2O_8$ calcd. (M$^+$) 407.8727, found 407.8705.

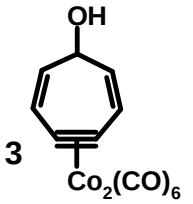


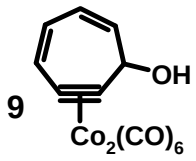
7

Hexacarbonyl[μ-η^4-(cyclohepta-2,6-dien-4-ynone)]dicobalt (8): To a solution of **7** (0.200 g, 0.490 mmol) in CH_2Cl_2 (10 mL) was added HBF_4 (0.5 mL, 54 wt. % in Et_2O, excess) in a dropwise fashion. After 20 min $NaHCO_{3(sat)}$ was added, and followed by a conventional extractive workup (CH_2Cl_2). Flash chromatographic purification (5:1 petroleum ether:Et_2O) afforded **8** (0.095 g, 50% yield); (**8**), (R_f = 0.45, 4:1 petroleum ether : Et_2O); (neat, NaCl) ν_{max} 3031, 2927, 2102, 2064, 2032, 1699 cm^{-1}; ^{1}H NMR ($CDCl_3$) δ 7.61 (d, J = 10.0, 2H, vinyl-C*H*), 6.59 (d, J = 10.0, 2H, vinyl-C*H*); ^{13}C NMR ($CDCl_3$) 198.0 (br), 191.1, 140.5, 135.3, 80.5; MS (EI, 20 eV) m/e 390 (M^+), 362(M-CO^+), 334(M-2CO^+), 306(M-3CO^+), 278(M-4CO^+), 250(M-5CO^+), 222(M-6CO^+); HRMS (TOF) m/e for $C_{13}H_4Co_2O_7$ calcd. (M^+) 389.8621, found 389.8625.

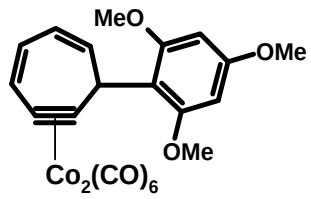


Hexacarbonyl[μ-η^4-(cyclohepta-2,6-dien-4-ynol)]dicobalt (3) and **Hexacarbonyl[μ-η^4-(cyclohepta-2,4-dien-6-ynol)]dicobalt (9):** To a solution of **8** (0.0768 g, 0.197 mmol) in Et_2O (10 mL) at -78 ^{o}C was added DIBAL-H (0.5 mL of 1M solution, 0.5 mmol). After stirred 2 h at -78 ^{o}C, saturated $NH_4Cl_{(aq)}$ was added, and the reaction subjected to a conventional extractive workup (Et_2O). Flash chromatographic purification (100% petroleum ether – 5:1 petroleum ether: Et_2O gave the sequential elution of recovered **8** (0.0036g, 5% recovery), alcohol **9** (0.0038 g, 5% yield), and **3** (0.0633 g, 82% yield, 86% based on recovered **8**); (**3**), (R_f = 0.20, 5:1 petroleum ether : Et_2O); IR (neat, NaCl) ν_{max} 3324,3021, 2923, 2099, 2053, 2053, 2028, 2009 cm^{-1}; ^{1}H NMR ($CDCl_3$) δ 6.79 (dd, J = 10.0, 1.8, 1H, vinyl-C*H*), 5.93 (dd, J = 10.0, 3.8, 1H, vinyl-C*H*), 4.94 (br, 1H, C*H*-OH), 2.21 (br, 1H, O*H*); ^{13}C NMR ($CDCl_3$) 199.1, 133.0, 127.5, 84.8, 70.3; MS (EI, 20 eV) m/e 392 (M^+); HRMS m/e for $C_{13}H_6Co_2O_7$ calcd. 391.8763 (M^+) , found 391.8764. Compound (**9**), (R_f = 0.32, 5:1 petroleum ether : Et_2O) IR (neat, NaCl) ν_{max} 3400 (br), 3022, 2095, 2054, 2022 cm^{-1}; ^{1}H NMR ($CDCl_3$) δ 6.88 (d, J = 9.8, 1H, vinyl-C*H*), 6.17 (m, 1H, vinyl-C*H*), 5.92-5.98 (m, 2H, 2 vinyl-C*H*), 5.55 (d, J = 6.2, 1H, C*H*-OH), 2.18 (br, 1H, O*H*); ^{13}C NMR (CD_2Cl_2) 199.8 (br), 135.7, 131.4, 127.2, 126.4, 102.5, 83.1, 72.5; MS (EI, 20 eV) m/e 364 (M-CO^+), 336 (M-2CO^+), 308 (M-3CO^+), 280 (M-4CO^+), 252 (M-5CO^+), 224 (M-6CO^+),.





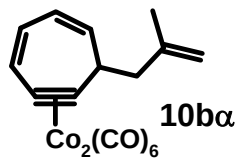
Hexacarbonyl[μ-η^4-(7-(2,4,6-trimethoxyphenyl)cyclohepta-1,3-dien-5-yne)]dicobalt (10aα):



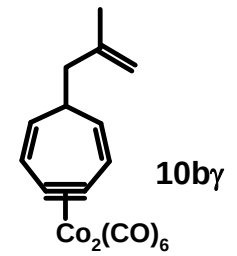
10aα

To a solution of compound **3** (0.023 g, 0.059 mmol) and 1,3,5-trimethoxybenzene (0.050 g, 0.29 mmol) in CH_2Cl_2 (5 mL) at 0 ^oC was added BF_3-OEt_2 (21 μL, 0.18 mmol). After 15 min, saturated $NaHCO_{3(aq)}$ was added and the mixture subjected to a conventional extractive workup (CH_2Cl_2). The combined organic layer were dried over $MgSO_4$ and concentrated under reduced pressure. Flash chromatography (10:1 petroleum ether : Et_2O) afforded **10aα** (0.028 g, 88% yield); (**10aα**), (R_f = 0.38, 10:1 petroleum ether : Et_2O); IR (neat, NaCl) ν_{max} 3019, 2924, 2090, 2050, 2020 cm^{-1}; ^{1}H NMR ($CDCl_3$) δ 6.74 (d, J = 9.6, 1H, vinyl-C*H*), 6.17 (s, 2H, aryl-C*H*), 6.12 (dd, J = 9.6, 7.5, 1H, vinyl-C*H*), 5.95 (dd, J = 11.9, 1.9, 1H, vinyl-C*H*), 5.83 (m, 1H, vinyl-C*H*), 5.59 (br s, 1H, alkyl-C*H*), 3.86 (s, 3H, OC*H*$_3$), 3.80 (s, 3H, OC*H*$_3$), 3.78 (s, 3H, OC*H*$_3$); ^{13}C NMR ($CDCl_3$) 199.8 (br), 160.3, 159.7, 158.2, 137.7, 129.3, 127.4, 124.7, 110.8, 106.4, 90.7, 90.1, 85.6, 55.3, 55.2, 54.5, 40.0; MS (EI, 20 eV) m/e 514 (M-CO^+), 486 (M-2CO^+), 458 (M-3CO^+), 430 (M-4CO^+), 402 (M-5CO^+), 374 (M-6CO^+); HRMS (TOF) m/e for $C_{22}H_{16}Co_2O_9$ calcd. (M-2CO^+) 485.9560, found 485.9538.

Hexacarbonyl[μ-η^4-(7-(2-methylallyl)cyclohepta-1,3-dien-5-yne)]dicobalt (10bα) and **Hexacarbonyl[μ-η^4-(7-(2-methylallyl)cyclohepta-1,5-dien-3-yne)]dicobalt (10bγ)**: Reaction of **3** (0.020 g, 0.051 mmol) with methallyltrimethylsilane (35 μL, 0.20 mmol) under the standard conditions afforded **10b** (0.016 g, 73%) as a 67:33 mixture of **10bα:10bγ** following purification by flash chromatography (100% hexanes); (**10b**), (R_f = 0.69, 100% petroleum ether); IR (neat, NaCl) ν_{max} 2091, 2050, 2021 cm^{-1}; ^{1}H NMR ($CDCl_3$) δ (major isomer) 6.79 (d, J = 9.6, 1H, vinyl-C*H*), 6.12 (dd, J = 9.6, 7.2, 1H, vinyl-C*H*), 5.90 (ddd, J = 11.9, 7.2, 2.4, 1H, vinyl-C*H*), 5.73 (ddd, J = 11.9, 3.0, 0.9, 1H, vinyl-C*H*), 4.93 (s, 1H, =CH*H*), 4.87 (s, 1H, =C*H*H), 3.83 (m, 1H, alkyl-C*H*), 2.59 (dd, J = 14.1, 5.1, 1H, C*H*H), 2.44 (dd, J = 14.1, 10.2, 1H, CH*H*), 1.80 (s, 3H, C*H*$_3$); (minor isomer) 6.71 (br d, J = 9.7, 2.2, 2H, vinyl-C*H*), 5.65 (dd, J = 9.7, 4.2, 2H, vinyl-C*H*), 4.87 (s, 1H, =C*H*H), 4.76 (s, 1H, =CH*H*), 3.15 (m, 1H, alkyl-C*H*), 2.33 (d, 7.7, 2H, C*H*$_2$), 1.70 (s, 3H, C*H*$_3$); ^{13}C NMR ($CDCl_3$) (major isomer) 199.7 (br), 142.6, 134.0, 127.61, 127.2, 113.2, 105.7, 85.8, 45.5, 41.1, 22.2; resonances from the minor isomer could be detected at 142.2, 135.0, 127.58, 113.4, 87.3, 44.8, 39.8, 22.0; MS (EI, 20 eV) m/e 402



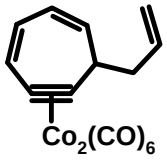
10bα



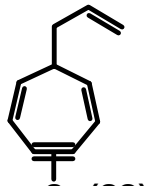
10bγ

(M-CO^+), 374 (M-$2CO^+$), 346 (M-$3CO^+$), 318 (M-$4CO^+$), 290 (M-$5CO^+$), 262 (M-$6CO^+$); HRMS (TOF) m/e for $C_{17}H_{12}Co_2O_6$ calcd. (M-CO^+) 401.9349, found 401.9334.

Hexacarbonyl[μ-η^4-(7-allylcyclohepta-1,3-dien-5-yne)]dicobalt (10cα) and Hexacarbonyl[μ-η^4-(7-allylcyclohepta-1,5-dien-3-yne)]dicobalt (10cγ): Reaction of **3** (0.028 g, 0.071 mmol) with allyltrimethylsilane (56 μL, 0.36 mmol) under the standard conditions afforded **10c** (0.021 g, 70%) as a 83:17 mixture of **10cα:10cγ** following purification by flash chromatography (100% hexanes); (**10c**), (R_f = 0.65, 100% petroleum ether); (neat, NaCl) ν_{max} cm^{-1}; ^{1}H NMR ($CDCl_3$) (major isomer) δ 6.79 (d, J = 10.0, 1H, vinyl-C*H*), 6.11 (dd, J = 10.0, 7.5, 1H, vinyl-C*H*), 5.96 (m, 1H, vinyl-C*H*), 5.90 (m, 1H, vinyl-C*H*), 5.74 (ddd, J = 12.0, 3.0, 1.0, 1H), 5.22 (dd, J = 17.0, 1.5, 1H, =C*H*H), 5.17 (dd, J = 10.5, 1.5, 1H, CH*H*), 3.74 (m, 1H, alkyl-C*H*), 2.67 (m, 1H, C*H*H), 2.51 (m, 1H, CH*H*); (minor isomer) δ 6.69 (dd, J = 9.5, 2.0, 2H, 2 vinyl-C*H*), 5.79 (m, 1H, vinyl-C*H*), 5.64 (dd, J = 9.5, 4.3, 2H, 2 vinyl-C*H*), 5.10 (d, J = 9.4, 1H, vinyl-C*H*), 5.09 (d, J = 17.7, 1H, vinyl-C*H*), 3.16 (m, 1H, alkyl-C*H*), 2.37 (apparent t, J = 6.8, 2H, CH_2); ^{13}C NMR ($CDCl_3$) (major isomer) 199.6 (br), 136.0, 135.0, 130.2, 127.7, 127.1, 117.4, 104.9, 85.8, 43.5, 41.3; resonances from the minor isomer could be detected at 135.5, 133.8, 127.4, 42.5, 41.1; MS (EI, 20 eV) m/e 418 (M^+), 388 (M-CO^+), 360 (M-$2CO^+$), 332 (M-$3CO^+$), 304 (M-$4CO^+$), 276 (M-$5CO^+$), 248 (M-$6CO^+$); HRMS (TOF) m/e for $C_{16}H_{10}Co_2O_6$ calcd. (M-CO^+) 387.9192, found 387.9166.

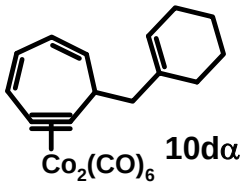


10cα

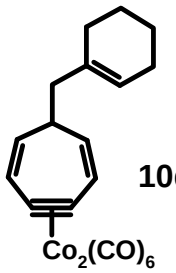


10cγ

Hexacarbonyl[μ-η^4-(7-(cyclohexenylmethyl)cyclohepta-1,3-dien-5-yne)]dicobalt (10dα) and Hexacarbonyl[μ-η^4-(7-(cyclohexenylmethyl)cyclohepta-1,5-dien-3-yne)]dicobalt (10dγ): Reaction of **3** (0.027 g, 0.068 mmol) with methylenecyclohexane (33 μL, 0.28 mmol) under the standard conditions afforded **10d** (0.016 g, 50%) as a 90:10 mixture of **10dα:10dγ** following purification by flash chromatography (10:1 petroleum ether : Et_2O); (**10d**), (R_f = 0.75, 100% petroleum ether); (neat, NaCl) ν_{max} 3018, 2929, 2090, 2050, 2020 cm^{-1}; ^{1}H NMR ($CDCl_3$) (major isomer) δ 6.77 (d, J = 9.5, 1H, vinyl-C*H*), 6.11 (dd, J = 9.5, 7.0, 1H, vinyl-C*H*), 5.88 (m, 1H, vinyl-C*H*), 5.73 (dd, J = 12.0, 1.0, 1H, vinyl-C*H*), 5.58 (br s, 1H, vinyl-C*H*), 3.82 (m, 1H, alkyl-C*H*), 2.53 (m,



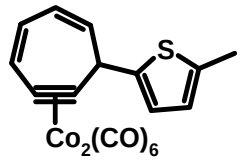
10dα



10dγ

1H, C*H*H), 2.34 (m, 1H, CH*H*), 2.00-2.10 (m, 4H, 2 CH_2), 1.55-1.75 (m, 4H, 2 CH_2); resonances from the minor isomer could be detected at 6.49 (dd, J = 9.5, 2.2, 1H, 2 vinyl-C*H*), 5.64 (dd, J = 9.5, 4.5, 1H, 2 vinyl-C*H*), 5.49 (br s, 1H, vinyl-C*H*), 3.16 (m, 1H, alkyl-C*H*), 2.24 (d, J = 7.5, 2H, CH_2); ^{13}C NMR ($CDCl_3$) (major isomer) 199.7 (br), 135.4, 134.8, 130.0, 127.3, 127.2, 124.2, 106.1, 85.9, 46.0, 41.0, 28.2, 25.3, 22.9, 22.4; peaks from the minor isomer could be observed at 134.4, 124.5, 45.3, 40.0, 20.0; MS (EI, 20 eV) m/e 470 (M^+), 442 (M - CO^+), 414 (M - 2CO^+), 386 (M - 3CO^+), 358 (M - 4CO^+), 330 (M - 5CO^+), 302 (M - 6CO^+); HRMS (TOF) m/e for $C_{20}H_{16}Co_2O_6$ calcd. (M^+) 469.9611, found 469.9626.

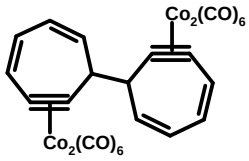
Hexacarbonyl[μ-η^4-(7-(5-methyl-2-thienyl)cyclohepta-1,3-dien-5-yne)]dicobalt (10eα):



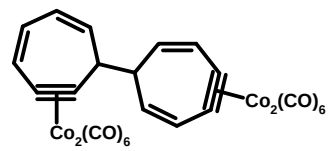
10eα

Reaction of **3** (0.018 g, 0.046 mmol) with 2-methylthiophene (23 μL, 0.23 mmol) under the standard conditions afforded **10eα** (0.018 g, 83% yield) following purification by flash chromatography (100% hexanes); (**10eα**), (R_f = 0.59, 100% petroleum ether); (neat, NaCl) ν_{max} 3020, 2923, 2091, 2052, 2022 cm^{-1}; ^{1} H NMR ($CDCl_3$) δ 6.84 (d, J = 9.0, 1H, vinyl-C*H*), 6.76 (d, J = 3.0, 1H, thienyl-C*H*), 6.61 (d, J = 3.0, 1H, thienyl-C*H*), 6.18 (m, 1H, vinyl-C*H*), 6.00-6.08 (m, 2H, 2 vinyl-C*H*), 5.16 (s, 1H, alkyl-C*H*), 2.46 (s, 3H, CH_3); ^{13}C NMR ($CDCl_3$) 199.0 (br), 145.0, 139.0, 134.3, 131.0, 127.9, 126.6, 124.7, 124.4, 105.9, 84.5, 45.7, 15.4; MS (EI, 20 eV) m/e 472 (M^+), 444 (M - CO^+), 416 (M - 2CO^+), 388 (M - 3CO^+), 360 (M - 4CO^+), 332 (M - 5CO^+), 304 (M - 6CO^+); HRMS (TOF) m/e for $C_{18}H_{10}Co_2O_6S$ calcd. (M^+) 471.8862, found 471.8851.

Hexacarbonyl[μ^4-η^2,η^2,η^2,η^2-(1,1'-bi(cyclohepta-2,4-dien-6-yne)]tetracobalt (11αα) and Hexacarbonyl[μ^4-η^2,η^2,η^2,η^2-(7-(cyclohepta-2,6-dien-4-ynyl)cyclohepta-1,3-dien-5-yne)]-tetracobalt (11αγ): To a solution of **3** (0.028 g, 0.071 mmol) and mesitylene (49 μL, 0.36 mmol) in CH_2Cl_2 (5 mL) at 0 °C was added BF_3-OEt_2 (26 μL, 0.21 mmol).). After 15 min, saturated $NaHCO_{3(aq)}$ was added and the mixture subjected to a conventional extractive workup (CH_2Cl_2). The combined organic layer were dried over $MgSO_4$ and concentrated under reduced pressure. Flash chromatography (100% hexanes) afforded **11** (0.0133 g, 50%) as a 33:67 mixture of **11αα:11αγ**. Compound **11αγ** slowly decomposed in



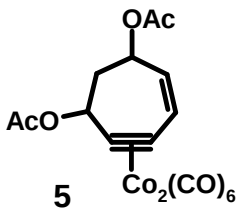
11αα



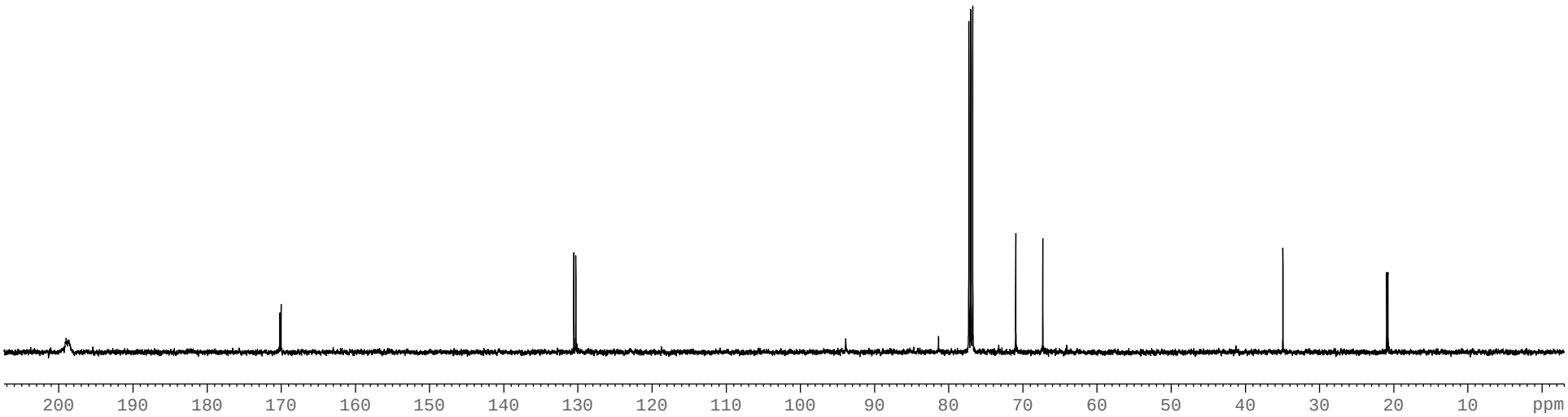
11αγ

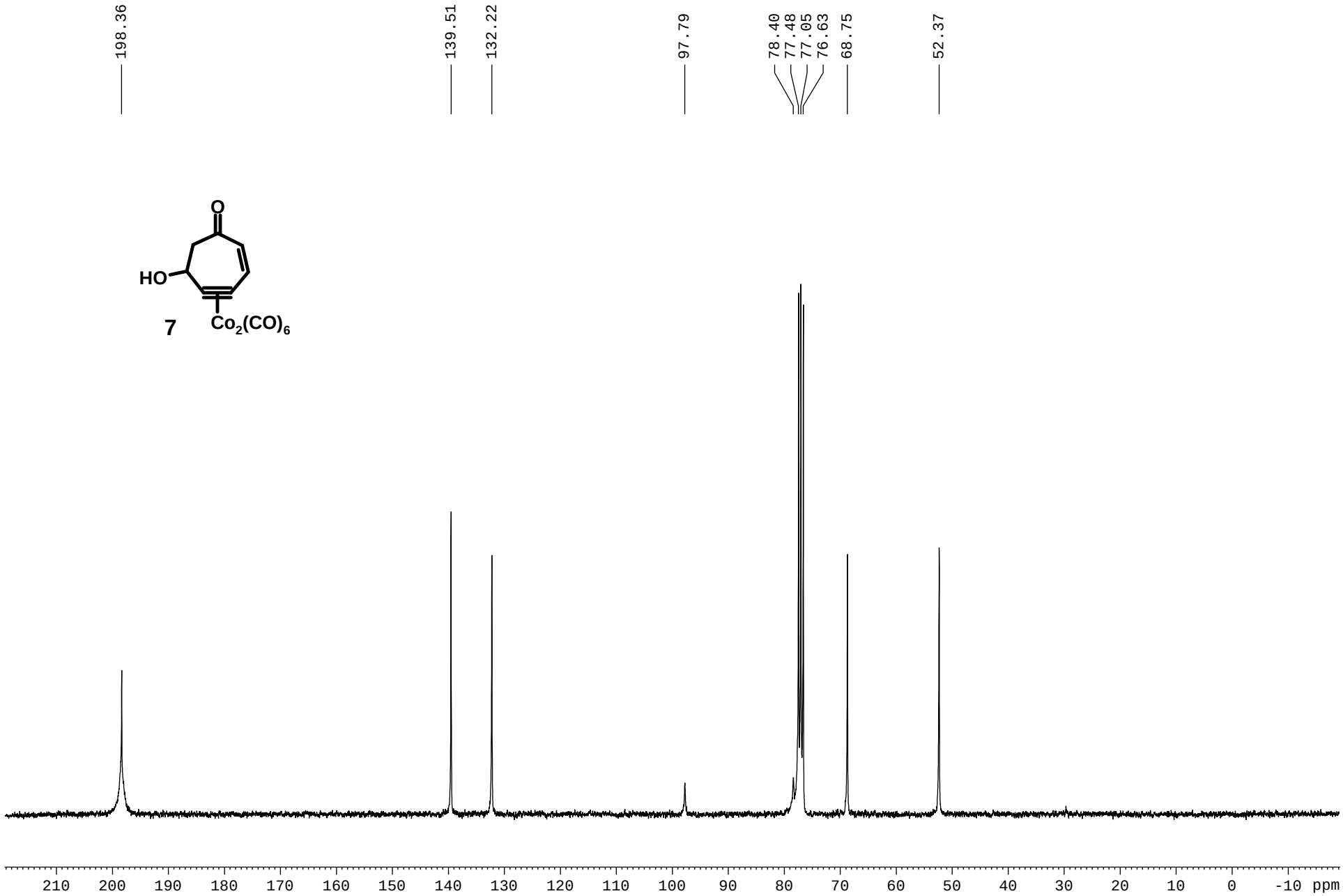
solution in $CDCl_3$; (**11**), (R_f = 0.52, 100% petroleum ether); IR (neat, NaCl) ν_{max} 3020, 2923, 2091, 2053, 2023 cm^{-1}; ^{1}H NMR ($CDCl_3$) (major isomer) δ 6.96 (dd, J = 9.8, 2.6, 1H, vinyl-C*H*), 6.94 (dd, J = 9.3, 2.6, 1H, vinyl-C*H*), 6.87 (d, J = 9.6, 1H, vinyl-C*H*), 6.17 (dd, J = 9.6, 7.3, 1H, vinyl-C*H*). 6.0-6.08 (m, 2H, 2 vinyl-C*H*), 5.96 (dd, J = 9.3, 3.6, 1H, vinyl-C*H*), 5.77 (ddd, J = 11.9, 3.1, 1.0, 1H, vinyl-C*H*), 3.96 (m, 1H, alkyl-C*H*), 3.38 (m, 1H, alkyl-C*H*); resonances from the minor isomer could be detected at 6.89 (d, J = 9.7, 2H, vinyl-C*H*), 6.25 (dd, J = 9.7, 7.3, 2H, vinyl-C*H*), 6.13 (m, 2H, vinyl-C*H*), 6.00 (ddd, J = 12.0, 2.5, 1.0, 2H, vinyl-C*H*), 4.16 (br s, 2H, alkyl-C*H*); ^{13}C NMR ($CDCl_3$) 199.3 (br), 133.4 (major), 132.8 (major), 132.3 (major), 131.6 (minor), 130.8 (major), 130.5 (major), 130.2 (minor), 129.8 (minor), 129.6 (major), 127.7 (minor), 126.9 (major), 104.2, 86.4, 48.5 (minor), 46.7 (major); MS (EI, 20 eV) m/e 638 (M^+-4CO), 610 (M^+-5CO), 582 (M^+-6CO), 554 (M^+-7CO), 526 (M^+-8CO), 498 (M^+-9CO), 470 (M^+-10CO), 442 (M^+-11CO), 414 (M^+-12CO); HRMS (TOF) m/e for $C_{26}H_{10}Co_4O_{12}$ calcd. (M^+) 749.7500, found 749.7515.

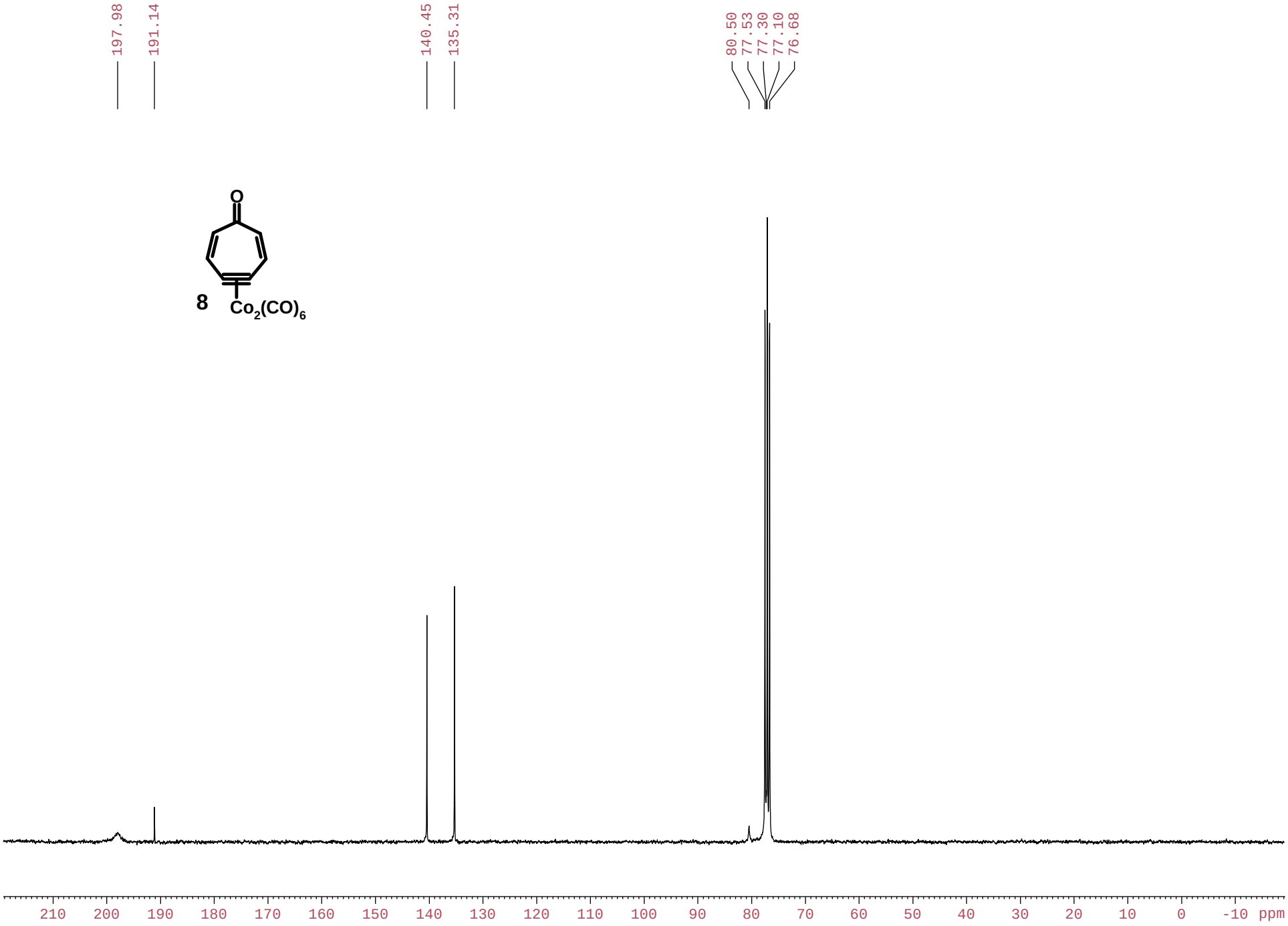
199.00
198.72
170.19
170.04
130.57
130.30
93.90
81.40
77.30
77.04
76.95
76.92
76.79
70.98
67.33
34.95
20.95
20.79

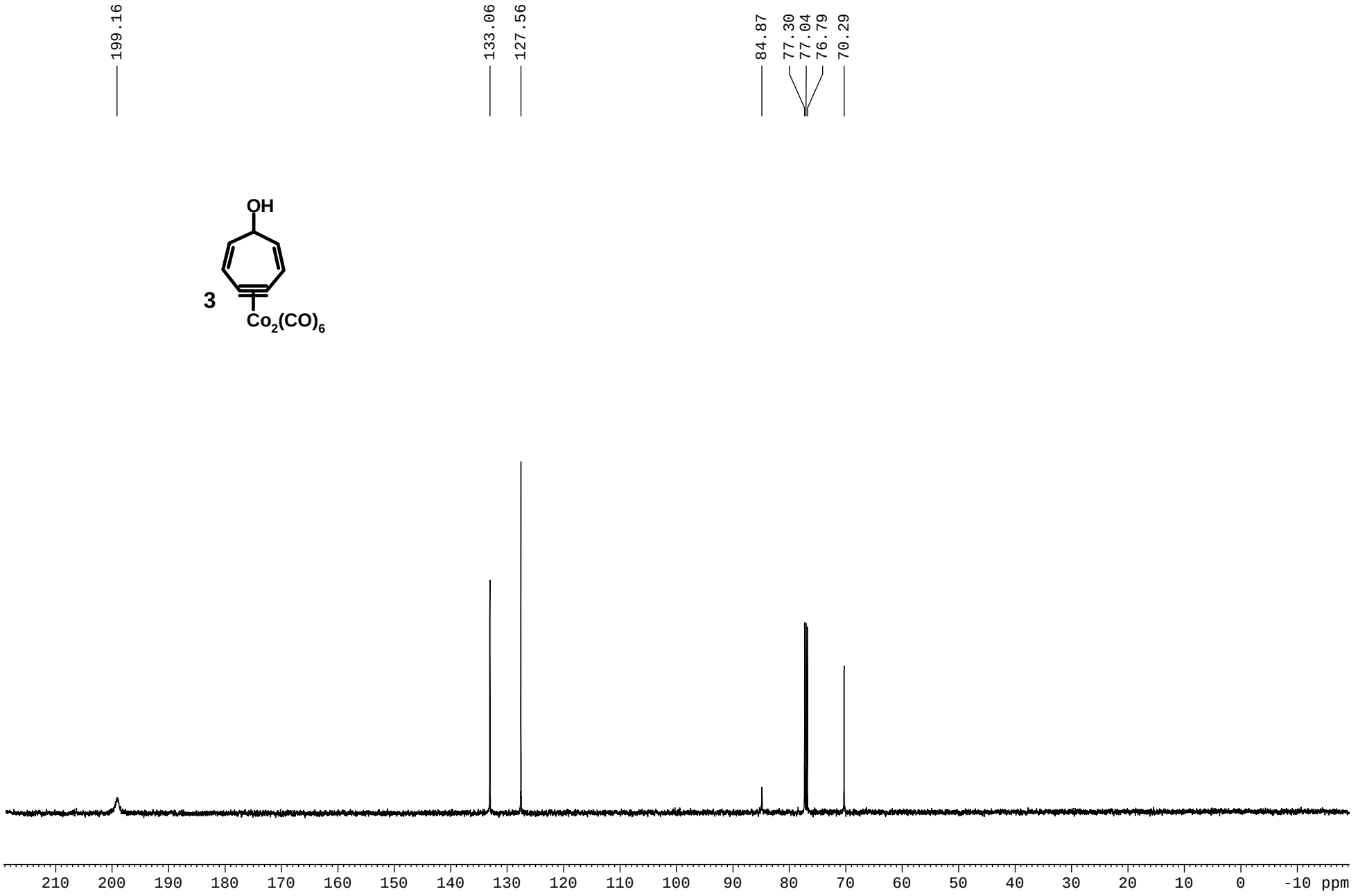


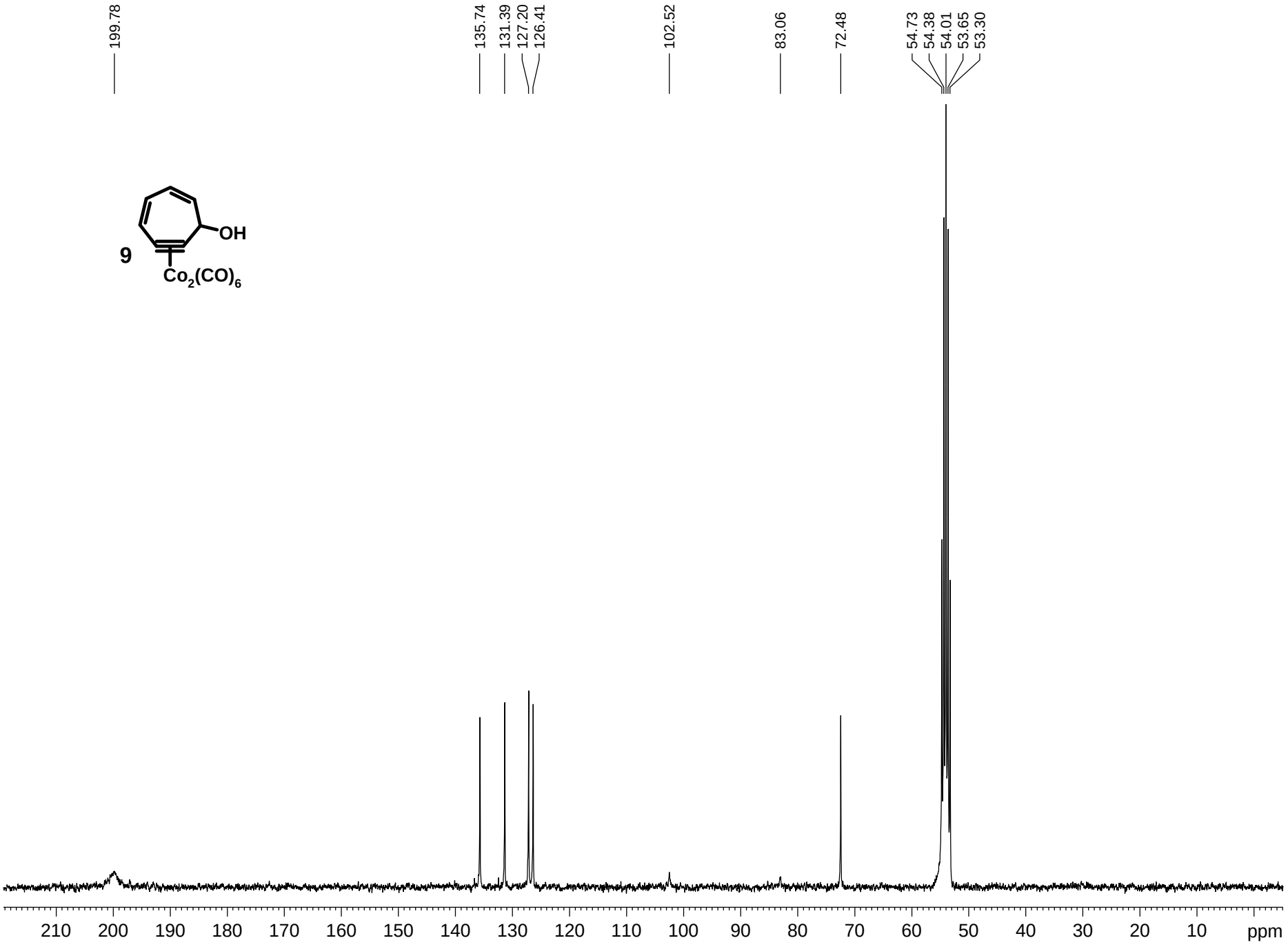
5

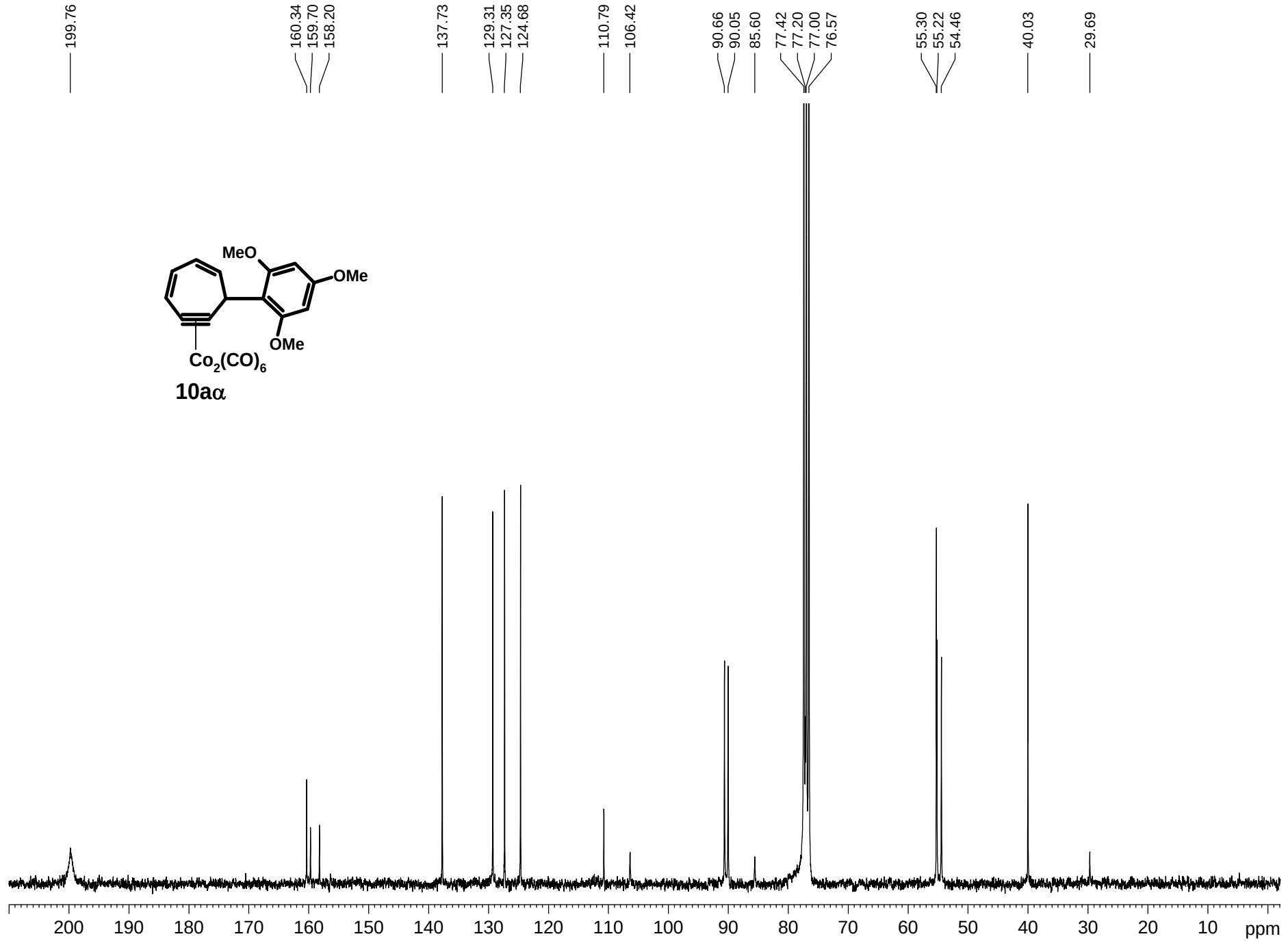


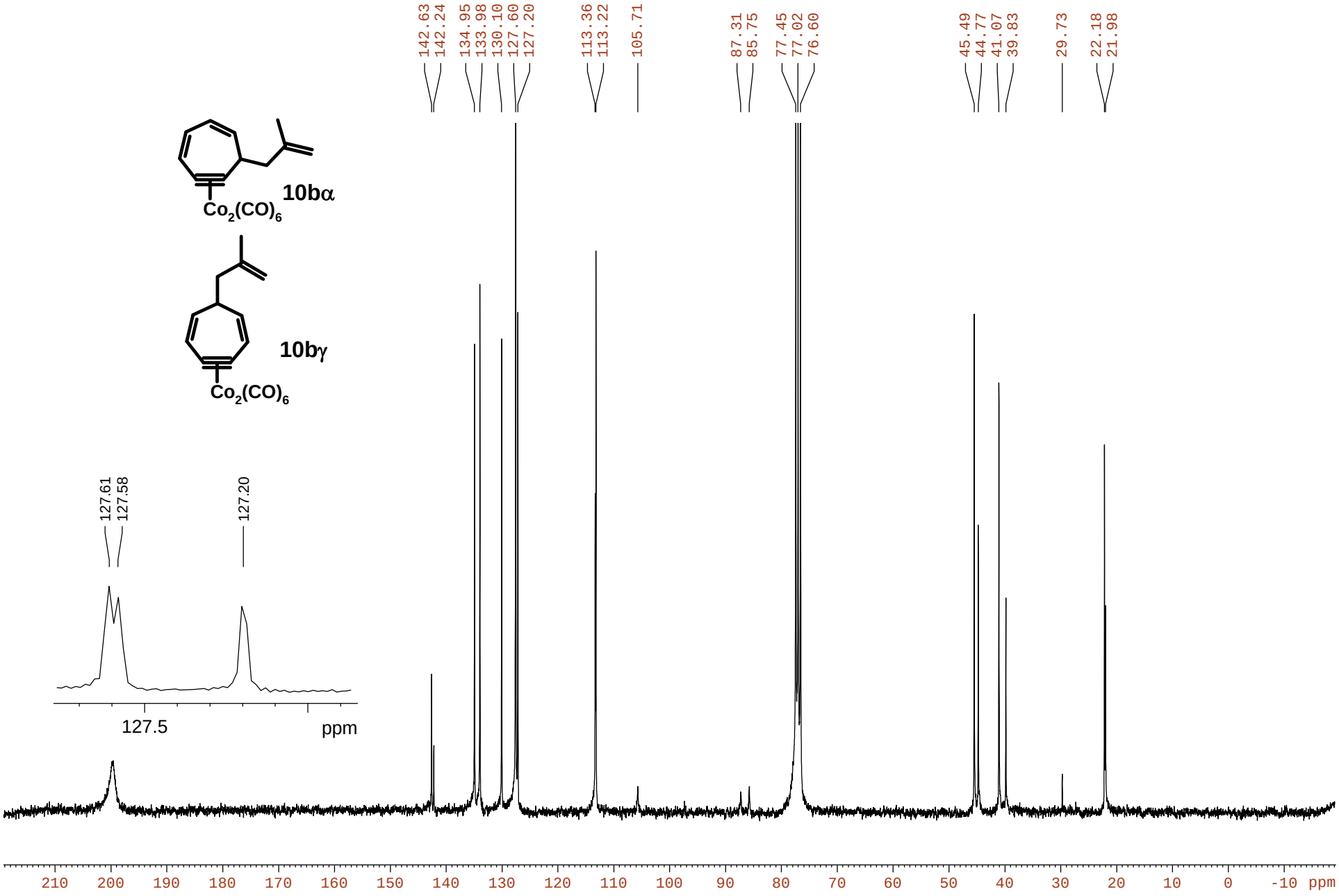

198.36
139.51
132.22
97.79
78.40
77.48
77.05
76.63
68.75
52.37
O
HO
7
Co2(CO)6
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
ppm

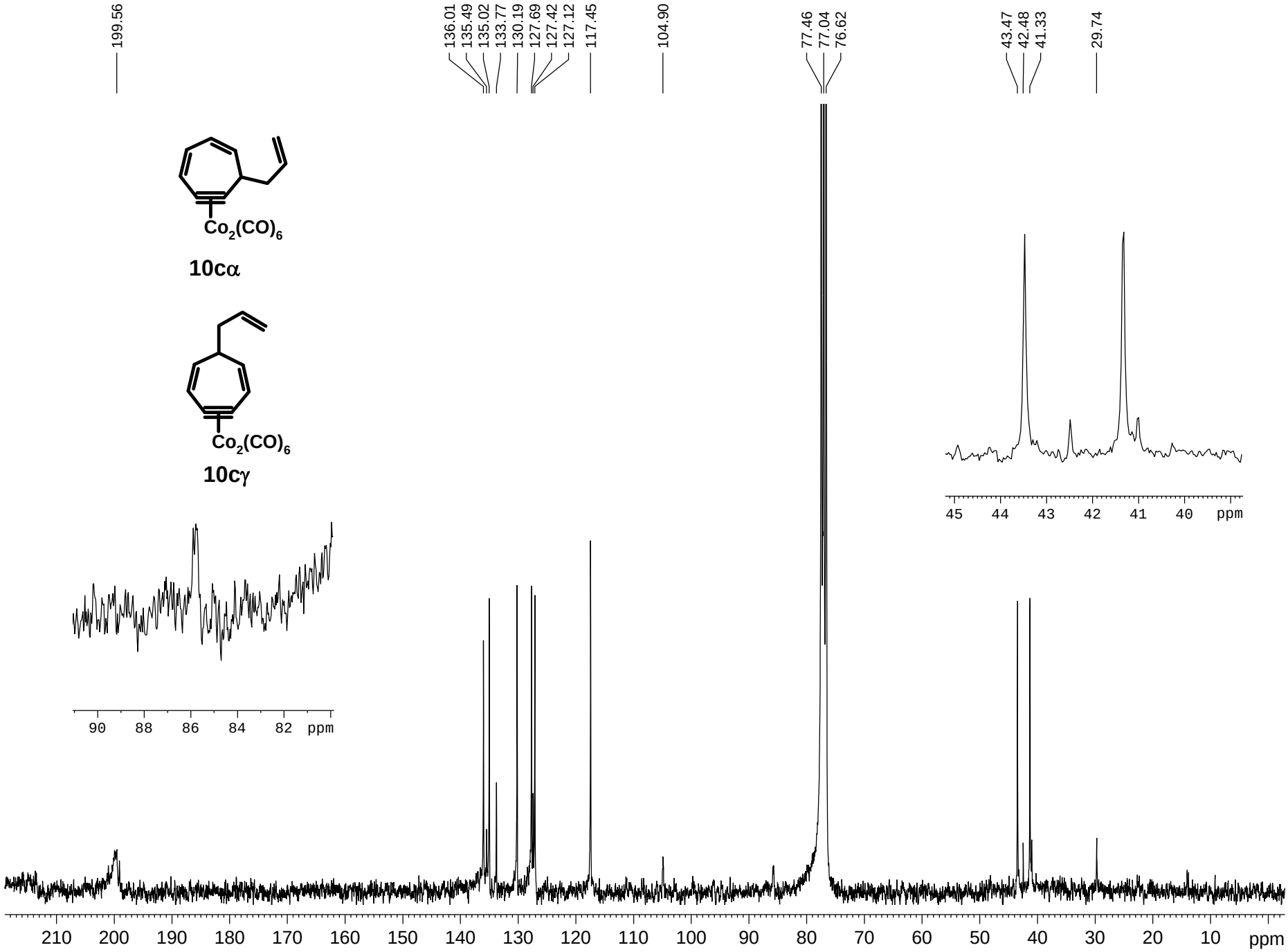

197.98
191.14
140.45
135.31
80.50
77.53
77.30
77.10
76.68
O
8
Co2(CO)6
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
ppm

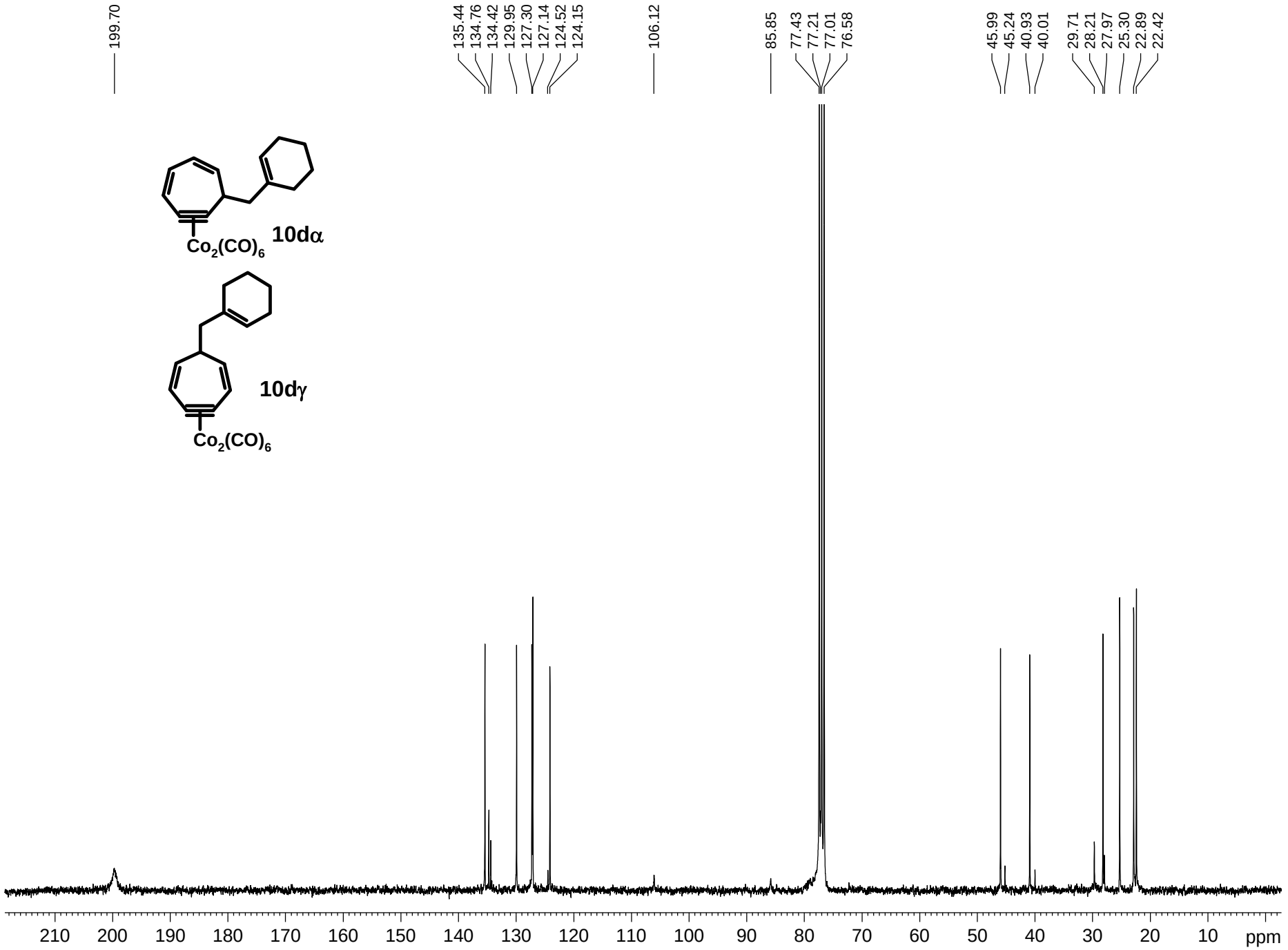

199.16
133.06
127.56
84.87
77.30
77.04
76.79
70.29
OH
3
Co2(CO)6
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10 ppm

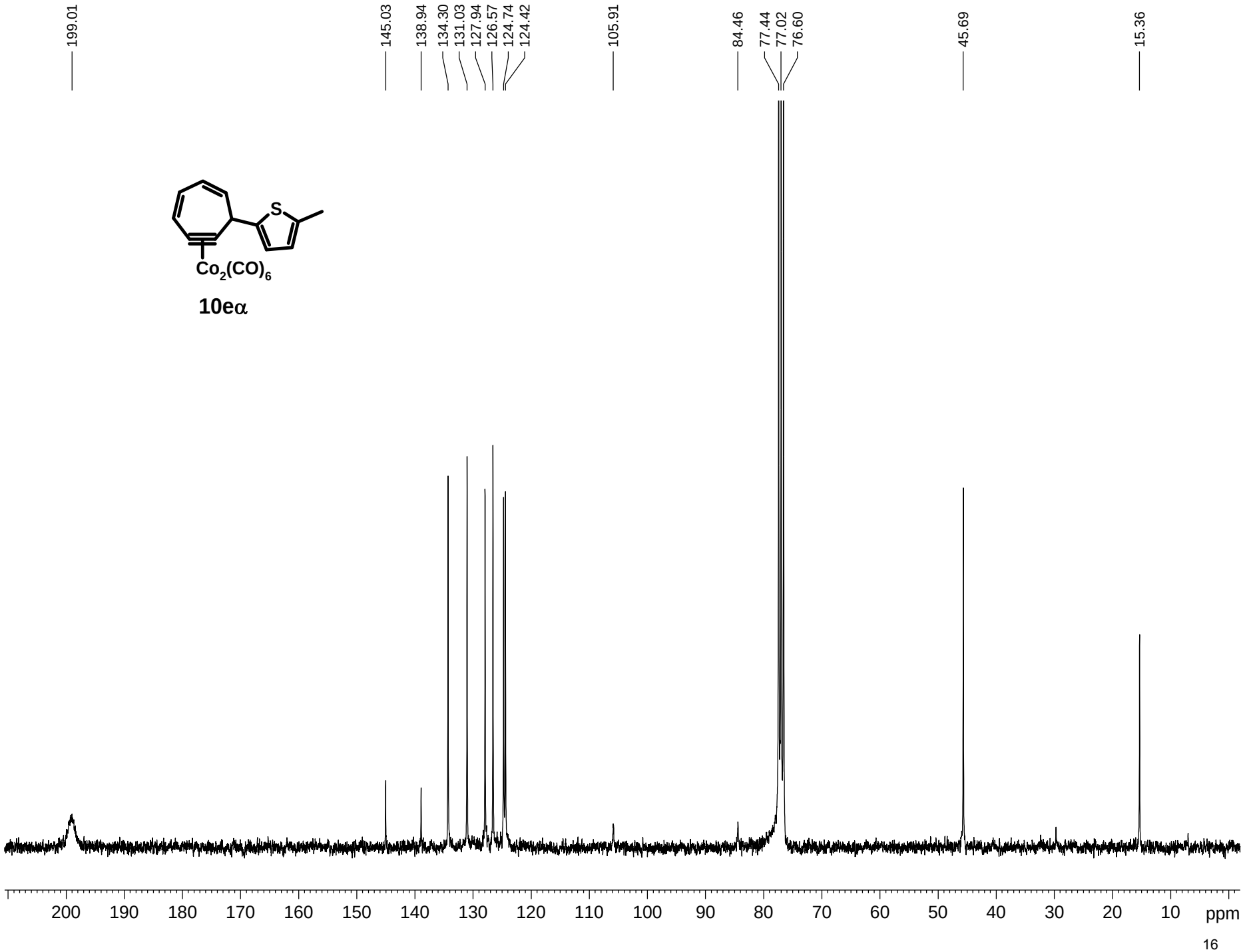

199.78
135.74
131.39
127.20
126.41
102.52
83.06
72.48
54.73
54.38
54.01
53.65
53.30
OH
9
Co2(CO)6
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

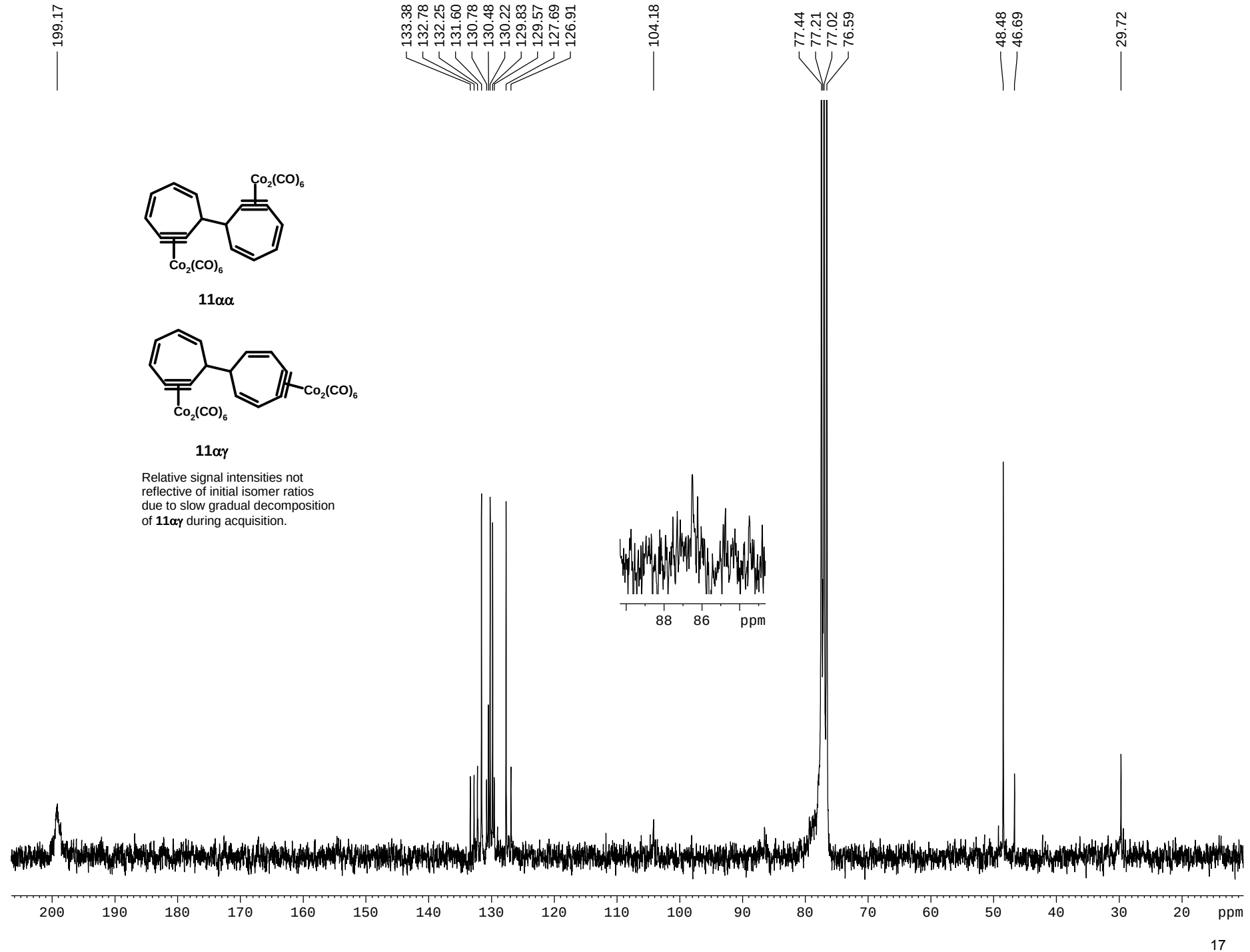

199.76
160.34
159.70
158.20
137.73
129.31
127.35
124.68
110.79
106.42
90.66
90.05
85.60
77.42
77.20
77.00
76.57
55.30
55.22
54.46
40.03
29.69
MeO
OMe
OMe
Co2(CO)6
10aα
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


142.63
142.24
134.95
133.98
130.10
127.60
127.20
113.36
113.22
105.71
87.31
85.75
77.45
77.02
76.60
45.49
44.77
41.07
39.83
29.73
22.18
21.98
10bα
Co2(CO)6
10bγ
Co2(CO)6
127.61
127.58
127.20
127.5
ppm
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
ppm


199.56
136.01
135.49
135.02
133.77
130.19
127.69
127.42
127.12
117.45
104.90
77.46
77.04
76.62
43.47
42.48
41.33
29.74
Co2(CO)6
10cα
Co2(CO)6
10cγ
90 88 86 84 82 ppm
45 44 43 42 41 40 ppm
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


199.70
135.44
134.76
134.42
129.95
127.30
127.14
124.52
124.15
106.12
85.85
77.43
77.21
77.01
76.58
45.99
45.24
40.93
40.01
29.71
28.21
27.97
25.30
22.89
22.42
Co2(CO)6
10dα
10dγ
Co2(CO)6
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


199.01
145.03
138.94
134.30
131.03
127.94
126.57
124.74
124.42
105.91
84.46
77.44
77.02
76.60
45.69
15.36
S
Co2(CO)6
10eα
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


199.17
133.38
132.78
132.25
131.60
130.78
130.48
130.22
129.83
129.57
127.69
126.91
104.18
77.44
77.21
77.02
76.59
48.48
46.69
29.72
Co2(CO)6
Co2(CO)6
11αα
Co2(CO)6
Co2(CO)6
11αγ
Relative signal intensities not reflective of initial isomer ratios due to slow gradual decomposition of 11αγ during acquisition.
88
86
ppm
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm