

Orthogonal Pd- and Cu-Based Catalyst Systems for the C- and N-Arylation of Oxindoles

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Supporting Information

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General Considerations.

All reactions were carried out in resealable test tubes with teflon septa under a dry argon or nitrogen atmosphere. Copper(I) iodide (98%) and Pd₂dba₃ were purchased from Strem. Copper(I) mesityl was prepared according to literature precedent and stored in a -20 °C freezer in a nitrogen-filled glovebox.ⁱ Diamine ligands were purchased from Aldrich and used without further purification. XPhos was generously provided by Saltigo. RuPhos was prepared according to literature precedent.ⁱⁱ Anhydrous K₂CO₃ (99%) and NaOt-Bu (98%) were purchased from Aldrich and stored under nitrogen in a Vacuum Atmospheres glovebox. Small portions (~5 g) were removed from the glovebox in glass vials, stored in the air in a desiccator filled with anhydrous calcium sulfate, and weighed in the air. Oxindoles were purchased from commercial sources and used without further purification. Aryl halides were purchased from commercial sources and, when necessary, filtered through neutral alumina or distilled. Anhydrous 1,4-dioxane was purchased from Aldrich in Sure-Seal® bottles. Anhydrous THF was purchased from J. T. Baker in CYCLE-TRAINER® solvent delivery kegs and vigorously purged with argon for 2 h. The solvent was further purified by passing it through two packed columns of neutral alumina under argon. The solvents were transferred by syringe from the solvent purification system or bottle to the reaction flask. Flash column chromatography was performed using a Biotage SP4 Flash Purification System using KP-Sil silica cartridges. In all cases, dichloromethane was used to transfer the crude reaction material onto the silica gel samplelet, which was subsequently air-dried before usage. A gradient elution technique was performed, based on the recommendation from the Biotage TLC Wizard. *In situ* monitoring of reactions using infrared spectroscopy was performed with a Mettler Toledo iC10 ReactIR instrument equipped with a C1Fiber with a diamond-tipped probe.

Yields reported in the publication are of the isolated material and represent an average of at least two independent runs. Yields reported in the supporting information refer to a single experiment.

Compounds described in the literature were characterized by comparing their ^1H NMR and ^{13}C NMR spectra, and melting points (m.p.) to the previously reported data; their purity was confirmed by gas chromatography (GC) or elemental analysis. GC analyses were performed on a Hewlett Packard 6890 instrument with an FID detector and a Hewlett Packard 10 m x 0.2 mm i.d. HP-1 capillary column using dodecane as an internal standard. Elemental analyses were performed by Atlantic Microlabs, Inc., Norcross, GA. Previously unknown compounds were synthesized, purified and analyzed from a single run and were then repeated to determine an average yield. They were characterized by ^1H NMR, ^{13}C NMR, m.p., IR and elemental analysis. For those compounds that did not give a satisfactory elemental analysis, a copy of their ^1H NMR spectra is included. ^1H NMR and ^{13}C NMR spectra were recorded on Varian 500 MHz instruments with chemical shifts reported relative to the deuterated solvent or TMS. IR spectra were recorded on a Perkin-Elmer System 2000 FT-IR instrument for all previously unknown compounds (KBr disc). Melting points (uncorrected) were obtained on a Mel-Temp II capillary melting point apparatus.

General procedure for the C-arylation of oxindoles

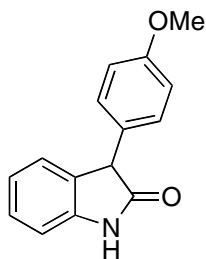
An oven-dried screw-cap test tube was charged with Pd_2dba_3 (0.010-0.020 mmol), XPhos (0.04-0.08 mmol), oxindole (1.00 mmol), aryl halide (1.20 mmol, if solid), K_2CO_3 (2.0 mmol), and a magnetic stir bar. The reaction vessel was fitted with a rubber septum. The test tube was evacuated and back-filled with dry argon twice. Aryl halide (1.20 mmol, if liquid), and solvent (0.50-1.0 mL) were then added successively. The rubber septum was removed and the reaction tube was quickly sealed with a Teflon-lined septum. The vessel was immersed in a pre-heated oil bath and stirred vigorously until TLC and/or GC analysis of the crude reaction mixture indicated that the limiting reagent had been completely consumed. The reaction mixture was cooled to room temperature, diluted with dichloromethane (15

mL), and filtered through a plug of celite, eluting with additional ethyl acetate (50 mL). The filtrate was concentrated and the resulting residue was purified by flash chromatography (hexanes/ethyl acetate or hexanes/dichloromethane) to provide the desired product.

General procedure for the *N*-arylation of oxindoles

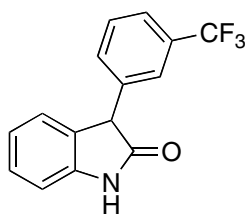
An oven-dried screw-cap test tube was charged with CuI (0.010-0.10 mmol), oxindole (1.00 mmol), aryl halide (1.20 mmol, if solid), K₂CO₃ (2.0 mmol), and a magnetic stir bar. The reaction vessel was fitted with a rubber septum. The test tube was evacuated and back-filled with dry argon. Aryl halide (1.20 mmol, if liquid), *rac-trans*-*N,N'*-dimethylcyclohexane-1,2-diamine (0.040-0.20 mmol) and 1,4-dioxane (0.50-1.0 mL) were then added successively. The rubber septum was removed and the reaction tube was quickly sealed with a Teflon-lined septum. The vessel was immersed in a pre-heated oil bath and stirred vigorously until TLC and/or GC analysis of the crude reaction mixture indicated that the limiting reagent had been completely consumed. The reaction mixture was cooled to room temperature, diluted with ethyl acetate (15 mL), and filtered through a plug of silica, eluting with additional ethyl acetate (50 mL). The filtrate was concentrated and the resulting residue was purified by flash chromatography (hexanes/ethyl acetate) to provide the desired product.

Experimental procedures for compounds in Table 1



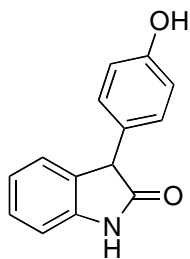
3-(4-methoxyphenyl)indolin-2-one (Entry 1)

The general procedure was followed using Pd₂dba₃ (9.1 mg, 0.010 mmol), XPhos (24 mg, 0.050 mmol), K₂CO₃ (0.28 g, 2.0 mmol), 4-chloroanisole (128 mg, 1.20 mmol), and oxindole (133 mg, 1.00 mmol) with THF (1.0 mL) as solvent for 24 h at 80 °C. Isolation and chromatographic purification (hexane / ethyl acetate) afforded the title compound as white solid (226 mg, 94%). ¹H NMR (500 MHz, CDCl₃) δ 9.53 (s, 1H), 7.25-6.86 (m, 8H), 4.60 (s, 1H), 3.80 (s, 3H). ¹³C NMR (125 MHz, CDCl₃) δ 179.7, 159.2, 142.0, 130.1, 129.7, 128.7, 128.5, 125.3, 122.8, 114.6, 110.3, 55.4, 52.2. m.p. 161-163 °C. (Lit. 163-165 °C).ⁱⁱⁱ



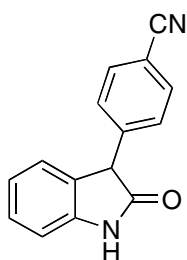
3-(3-(trifluoromethyl)phenyl)indolin-2-one (Entry 2)

The general procedure was followed using Pd₂dba₃ (9.1 mg, 0.010 mmol), XPhos (24 mg, 0.050 mmol), K₂CO₃ (0.28 g, 2.0 mmol), (136 μL, 1.00 mmol), and oxindole (146 mg, 1.10 mmol) with 1,4-dioxane (1.0 mL) as solvent for 24 h at 100 °C. Isolation and chromatographic purification (hexane / ethyl acetate) afforded the title compound as white solid (228 mg, 82 %). ¹H NMR (500 MHz, CDCl₃) δ 9.29 (s, 1H), 7.58 (d, 1H, *J* = 7.5 Hz), 7.52 (s, 1H), 7.47 (t, 1H, *J* = 7.8 Hz), 7.28 (td, 1H, *J* = 0.6 Hz, 7.8 Hz), 7.12 (d, 1H, *J* = 7.3 Hz), 7.07 (m, 1H), 6.96 (d, 1H, *J* = 7.9 Hz), 4.71 (s, 1H). ¹³C NMR (125 MHz, CDCl₃) δ 178.3, 141.9, 137.6, 132.2, 131.4, 129.6, 129.0, 128.7, 128.1, 125.5, 125.4, 124.8, 123.2, 110.6, 52.5. IR (KBr disc, cm⁻¹) 3226, 1712, 1621, 1472, 1332, 1221, 1167, 1127, 1075, 751, 700, 671, 592. Anal. Calc. for C₁₅H₁₀F₃NO: C 64.98, H 3.64. Found: C 65.08, H 3.89. m.p. 169-171 °C.



3-(4-hydroxyphenyl)indolin-2-one (Entry 3)

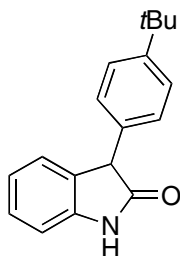
The general procedure was followed using Pd_2dba_3 (9.1 mg, 0.010 mmol), XPhos (24 mg, 0.050 mmol), K_2CO_3 (0.42 g, 3.0 mmol), (129 mg, 1.00 mmol), and oxindole (160 mg, 1.20 mmol) with 1,4-dioxane (1.0 mL) as solvent for 24 h at 100 °C. After cooling to room temperature, the reaction mixture was dissolved in 2M HCl (5mL) and extracted with EtOAc (3 x 15 mL). The combined organic fractions were dried over MgSO_4 and concentrated. The residue was stirred in 5 mL CH_2Cl_2 to dissolve the soluble impurities. The product was then isolated by filtration and washed with hexane to provide the title compound as an orange solid (240 mg, 90%). ^1H NMR (500 MHz, CD_3OD) δ 7.13 (tt, 1H, J = 0.9, 7.6 Hz), 6.98 (m, 1H), 6.92-6.89 (m, 3H), 6.85 (d, 1H, J = 7.8 Hz), 6.67-6.89 (m, 2H), 3.27 (s, 1H). ^{13}C NMR (125 MHz, CD_3OD) δ 180.7, 157.3, 143.0, 131.4, 130.3, 128.9, 128.5, 125.7, 123.3, 116.4, 110.6, 54.4. IR (KBr disc, cm^{-1}) 3266, 1700, 1616, 1559, 1541, 1512, 1471, 1219, 824, 751. m.p. 234-239 °C.



4-(2-oxoindolin-3-yl)benzonitrile (Entry 4)

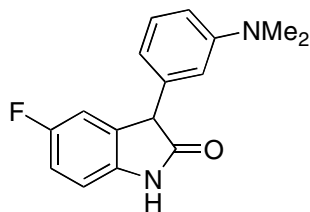
The general procedure was followed using Pd_2dba_3 (9.1 mg, 0.010 mmol), XPhos (24 mg, 0.050 mmol), K_2CO_3 (0.28 g, 2.0 mmol), 4-chlorobenzonitrile (166 mg, 1.20 mmol), oxindole (133 mg, 1.00 mmol), and 200 mg flame activated 4Å mol sieves with THF (1.0 mL) as solvent for 24 h at 80 °C. Isolation and

chromatographic purification (hexane / ethyl acetate) afforded the title compound as white solid (135 mg, 58 %). ^1H NMR (500 MHz, CDCl_3) δ 9.29 (s, 1H), 7.66-7.64 (m, 2H), 7.38-7.36 (m, 2H), 7.31-7.28 (m, 1H), 7.12-7.06 (m, 2H), 6.97 (d, 1H, $J = 7.8$ Hz), 4.71 (s, 1H). ^{13}C NMR (125 MHz, CDCl_3) δ 177.7, 141.9, 132.9, 129.5, 129.2, 128.2, 125.4, 124.7, 123.3, 118.7, 111.8, 110.6, 52.7. IR (KBr disc, cm^{-1}) 3250 (br), 2230, 1711, 1620, 1471, 1328, 1219, 1097, 1019, 914, 818, 752, 678. m.p. 176-178 °C.



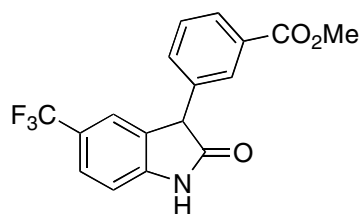
3-(4-*tert*-butylphenyl)indolin-2-one (Entry 5)

The general procedure was followed using Pd_2dba_3 (9.1 mg, 0.010 mmol), XPhos (24 mg, 0.050 mmol), K_2CO_3 (0.28 g, 2.0 mmol), 4-*t*-butyl-4-methylbenzenesulfonate (334 mg, 1.10 mmol), and oxindole (133 mg, 1.00 mmol) with *t*-BuOH (1.0 mL) as solvent for 24 h at 80 °C. Isolation and chromatographic purification (hexane / ethyl acetate) afforded the title compound as white solid (164 mg, 64%). ^1H NMR (500 MHz, CDCl_3) δ 9.21 (s, 1H), 7.38-7.35 (m, 2H), 7.23 (t, 1H, $J = 7.8$ Hz), 7.21-7.13 (m, 3H), 7.02, (1H, td, $J = 7.9, 1.0$ Hz) 6.88 (d, 1H, 7.8 Hz), 4.62 (s, 1H), 1.31 (s, 9H). ^{13}C NMR (125 MHz, CDCl_3) δ 150.6, 141.9, 133.5, 130.0, 128.5, 128.2, 126.1, 125.4, 122.8, 110.2, 52.4, 34.9, 31.5. IR (KBr disc, cm^{-1}) 3211 (br), 2963, 1709, 1620, 1515, 1471, 1328, 1269, 1220, 1018, 910, 818, 751, 677, 564. m.p. 170-172 °C.



3-(3-(Dimethylamino)phenyl)-5-fluoroindolin-2-one (Entry 6)

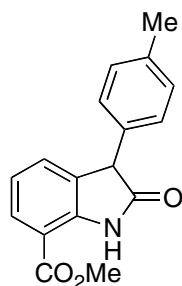
The general procedure was followed using Pd₂dba₃ (9.1 mg, 0.010 mmol), XPhos (24 mg, 0.050 mmol), K₂CO₃ (0.28 g, 2.0 mmol), (171 mg, 1.10 mmol), and 5-fluorooxindole (157 mg, 1.00 mmol) with 1,4-dioxane (1.0 mL) as solvent for 24 h at 100 °C. Isolation and chromatographic purification (hexane / ethyl acetate) afforded the title compound as white solid (203 mg, 75 %). ¹H NMR (500 MHz, CDCl₃) δ 9.44 (s, 1H), 7.22 (dd, 1H, *J* = 7.5, 8.2 Hz), 6.94-6.82 (m, 3H), 6.69 (dd, 1H, *J* = 2.3, 5.9 Hz), 6.56 (t, 1H, *J* = 1.6 Hz), 6.50 (d, 1H, *J* = 7.6 Hz), 4.57, (s, 1H), 2.94 (s, 6H). ¹³C NMR (125 MHz, CDCl₃) δ 180.0, 159.8, 151.7, 138.4, 137.4, 132.4, 132.3, 130.4, 116.9, 115.3, 113.7, 113.1, 112.7, 111.3, 54.4, 41.2. IR (KBr disc, cm⁻¹) 3219 (br), 3085, 2877, 2808, 1712, 1601, 1501, 1486, 1356, 1302, 1231, 1194, 1126, 999, 910, 815, 761, 732, 694, 592. Anal. Calc. for C₁₆H₁₅FN₂O: C 71.10, H 5.59. Found: C 70.87, H 5.61. m.p. 126-128 °C.



Methyl 3-(2-oxo-5-(trifluoromethyl)indolin-3-yl)benzoate (Entry 7)

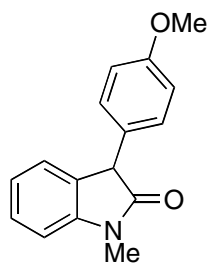
The general procedure was followed using Pd₂dba₃ (9.1 mg, 0.010 mmol), XPhos (24 mg, 0.050 mmol), K₂CO₃ (0.28 g, 2.0 mmol), methyl 3-chlorobenzoate (153 μL, 1.10 mmol), and 5-trifluoromethyloxindole (120 mg, 1.00 mmol) with THF (2.0 mL) as solvent for 24 h at 80 °C. Isolation and chromatographic purification (dichloromethane / ethyl acetate, 1:0 → 9:1) afforded the title compound as a slightly yellow foam (265 mg, 79%). ¹H NMR (500 MHz, CDCl₃) δ 9.94 (s, 1H), 8.01 (dt, 1H, *J* = 1.4, 7.8 Hz), 7.92 (t, 1H, *J* = 1.7 Hz), 7.52 (dt, 1H, *J* = 0.9, 8.2 Hz), 7.45 (m, 1H), 7.39 (dt, 1H, *J* = 1.4, 7.6 Hz), 7.34 (s, 1H), 7.01 (d, 1H, *J* = 8.2 Hz), 4.74 (s, 1H), 3.90 (s, 3H). ¹³C NMR (125 MHz, CDCl₃) δ 178.9, 166.8, 145.0, 136.0, 133.1, 131.3, 129.9, 129.8, 129.6, 129.5, 126.6, 125.6, 122.3, 121.8, 110.5, 52.5, 36.3. IR (KBr disc, cm⁻¹) 3256, 2957, 1722, 1631, 1499, 1415, 1330, 1303,

1264, 1221, 1159, 1117, 1060, 910, 829, 732, 695, 635, 543. m.p. 132-136 °C.



methyl 2-oxo-3-*p*-tolylindoline-7-carboxylate (Entry 8)

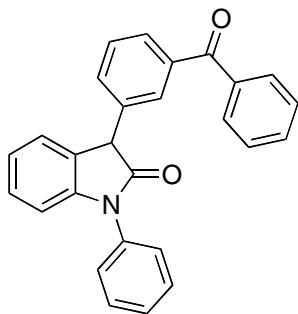
The general procedure was followed using Pd₂dba₃ (9.1 mg, 0.010 mmol), XPhos (24 mg, 0.050 mmol), K₂CO₃ (0.28 g, 2.0 mmol), 4-chlorotoluene (130 µL, 1.10 mmol), and methyl oxindole-7-carboxylate (191 mg, 1.00 mmol) with THF (2.0 mL) as solvent for 24 h at 80 °C. Isolation and chromatographic purification (hexane / ethyl acetate) afforded the title compound as a white solid (160 mg, 57%). ¹H NMR (500 MHz, CDCl₃) δ 9.22 (s, 1H), 7.86 (dt, 1H, *J* = 0.9, 8.1 Hz.), 7.29 (dd, 1H, *J* = 0.5, 7.3 Hz), 7.16 (d, 2H, *J* = 7.9 Hz), 7.01-7.03 (m, 3H), 4.60 (s, 1H), 3.96 (s, 3H), 2.34 (s, 3H). ¹³C NMR (125 MHz, CDCl₃) δ 177.4, 166.6, 144.3, 137.7, 133.0, 131.1, 129.9, 129.8, 129.2, 128.4, 122.1, 111.6, 52.4, 51.5, 21.3. IR (KBr disc, cm⁻¹) 3267 (br), 3024, 3004, 2952, 1707, 1608, 1514, 1454, 1430, 1312, 1285, 1198, 1133, 1060, 993, 941, 916, 804, 774, 753, 737, 661, 496, 460. m.p. 155-163 °C.



3-(4-methoxyphenyl)-1-methylindolin-2-one (Entry 9)

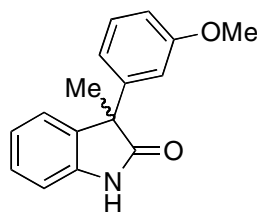
The general procedure was followed using Pd₂dba₃ (9.1 mg, 0.010 mmol), XPhos (24 mg, 0.050 mmol), K₂CO₃ (0.28 g, 2.0 mmol), 4-chloroanisole (134 µL, 1.00 mmol), and 1-methyl oxindole (147 mg, 1.10 mmol) with THF (1.0 mL) as solvent for 24 h at 80 °C. Isolation and chromatographic purification

(hexane / ethyl acetate) afforded the title compound as white solid (201 mg, 79%). ^1H NMR (500 MHz, CDCl_3) δ 7.34 (tt, 1H, J = 0.8, 7.6 Hz), 7.20-7.12 (m, 4H), 7.08 (dt, 1H, J = 0.8, 8.5 Hz), 9.91-6.81 (m, 3H), 4.57 (s, 1H), 3.79 (s, 3H), 3.26 (s, 3H). ^{13}C NMR (125 MHz, CDCl_3) δ 176.5, 159.2, 144.6, 129.6, 129.2, 128.8, 128.5, 125.2, 122.8, 114.5, 108.3, 55.5, 51.4, 26.6. Anal. Calc. for $\text{C}_{16}\text{H}_{15}\text{NO}_2$: C 75.97, H 5.97. Found: C 75.58, H 6.00. m.p. 85-88 °C. (Lit. 90-91°C).^{iv}



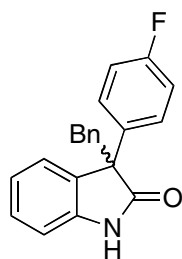
1-phenyl-3-(3-(phenylcarbonyl)phenyl)indolin-2-one (Entry 10)

The general procedure was followed using Pd_2dba_3 (9.1 mg, 0.010 mmol), XPhos (24 mg, 0.050 mmol), K_3PO_4 (0.42 g, 2.0 mmol), 3-chlorobenzophenone (217 mg, 1.00 mmol), and 1-phenyloxindole (251 mg, 1.20 mmol) with 1,4-dioxane (1.0 mL) as solvent for 24 h at 80 °C. Isolation and chromatographic purification (hexane / ethyl acetate) afforded the title compound as white solid (341 mg, 88 %). ^1H NMR (500 MHz, CDCl_3) δ 7.95-7.81 (m, 3H), 7.75 (dt, 1H, J = 1.6, 7.4 Hz), 7.62-7.41 (m, 10H), 7.30-7.25 (m, 2H), 7.12 (td, 1H, J = 0.8, 7.5 Hz), 6.90 (d, 1H, J = 7.8 Hz), 4.89 (s, 1H). ^{13}C NMR (125 MHz, CDCl_3) δ 196.5, 175.0, 144.6, 138.3, 137.5, 137.3, 134.5, 132.7, 132.6, 130.4, 130.3, 129.8, 129.7, 129.0, 128.8, 128.5, 128.4, 128.1, 126.8, 125.5, 123.5, 109.9, 52.1. IR (KBr disc, cm^{-1}) 1722, 1658, 1612, 1596, 1500, 1465, 1369, 1320, 1283, 1219, 1176, 911, 754, 722, 714, 698, 603. Anal. Calc. for $\text{C}_{27}\text{H}_{19}\text{NO}_2$: C 83.27, H 4.92. Found: C 83.62, H 4.92. m.p. 133-135 °C.



3-(3-methoxyphenyl)-3-methylindolin-2-one (Entry 11)

The general procedure was followed using Pd_2dba_3 (9.1 mg, 0.010 mmol), RuPhos (23 mg, 0.050 mmol), NaOt-Bu (0.20 g, 2.0 mmol), 3-bromoanisole (152 μL , 1.20 mmol), and 3-methyloxindole (146 mg, 1.00 mmol) with toluene (1.0 mL) as solvent for 9 h at 100 °C. Isolation and chromatographic purification (CH_2Cl_2 / ethyl acetate) afforded the title compound as yellow solid (228 mg, 90 %). ^1H NMR (500 MHz, CDCl_3) δ 9.60 (s, 1H), 7.26-7.20 (m, 2H), 7.13 (td, 1H, $J = 0.6, 7.5$ Hz), 7.04 (td, 1H, $J = 0.9, 7.65$ Hz), 7.697 (d, 1H, $J = 7.6$ Hz), 6.93-6.90 (m, 2H), 6.81 (ddd, 1H, $J = 0.9, 2.5, 8.2$ Hz), 3.77 (s, 3H), 1.83 (s, 3H). ^{13}C NMR (125 MHz, CDCl_3) δ 174.0, 159.7, 143.9, 143.6, 129.7, 129.4, 128.0, 128.0, 120.1, 113.1, 112.5, 55.3, 43.3, 37.9, 20.4. IR (KBr disc, cm^{-1}) 3215, 1710, 1618, 1599, 1485, 1472, 1372, 1324, 1259, 1204, 1167, 1118, 1043, 912, 754, 696, 660. m.p. 131-133 °C.

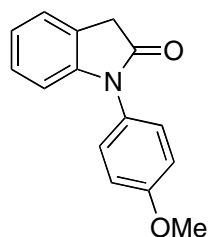


3-(4-fluorophenyl)-3-benzylindolin-2-one (Entry 12)

The general procedure was followed using Pd_2dba_3 (9.1 mg, 0.010 mmol), RuPhos (19 mg, 0.040 mmol), NaOt-Bu (0.20 g, 2.0 mmol), 1-bromo-3-fluorobenzene (132 μL , 1.20 mmol), and 3-benzyloxindole (223 mg, 1.00 mmol) with toluene (1.0 mL) as solvent for 20 h at 100 °C. Isolation and chromatographic purification (hexane / ethyl acetate) afforded the title compound as yellow solid (253 mg, 80 %). ^1H NMR (500 MHz, CDCl_3) δ 8.18 (bs 1H), 7.49-7.42 (m, 2H), 7.20-7.15 (m, 2H), 7.10-

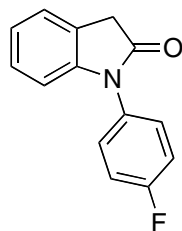
6.88 (m, 5H), 6.86-6.63 (m, 2H), 6.73-6.70 (m, 2H), 3.66 (d, 1H, $J = 12.8$ Hz), 3.44 (d, 1H, $J = 12.8$ Hz). ^{13}C NMR (125 MHz, CDCl_3) δ 180.3, 164.0, 141.0, 135.5, 131.7, 130.2, 129.1, 129.1, 128.6, 127.8, 126.9, 126.0, 122.5, 115.8, 110.2, 58.2, 44.0. IR (KBr disc, cm^{-1}) 3198, 1697, 1617, 1507, 147, 1225, 1201, 1163, 1014, 855, 815, 754, 697. m.p. 189-191 °C.

Experimental procedures for compounds in Table 2



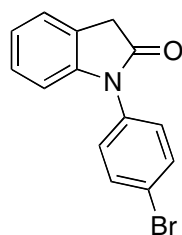
1-(4-methoxyphenyl)indolin-2-one (Entry 1)

The general procedure was followed using CuI (9.5 mg, 0.050 mmol), *rac-trans-N,N'*-dimethylcyclohexane-1,2-diamine (16 μL , 0.10 mmol), K_2CO_3 (0.28 g, 2.0 mmol), 4-iodoanisole (234 mg, 1.00 mmol), and oxindole (160 mg, 1.20 mmol) with 1,4-dioxane (1.0 mL) as solvent for 24 h at 100 °C. Isolation and chromatographic purification (hexane / ethyl acetate) afforded the title compound as white solid (204 mg, 85%). ^1H NMR (500 MHz, CDCl_3) δ 7.33-7.30 (m, 3H), 7.21 (td, $J = 1.2, 7.8$ Hz), 7.09-7.04 (m, 3H), 6.74 (dd, 1H, $J = 0.3, 7.9$ Hz), 3.87 (s, 3H), 2.71 (s, 2H). ^{13}C NMR (125 MHz, CDCl_3) δ 174.9, 159.3, 145.88, 128.1, 127.9, 127.2, 124.7, 124.4, 122.8, 115.9, 109.4, 55.7, 36.1. Anal. Calc. for $\text{C}_{15}\text{H}_{13}\text{NO}_2$: C 75.30, H 5.48. Found: C 75.17, H 5.41. m.p. 131-132 °C. (Lit. 118-122 °C).^v



1-(4-fluorophenyl)indolin-2-one (Entry 2)

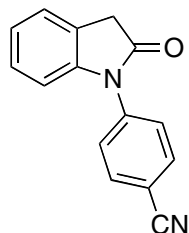
The general procedure was followed using CuI (1.9 mg, 0.010 mmol), *rac-trans-N,N'*-dimethylcyclohexane-1,2-diamine (6.4 μ L, 0.040 mmol), K₂CO₃ (0.28 g, 2.0 mmol), 4-fluoriodobenzene (115 μ L, 1.00 mmol), and oxindole (160 mg, 1.20 mmol) with 1,4-dioxane (1.0 mL) as solvent for 24 h at 100 °C. Isolation and chromatographic purification (hexane / ethyl acetate) afforded the title compound an orange solid (221 mg, 97 %). ¹H NMR (500 MHz, CDCl₃) δ 7.42-7.39 (m, 2H), 7.34-7.32 (m, 1H), 7.25-7.21 (m, 2H), 7.10 (td, 1H, *J* = 0.9, 7.3 Hz), 6.75 (dd, *J* = 0.5, 7.9 Hz), 3.72 (s, 2H). ¹³C NMR (125 MHz, CDCl₃) δ 174.7, 163.0, 161.1, 145.3, 128.7, 128.0, 124.9, 123.1, 116.9, 116.8, 109.4, 36.1. IR (KBr disc, cm⁻¹) 1710, 1612, 1602, 1512, 1481, 1461, 1371, 1322, 1244, 1222, 1201, 1174, 1100, 952, 840, 814, 746. Anal. Calc. for C₁₄H₁₀FNO: C 74.00, H 4.44. Found: C 73.68, H 4.37. m.p. 129-132 °C.



1-(4-bromophenyl)indolin-2-one (Entry 3)

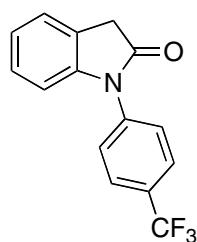
The general procedure was followed using CuI (9.5 mg, 0.050 mmol), *rac-trans-N,N'*-dimethylcyclohexane-1,2-diamine (16 μ L, 0.10 mmol), K₂CO₃ (0.28 g, 2.0 mmol), 1-bromo-4-iodobenzene (340 mg, 1.20 mmol), and oxindole (133 mg, 1.00 mmol) with 1,4-dioxane (1.0 mL) as solvent for 24 h at 40 °C. Isolation and chromatographic purification (hexane / ethyl acetate) afforded the title compound as white solid (148 mg, 57%). ¹H NMR (500 MHz, CDCl₃) δ 7.67-7.65 (m, 2H), 7.33-7.30 (m, 2H), 7.25-7.18 (m, 2H), 7.10 (t, 1H, *J* = 7.6 Hz), 6.81 (d, 1H, *J* = 7.8 Hz), 3.72 (s, 2H). ¹³C NMR (125 MHz, CDCl₃) δ 174.3, 144.7, 138.9, 133.0, 128.3, 128.0, 124.9, 124.4, 123.2, 121.8, 109.4, 36.1. IR (KBr disc, cm⁻¹) 1722, 1612, 1493, 1464, 1370, 1324, 1240, 1172, 1094, 1070, 1012,

821, 751, 673. m.p. 115-117 °C.



4-(2-oxoindolin-1-yl)benzonitrile (Entry 4)

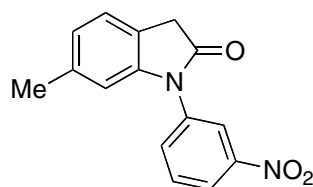
The general procedure was followed using CuI (9.5 mg, 0.050 mmol), *rac-trans-N,N'*-dimethylcyclohexane-1,2-diamine (16 μ L, 0.10 mmol), K₂CO₃ (0.28 g, 2.0 mmol), 4-iodobenzonitrile (343 mg, 1.20 mmol), oxindole (133 mg, 1.00 mmol) and 200 mg 4Å flame activated mol sieves with 1,4-dioxane (1.0 mL) as solvent for 24 h at 80 °C. Isolation and chromatographic purification (hexane / ethyl acetate) afforded the title compound as white solid (167 mg, 71%). ¹H NMR (500 MHz, CDCl₃) δ 7.85-7.82 (m, 2H), 7.64-7.61 (m, 2H), 7.37-7.34 (m, 1H), 7.26 (td, 1H, *J* = 1.3, 8.0 Hz), 7.14 (td, 1H, *J* = 0.9 7.5, Hz), 6.90 (dd, 1H, *J* = 0.5, 8.0 Hz), 3.776 (s, 2H). ¹³C NMR (125 MHz, CDCl₃) δ 174.1, 143.7, 138.8, 133.7, 128.1, 126.9, 125.2, 124.4, 123.8, 118.4, 111.4, 109.5, 39.7. IR (KBr disc, cm⁻¹) 2231, 1714, 1607, 1513, 1463, 1365, 1242, 1167, 743, 630. m.p. 190-192 °C.



1-(4-(trifluoromethyl)phenyl)indolin-2-one (Entry 5)

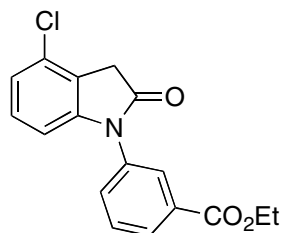
The general procedure was followed using CuI (1.9 mg, 0.010 mmol), *rac-trans-N,N'*-dimethylcyclohexane-1,2-diamine (6.4 μ L, 0.04 mmol), K₂CO₃ (0.28 g, 2.0 mmol), 4-iodobenzotrifluoride (176 μ L, 1.20 mmol), and oxindole (133 mg, 1.00 mmol) with 1,4-dioxane (1.0 mL) as solvent for 24 h at 100 °C. Isolation and chromatographic purification (hexane / ethyl acetate)

afforded the title compound as white solid (242 mg, 87%). ^1H NMR (500 MHz, CDCl_3) δ 7.81 (d, 2H, J = 8.3 Hz), 7.61 (d, 2H, J = 8.2 Hz), 7.36 (dd, 1H, J = 0.5, 7.3 Hz), 7.26 (td, 1H, J = 1.0, 7.7 Hz), 7.14 (td, 1H, J = 0.8, 7.5 Hz), 6.88 (d, 1H, J = 8.0 Hz), 3.76 (s, 2H). ^{13}C NMR (125 MHz, CDCl_3) δ 174.3, 144.2, 137.9, 129.9, 128.0, 127.0, 126.9, 126.8, 125.1, 124.4, 123.5, 109.5, 36.1. IR (KBr disc, cm^{-1}) 1724, 1613, 1483, 1370, 1324, 1240, 1169, 1123, 1068, 1019, 750. Anal. Calc. for $\text{C}_{15}\text{H}_{10}\text{F}_3\text{NO}$: C 64.98, H 3.64. Found: C 64.83, H 3.57. m.p. 125-125 °C.



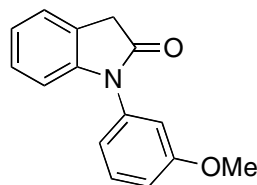
6-methyl-1-(3-nitrophenyl)indolin-2-one (Entry 6)

The general procedure was followed using CuI (9.5 mg, 0.050 mmol), *rac-trans-N,N'*-dimethylcyclohexane-1,2-diamine (16 μL , 0.10 mmol), K_2CO_3 (0.28 g, 2.0 mmol), 3-iodonitrobenzene (275 mg, 1.1 mmol), and 6-methyloxindole (147 mg, 1.00 mmol) with 1,4-dioxane (0.5 mL) as solvent for 24 h at 80 °C. Isolation and chromatographic purification (hexane / ethyl acetate) afforded the title compound as red/brown solid (196 mg, 73%). ^1H NMR (500 MHz, CDCl_3) δ 8.35-8.32 (m, 2H), 7.84-7.77 (m, 2H), 7.65 (d, 1H, J = 7.7 Hz), 7.07-7.04 (m, 1H), 6.75 (s, 1H), 2.43 (s, 3H). ^{13}C NMR (125 MHz, CDCl_3) δ 181.1, 157.9, 151.5, 150.8, 149.3, 134.4, 132.4, 131.2, 126.4, 123.6, 121.2, 115.77, 111.8, 39.8, 17.1. IR (KBr disc, cm^{-1}) 3093, 2922, 2865, 1728, 1626, 1533, 1369, 1352, 1242, 1179, 1112, 912, 805, 738, 690, 602. m.p. 170-180 °C (dec.).



methyl 3-(4-chloro-2-oxoindolin-1-yl)benzoate (Entry 7)

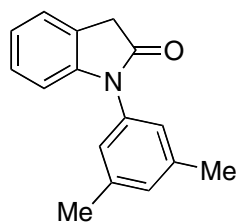
The general procedure was followed using CuI (9.5 mg, 0.050 mmol), *rac-trans-N,N'*-dimethylcyclohexane-1,2-diamine (16 μ L, 0.10 mmol), K₂CO₃ (0.28 g, 2.0 mmol), ethyl 3-iodobenzoate (202 μ L, 1.20 mmol), and 4-chlorooxindole (168 mg, 1.00 mmol) with 1,4-dioxane (0.5 mL) as solvent for 24 h at 80 °C. Isolation and chromatographic purification (hexane / ethyl acetate) afforded the title compound as white solid (276 mg, 88 %). ¹H NMR (500 MHz, CDCl₃) δ 8.13-8.08 (m, 2H), 7.65-7.60 (m, 2H), 7.17 (tt, 1H, *J* = 0.8, 8.0 Hz), 7.09 (dd, 1H, *J* = 0.8, 8.2 Hz), 6.68 (dd, 1H, *J* = 0.5, 7.9 Hz), 4.40 (q, 2H, *J* = 7.1 Hz), 3.73 (s, 2H), 1.40 (t, 3H, *J* = 7.1 Hz). ¹³C NMR (125 MHz, CDCl₃) δ 173.5, 165.7, 145.9, 134.7, 132.5, 131.2, 131.0, 130.5, 129.6, 129.4, 127.8, 123.4, 123.1, 107.8, 61.6, 35.7, 14.5. IR (KBr disc, cm⁻¹) 1726, 1609, 1587, 1491, 1456, 1366, 1262, 1182, 1164, 1142, 1105, 1081, 1023, 755, 717, 687, 614. Anal. Calc. for C₁₆H₁₂ClNO₃: C 64.67, H 4.47. Found: C 64.41, H 4.48. m.p. 114-116 °C.



1-(3-methoxyphenyl)indolin-2-one (Entry 8)

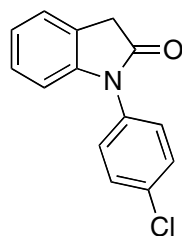
The general procedure was followed using CuI (19 mg, 0.10 mmol), *rac-trans-N,N'*-dimethylcyclohexane-1,2-diamine (32 μ L, 0.20 mmol), K₂CO₃ (0.28 g, 2.0 mmol), 3-bromoanisole (152 μ L, 1.20 mmol), and oxindole (133 mg, 1.00 mmol) with 1,4-dioxane (1.0 mL) as solvent for 24 h at 100 °C. Isolation and chromatographic purification (hexane / ethyl acetate) afforded the title compound as a slightly orange solid (139 mg, 58 %). ¹H NMR (500 MHz, CDCl₃) δ 7.46-7.43 (m, 1H), 7.32 (dd, *J* = 0.6, 7.2 Hz), 7.22 (td, 1H, *J* = 1.1, 7.9 Hz), 7.07 (td, 1H, *J* = 1.1, 7.5 Hz), 7.02-6.96 (m, 3H), 6.83 (dd, 1H, *J* = 0.3, 7.9 Hz), 3.84 (s, 3H), 3.72 (s, 2H). ¹³C NMR (125 MHz, CDCl₃) δ 174.5, 160.7, 145.3,

135.7, 130.5, 127.9, 124.7, 124.4, 122.9, 118.9, 114.2, 112.4, 109.6, 55.6, 36.2. m.p. 101-104 °C (Lit. 104-106 °C).^{vi}



1-(3,5-dimethylphenyl)indolin-2-one (Entry 9)⁰

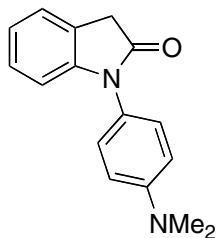
The general procedure was followed using CuI (19 mg, 0.10 mmol), *rac-trans-N,N'*-dimethylcyclohexane-1,2-diamine (32 μ L, 0.20 mmol), K₂CO₃ (0.28 g, 2.0 mmol), 5-bromo-*m*-xylene (163 μ L, 1.20 mmol), and oxindole (133 mg, 1.00 mmol) with 1,4-dioxane (0.5 mL) as solvent for 24 h at 100 °C. Isolation and chromatographic purification (hexane / ethyl acetate) afforded the title compound as slightly yellow solid (143 mg, 60%). ¹H NMR (500 MHz, CDCl₃) δ 7.31 (dd, 1H, *J* = 0.4, 7.3 Hz), 7.21 (td, 1H, *J* = 1.1, 7.6 Hz), 7.09-7.04 (m, 2H), 7.03 (d, 2H, *J* = 0.5 Hz), 6.7 (d, 1H, *J* = 7.6 Hz), 3.73 (s, 2H), 2.39 (s, 6H). ¹³C NMR (125 MHz, CDCl₃) δ 174.7, 145.7, 139.6, 134.4, 130.1, 127.9, 124.6, 124.5, 124.4, 122.8, 109.6, 36.2, 21.5. IR (KBr disc, cm⁻¹) 1725, 1614, 1593, 1489, 1465, 1369, 1325, 1304, 1240, 1197, 176, 1095, 848, 750, 733, 696, 619. m.p. 92-94 °C.



1-(4-chlorophenyl)indolin-2-one^{vii} (Entry 10)

The general procedure was followed using CuI (19 mg, 0.10 mmol), *rac-trans-N,N'*-dimethylcyclohexane-1,2-diamine (32 μ L, 0.20 mmol), K₂CO₃ (0.28 g, 2.0 mmol), 1-bromo-4-chlorobenzene (287, 1.50 mmol), and oxindole (133 mg, 1.00 mmol) with 1,4-dioxane (1.0 mL) as

solvent for 24 h at 100 °C. Isolation and chromatographic purification (hexane / ethyl acetate) afforded the title compound as white solid (192 mg, 79%). ^1H NMR (500 MHz, CDCl_3) δ 7.52-7.49 (m, 2H), 7.40-7.37 (m, 2H), 7.334-7.31 (m, 1H), 7.23 (td, 1H, $J = 0.8, 7.7$ Hz), 7.10 (td, 1H, $J = 0.9, 7.5$ Hz), 76.80 (dd, 1H, $J = 0.6, 7.9$ Hz). ^{13}C NMR (125 MHz, CDCl_3) δ 174.5, 144.8, 133.8, 133.1, 133.0, 130.0, 128.0, 124.9, 124.4, 123.2, 109.4, 36.1. m.p. 123-125 °C.



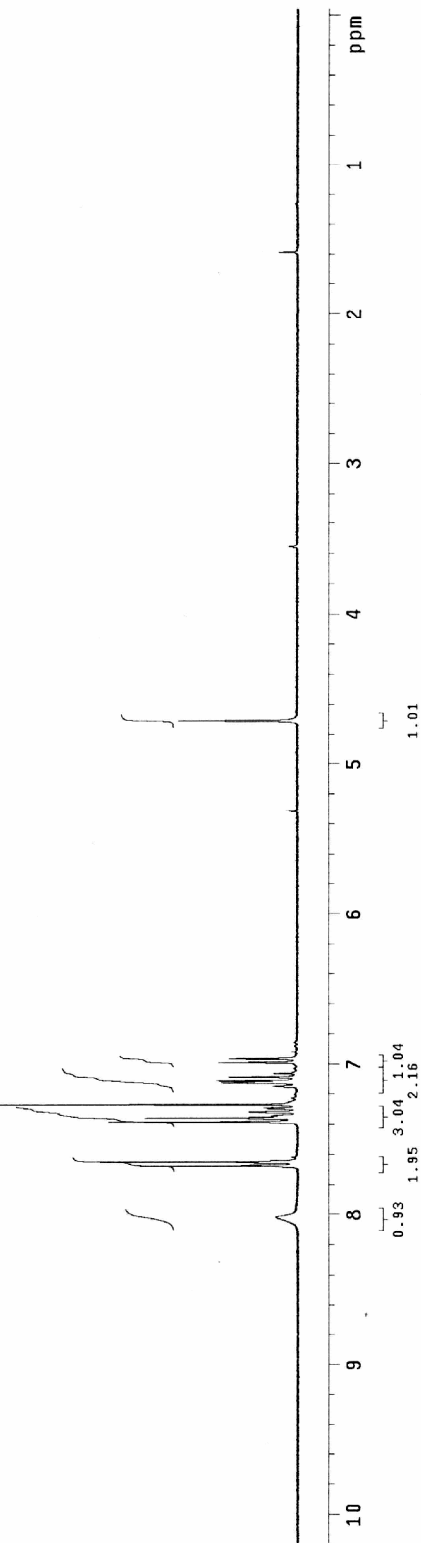
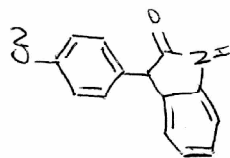
1-(4-(dimethylamino)phenyl)indolin-2-one (Entry 11)

The general procedure was followed using CuI (19 mg, 0.10 mmol), *rac-trans-N,N'*-dimethylcyclohexane-1,2-diamine (32 μL , 0.20 mmol), K_2CO_3 (0.28 g, 2.0 mmol), 4-bromo-*N,N'*-dimethylaniline (200 mg, 1.00 mmol), and oxindole (160 mg, 1.20 mmol) with 1,4-dioxane (1.0 mL) as solvent for 24 h at 100 °C. Isolation and chromatographic purification (hexane / ethyl acetate) afforded the title compound as a tan solid (127 mg, 50%). ^1H NMR (500 MHz, CDCl_3) δ 7.29 (dt, 1H, $J = 0.5, 7.3$ Hz), 7.24 (m 2H), 7.20 (td, 1H, $J = 0.4, 7.8$ Hz), 7.06 (td, 1H, $J = 0.9, 7.5$ Hz), 6.8 (d, 2H, $J = 8.8$ Hz), 6.74 (d, 1H, $J = 7.8$ Hz), 3.70 (s, 2H), 3.02 (s, 6H). ^{13}C NMR (125 MHz, CDCl_3) δ 175.2, 150.4, 146.4, 127.9, 127.7, 124.6, 124.5, 122.5, 113.2, 109.6, 105.3, 40.8, 36.2. IR (KBr disc, cm^{-1}) 1712, 1610, 1524, 1483, 1462, 1354, 1241, 1168, 1095, 950, 8821, 763, 631. Anal. Calc. for $\text{C}_{16}\text{H}_{16}\text{N}_2\text{O}$: C 76.16, H 6.39. Found: C 75.83, H 6.37. m.p. 171-172 °C.

RAAVI279

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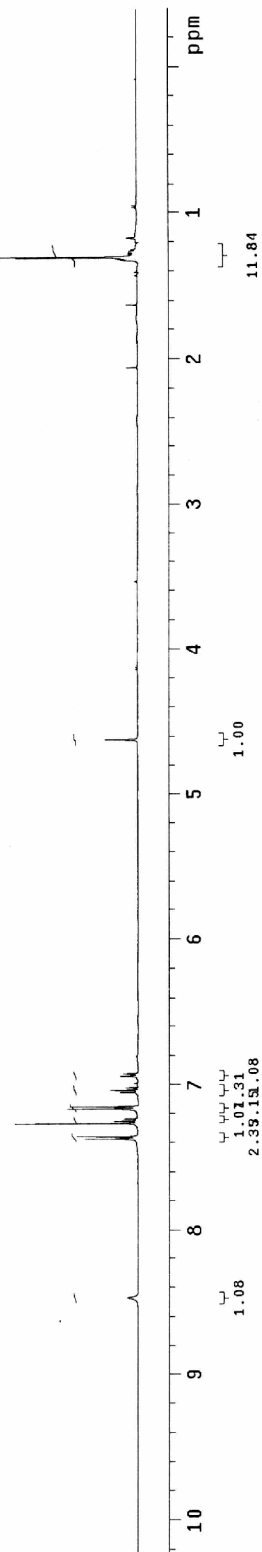
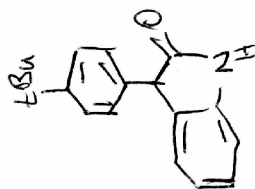


RAAVI280

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RAAVI278

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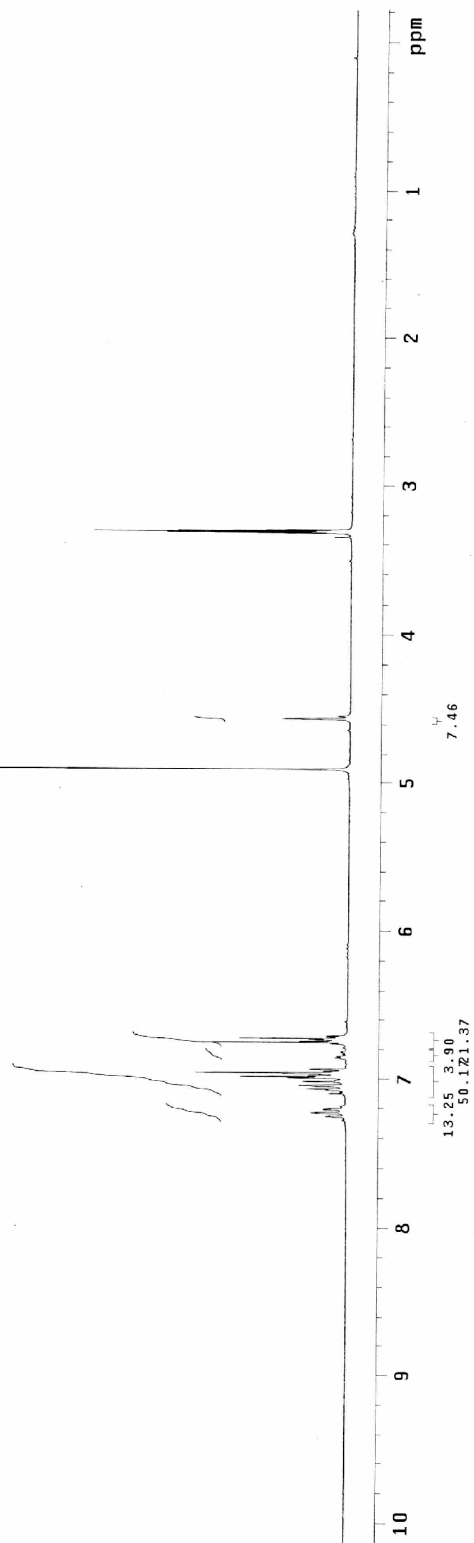
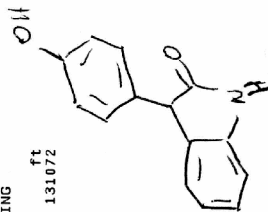
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STANDARD PROTON PARAMETERS

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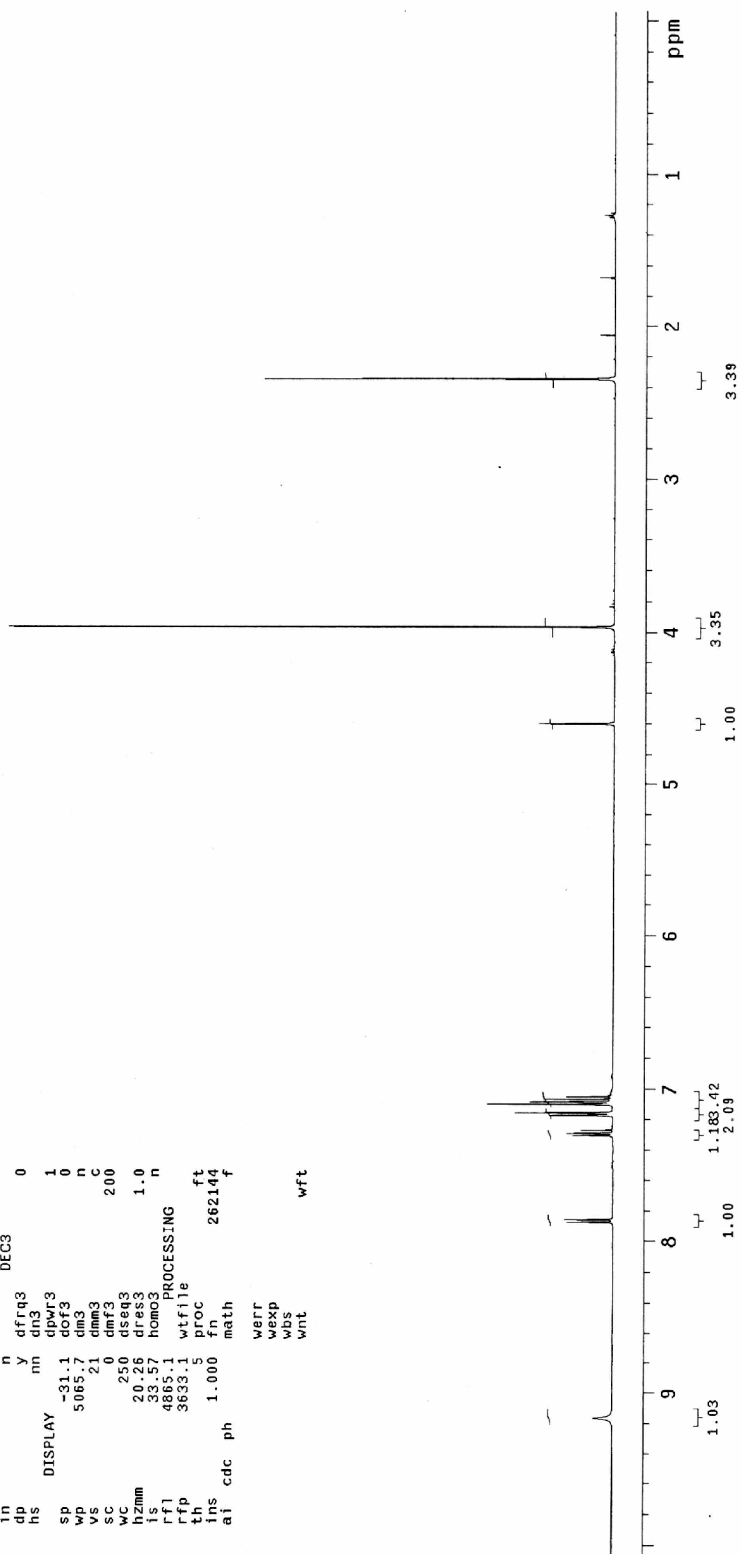
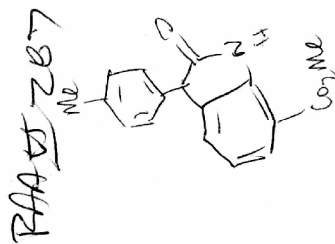
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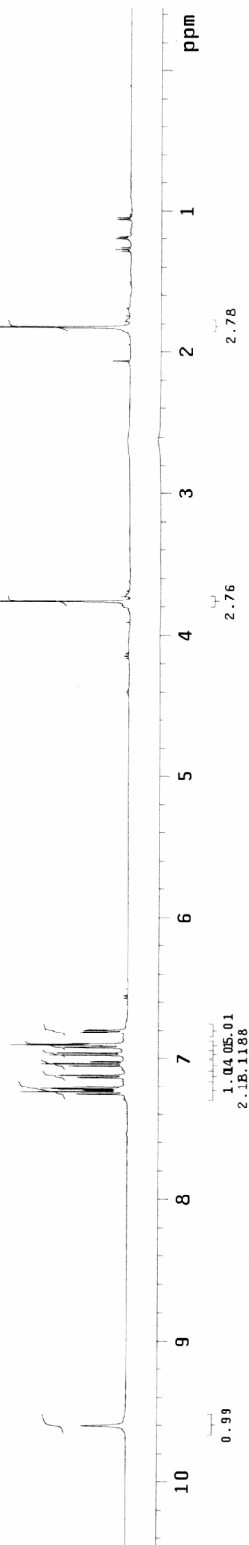
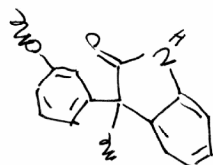
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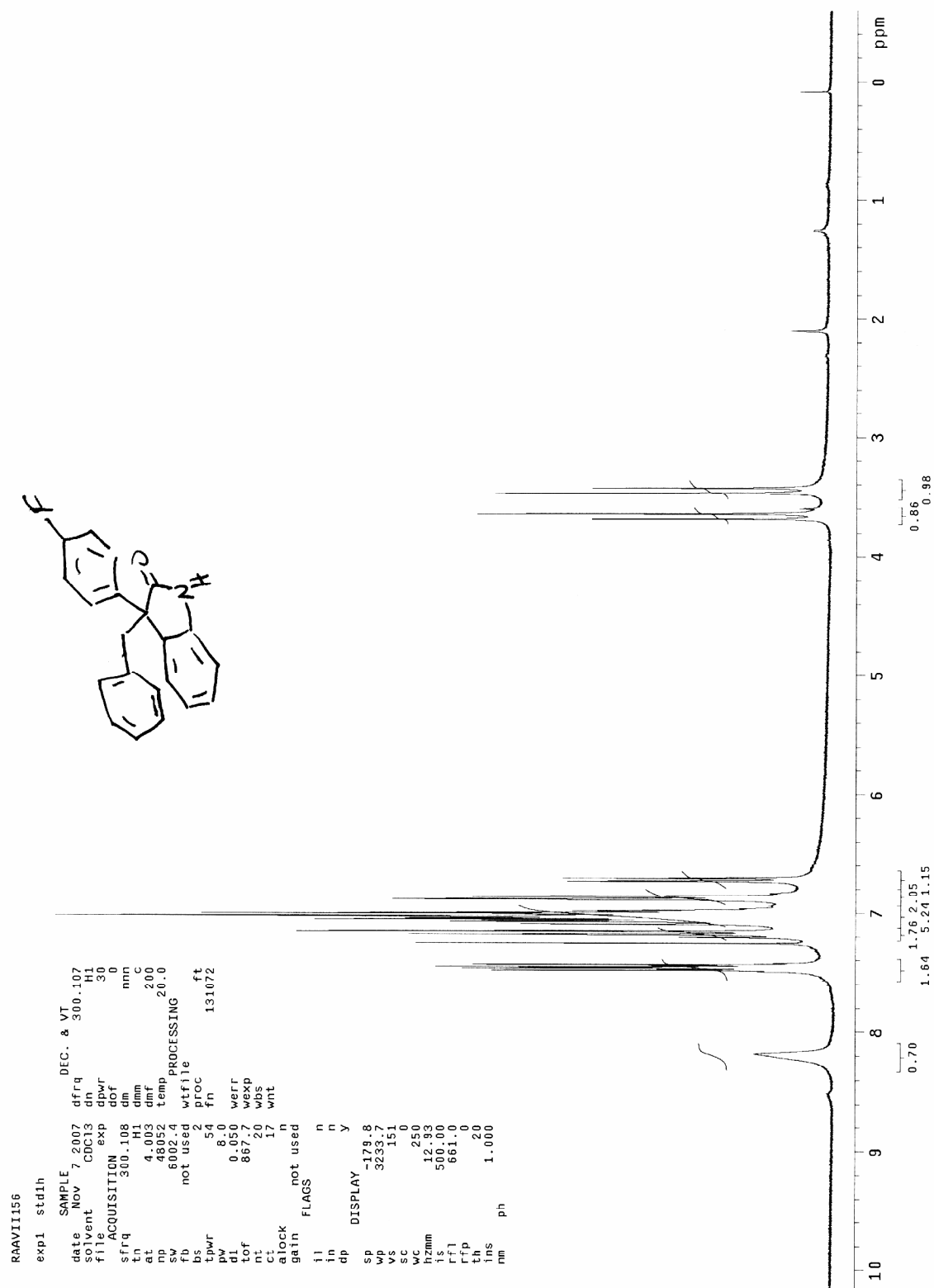


RAAVI186d

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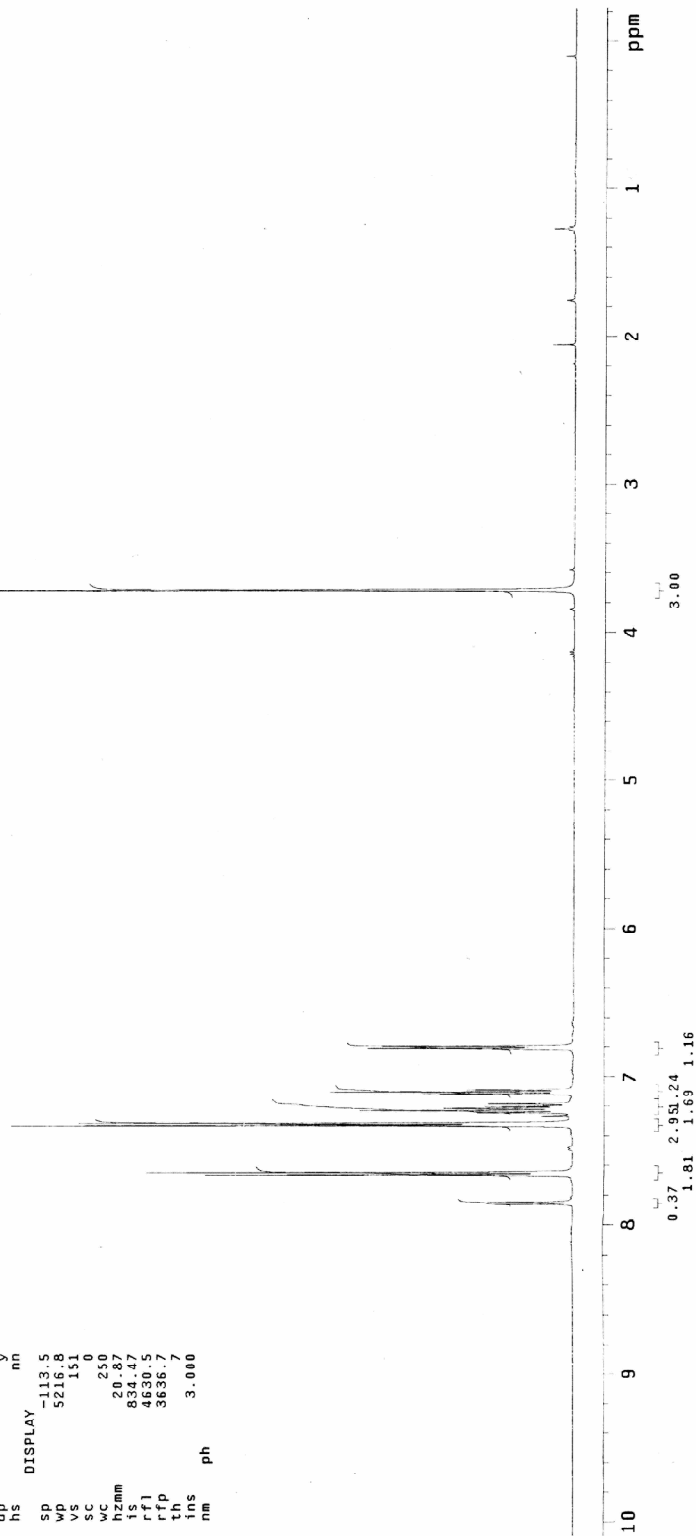
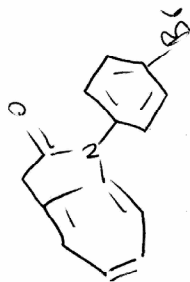


STANDARD PROTON PARAMETERS

exp1 szpu1

date	Jan 30 2007	DEC. & VT	125.795
solvent	CDCl3	dn	38
file	ACQUISITION	exp	0
sfreq	500.235	dm	nm
at	3.200	d1	10000
np	64000	dseq	1.0
sw	10000.0	dres	1.0
fb	not used	homo	n
bs	8	PROCESSING	
ss	1	wfile	ft
tpwr	53	proc	131072
pw	9.8	fn	f
d1	0	math	
tof	1498.2	werr	
nt	16	wexp	
clock	not used	wns	
gain	not used	wnt	
il	n		
in	n		
dp	y		
hs	nn		
sp	-113.5		
wp	5216.8		
vs	151		
sc	250		
h2mm	20.87		
is	834.47		
rfl	4630.5		
rfl	3636.7		
th	7		
ins	3.000		
nm	ph		

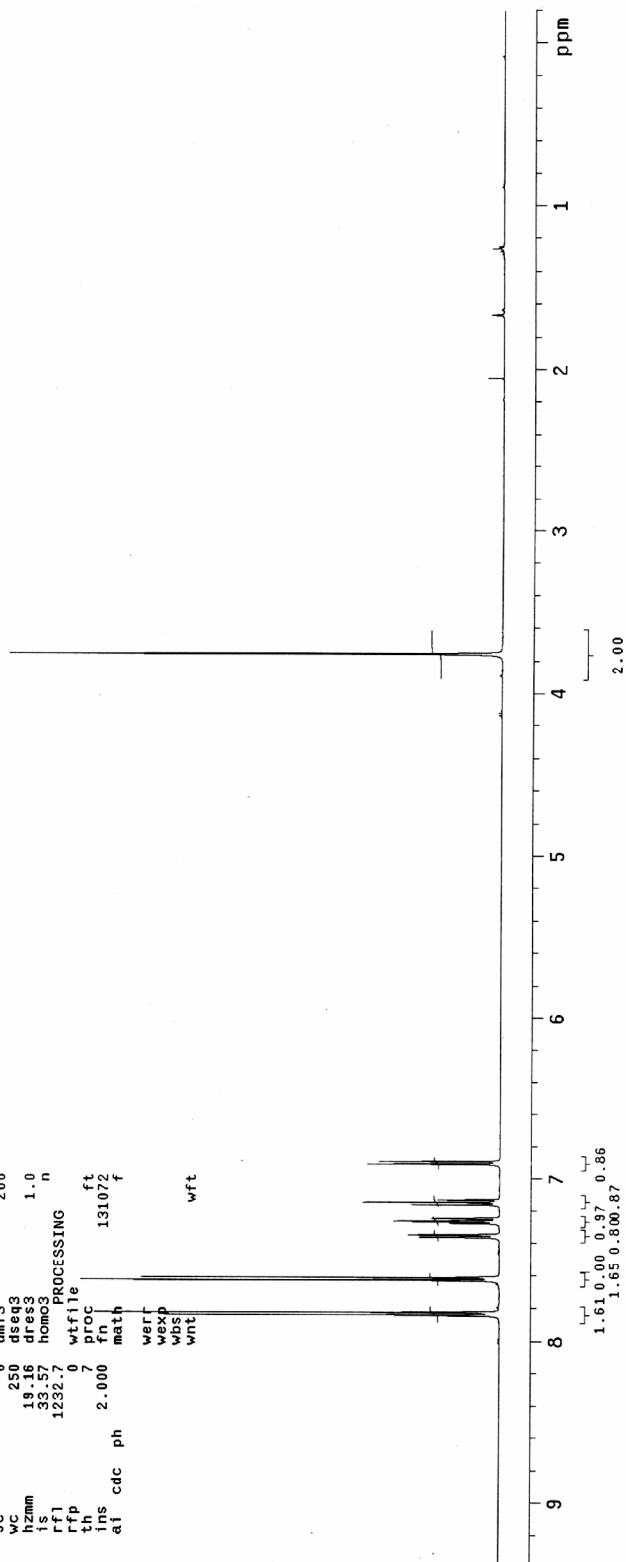
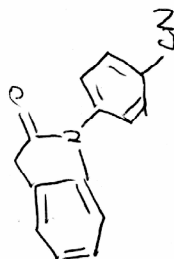
PAA VI 189

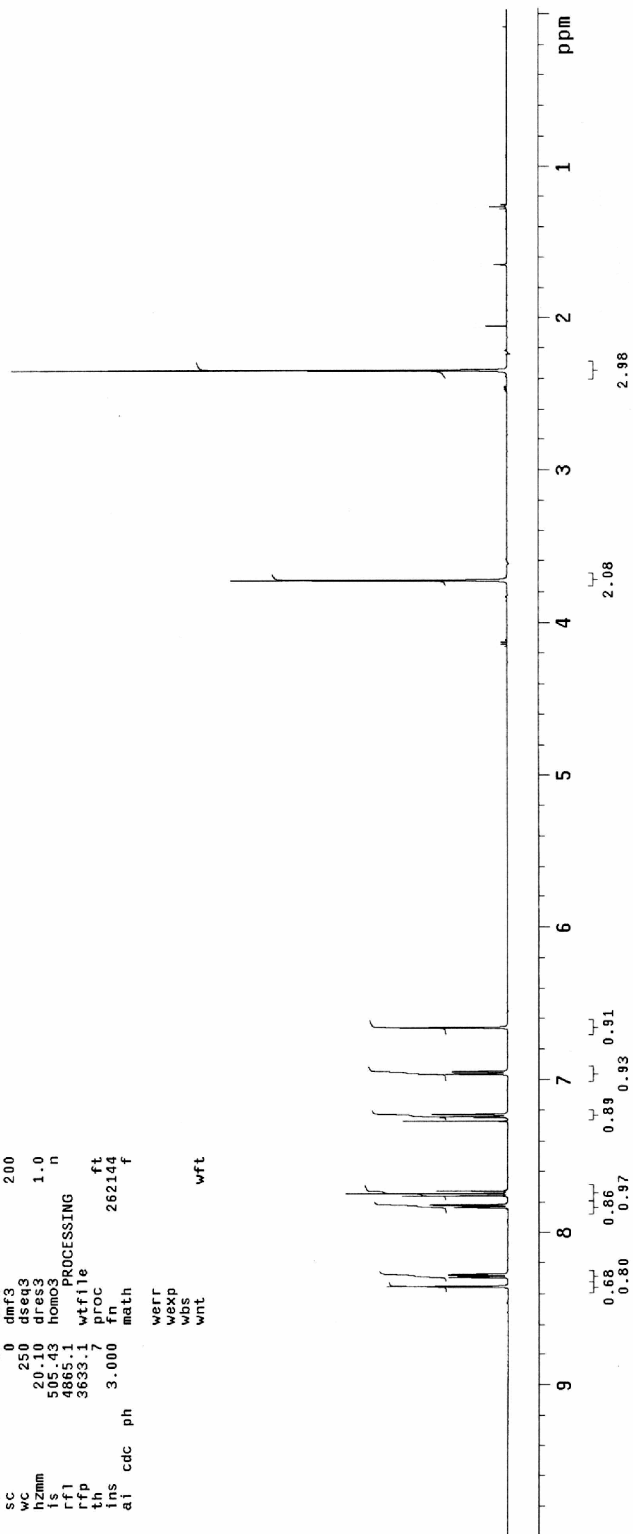
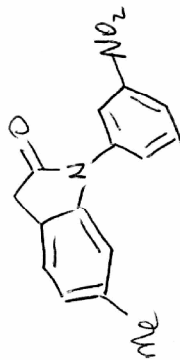


RAAVI245

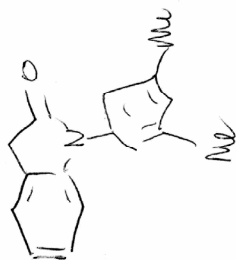
exp1 szpul

SAMPLE
 date Feb 25 2007
 solvent CDC13
 file ACQUISITION exp
 sfrq 499.746
 at 3.001
 nt 53050
 np 10504.2
 sw not used
 bs 8
 tpwr 56
 pw 8.9
 d1 2.000
 tof 1519.5
 nt 16
 ct 16
 a lock
 gain not used
 flags
 il n
 in n
 dp n
 hs n
 sp -100.8
 wp 4789.5
 vs 34
 sc 0
 wc 250
 icmm 19.18
 lzf 33.57
 rfl 1232.7
 rfp 0
 th 7
 ins 131072
 ai cdc ph
 DEC. & VT
 dn 125.672
 dpwr 30
 dof 0
 nm 10000
 dnm 1.0
 dres 1.0
 homo n
 DEC2
 dfrq2 0
 dn2 1
 dpwr2 0
 dof2 0
 nm2 n
 dnm2 200
 dfr2 n
 dres2 1.0
 homo2 n
 DEC3
 dfrq3 0
 dn3 1
 dpwr3 0
 dof3 n
 dnm3 200
 dfr3 n
 dres3 1.0
 homo3 n
 PROCESSING
 wfile
 ft
 fn 131072
 math
 werr
 wexp
 wbs
 wnt
 wft



[illegible]

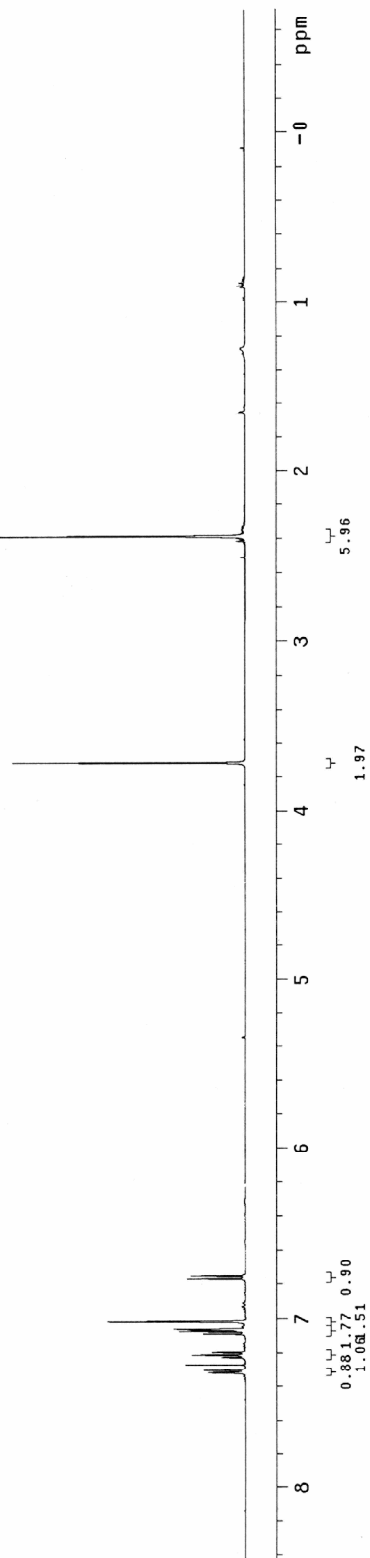
PAA VI 273



STANDARD PROTON PARAMETERS

exp3 s2pul

SAMPLE 6 2007 DEC. & VT
 date Apr CDC13 dn 125.672
 solvent file exp dnr C13
 file ACQUISITION exp 30
 sfrq 499.746 nm
 tn H1 dmm w
 at 3.001 dmf 19000
 ap 5.000 dseq
 sp 10500.2 dms
 fb not used homo 1.0
 bs 8 DEC2
 tpwr 56 dfrq2 0
 pw 8.6 dn2
 d1 2.000 dpwr2 1
 tof 1519.5 dof2 0
 nt 16 dm2 n
 ct 16 dmm2 c
 alock n dmf2 200
 gain not used dseq2
 flags n dres2 1.0
 il n homo2 DEC3
 in y dfrq3 0
 dp nn dn3
 hs DISPLAY
 sp -362.7 dpwr3 1
 wp 4582.6 dof3 0
 vs 15 dmm3 n
 sc 0 dmf3 c
 wc 250 dseq3 200
 hzmm 18.33 dres3 1.0
 ls 33.57 homo3 n
 rf1 4685.3 wfile
 rfp 3635.7 wfile
 ths ft
 ins proc 262144
 ai cdc ph fn math
 werr
 wexp
 wbs
 wnt wft



Cartesian Coordinates for Complexes 1-16 and Transition States 1-TS-4-TS

Complex 1

C -0.610381 2.338797 -0.191842
 C -1.205948 2.173304 -1.477423
 C -2.574743 1.904434 -1.550257
 C -3.386951 1.813495 -0.415244
 C -2.787394 1.984173 0.833708
 C -1.419580 2.251393 0.973850
 C 0.778703 2.925792 -0.108323
 C 1.989253 2.196228 -0.047975
 C 3.206258 2.903506 -0.093313
 C 3.249588 4.294298 -0.153380
 C 2.057475 5.015976 -0.160884
 C 0.845291 4.331700 -0.145143
 H -3.027399 1.757751 -2.526400
 H -3.398691 1.922058 1.728481
 H 4.146157 2.363585 -0.088523
 H 4.207648 4.805495 -0.189126
 H 2.068373 6.101993 -0.194242
 H -0.085748 4.889936 -0.177700
 P 1.982067 0.351523 0.189316
 Pd -0.183536 -0.557184 -0.208372
 C 3.466187 -0.214449 -0.818764
 C 3.882280 -1.679336 -0.559450
 C 3.210341 0.027788 -2.323464
 H 4.310491 0.418067 -0.511301
 C 5.106369 -2.058700 -1.411597
 H 3.053062 -2.349674 -0.800105
 H 4.114372 -1.830262 0.500536
 C 4.426851 -0.376409 -3.173576
 H 2.336742 -0.557323 -2.636153
 H 2.967539 1.081736 -2.503261
 C 4.846185 -1.828741 -2.906637
 H 5.365603 -3.108490 -1.225924
 H 5.974855 -1.460368 -1.096107
 H 4.193451 -0.232747 -4.236098
 H 5.269278 0.293965 -2.945285
 H 5.739004 -2.081327 -3.492711
 H 4.045629 -2.504692 -3.238932
 C 2.462274 0.227157 2.024295
 C 2.047231 -1.118817 2.653706
 C 3.925124 0.573978 2.371929
 H 1.826197 1.002331 2.475742

C 2.291677 -1.129153 4.172015
 H 2.607017 -1.940827 2.189786
 H 0.989612 -1.307148 2.441660
 C 4.157106 0.553443 3.894720
 H 4.602302 -0.150549 1.900543
 H 4.189810 1.561922 1.982077
 C 3.747590 -0.788446 4.516461
 H 2.020125 -2.110675 4.580642
 H 1.624532 -0.396417 4.649730
 H 5.212104 0.769927 4.106140
 H 3.573265 1.362190 4.358201
 H 3.887280 -0.761789 5.604439
 H 4.406892 -1.582011 4.134628
 C 0.429784 -2.419713 -0.653392
 C 0.651887 -3.403825 0.313089
 C 0.574285 -2.734021 -2.009718
 C 1.075770 -4.681553 -0.074733
 H 0.488100 -3.199889 1.365274
 C 1.000437 -4.012345 -2.388969
 H 0.320171 -2.004506 -2.771080
 C 1.264229 -4.986488 -1.423265
 H 1.249435 -5.438830 0.686628
 H 1.109851 -4.245673 -3.445748
 H 1.593461 -5.978818 -1.720470
 C -0.864503 2.554223 2.366787
 C -1.162226 1.442645 3.388891
 C -1.382811 3.913391 2.881392
 H 0.224515 2.639261 2.284375
 H -0.766573 0.479034 3.052480
 H -0.705423 1.684384 4.356534
 H -2.237636 1.316442 3.554607
 H -1.122699 4.726444 2.195117
 H -2.473477 3.904014 2.990896
 H -0.947998 4.144752 3.861346
 C -0.413606 2.389633 -2.769056
 C -0.642111 3.816434 -3.314821
 C -0.722655 1.356908 -3.867882
 H 0.650352 2.299992 -2.525981
 H -0.344628 4.586082 -2.595761
 H -0.061195 3.969308 -4.232610
 H -1.700281 3.971297 -3.557775
 H -0.719355 0.335341 -3.482857
 H -1.710583 1.524476 -4.312980
 H 0.014401 1.450268 -4.675049
 C -4.888371 1.607299 -0.583888
 C -5.589733 2.966395 -0.794517

C -5.552570 0.827236 0.561455
 H -5.024898 1.023457 -1.504616
 H -5.164592 3.507121 -1.647298
 H -6.661852 2.826119 -0.978549
 H -5.478886 3.601033 0.093493
 H -5.052892 -0.128821 0.746005
 H -5.549151 1.398830 1.497659
 H -6.601092 0.622865 0.315151
 C -2.774274 -2.076119 0.629983
 C -3.885170 -2.775443 0.103900
 N -2.079142 -1.379800 -0.363771
 C -3.900019 -2.527878 -1.378643
 H -3.812871 -3.436719 -1.986182
 C -4.717069 -3.508283 0.936370
 H -5.571635 -4.044718 0.529091
 C -4.443519 -3.558839 2.312718
 H -5.087173 -4.132687 2.973735
 C -3.343207 -2.871072 2.829433
 H -3.135744 -2.913461 3.896319
 C -2.500116 -2.122574 1.999010
 H -1.648683 -1.585663 2.405929
 C -2.647810 -1.647526 -1.586137
 O -2.237274 -1.258517 -2.678039
 H -4.791087 -1.992393 -1.730842

Complex 2

C 0.939518 -2.357536 -0.263768
 C 1.521942 -2.055544 -1.529013
 C 2.885006 -1.743613 -1.585645
 C 3.700099 -1.720363 -0.450134
 C 3.104412 -1.991560 0.785803
 C 1.747369 -2.311888 0.906259
 C -0.398764 -3.061125 -0.221911
 C -1.673581 -2.458445 -0.107273
 C -2.814677 -3.282167 -0.163272
 C -2.724235 -4.665390 -0.296476
 C -1.467870 -5.263235 -0.371995
 C -0.328941 -4.463465 -0.338934
 H 3.327686 -1.506563 -2.548608
 H 3.717208 -1.975394 1.682699
 H -3.802186 -2.838297 -0.108484
 H -3.628255 -5.266828 -0.337059
 H -1.372170 -6.341385 -0.467690
 H 0.650660 -4.925903 -0.419149
 P -1.842304 -0.627968 0.184285

Pd 0.239060 0.558808 -0.241123
 C -3.413186 -0.196759 -0.761122
 C -3.940606 1.225355 -0.468311
 C -3.184401 -0.394401 -2.276205
 H -4.192141 -0.901299 -0.438897
 C -5.217771 1.513182 -1.277582
 H -3.176177 1.965280 -0.721574
 H -4.152967 1.342611 0.600014
 C -4.454358 -0.082180 -3.085713
 H -2.370700 0.266195 -2.600741
 H -2.861133 -1.422002 -2.481077
 C -4.988009 1.325072 -2.783408
 H -5.556867 2.535428 -1.068162
 H -6.023264 0.840453 -0.945032
 H -4.241684 -0.190666 -4.156906
 H -5.230054 -0.824904 -2.844797
 H -5.918058 1.506758 -3.337193
 H -4.260121 2.071848 -3.130212
 C -2.281166 -0.596244 2.032521
 C -1.995974 0.777907 2.676368
 C -3.685846 -1.106548 2.414573
 H -1.551175 -1.304367 2.451704
 C -2.195779 0.736311 4.201059
 H -2.657857 1.540059 2.245449
 H -0.973362 1.089487 2.437060
 C -3.871566 -1.139615 3.943369
 H -4.451803 -0.450674 1.979475
 H -3.855859 -2.109786 2.009664
 C -3.593857 0.228525 4.580126
 H -2.022878 1.735102 4.621417
 H -1.437769 0.074798 4.646416
 H -4.888901 -1.475801 4.181894
 H -3.187248 -1.886467 4.372472
 H -3.696097 0.168187 5.671086
 H -4.349219 0.949622 4.234020
 C -0.548234 2.362485 -0.702094
 C -0.869848 3.308908 0.277031
 C -0.825582 2.647458 -2.045853
 C -1.507750 4.503734 -0.078977
 H -0.617973 3.133628 1.318111
 C -1.460604 3.844789 -2.397177
 H -0.527278 1.956261 -2.828587
 C -1.813790 4.772599 -1.414323
 H -1.757280 5.227060 0.694564
 H -1.666560 4.052858 -3.445149
 H -2.307317 5.701700 -1.688323

C 1.198425 -2.693696 2.281485
 C 1.456094 -1.610322 3.345312
 C 1.756901 -4.053929 2.747716
 H 0.113292 -2.807940 2.189012
 H 1.041714 -0.643798 3.038880
 H 0.992596 -1.895522 4.297632
 H 2.526822 -1.469870 3.532488
 H 1.522033 -4.848111 2.031192
 H 2.846583 -4.016428 2.862151
 H 1.326622 -4.333814 3.716825
 C 0.724223 -2.151932 -2.830637
 C 0.948750 -3.515945 -3.518572
 C 1.033377 -1.012083 -3.819806
 H -0.337482 -2.084523 -2.571122
 H 0.649090 -4.353242 -2.880993
 H 0.366371 -3.571986 -4.446225
 H 2.006201 -3.647586 -3.778178
 H 1.057173 -0.031663 -3.336249
 H 2.007413 -1.151689 -4.304028
 H 0.279265 -1.003609 -4.616256
 C 5.194620 -1.451517 -0.582664
 C 5.991156 -2.770402 -0.503165
 C 5.725445 -0.428982 0.437516
 H 5.354215 -1.029938 -1.583911
 H 5.654310 -3.484687 -1.262710
 H 7.061179 -2.586688 -0.657935
 H 5.869808 -3.244084 0.478883
 H 5.168898 0.512770 0.390738
 H 5.659205 -0.808316 1.464305
 H 6.781238 -0.211189 0.238779
 C 2.400198 2.490415 0.784108
 C 2.606862 3.766556 0.206255
 C 2.838377 4.900820 0.976272
 H 2.991992 5.873012 0.515153
 C 2.879465 4.750544 2.369106
 H 3.062029 5.622115 2.992423
 C 2.697997 3.497874 2.961499
 H 2.744621 3.399928 4.042962
 C 2.455729 2.365230 2.170680
 H 2.311989 1.393593 2.636606
 C 2.360627 2.304465 -1.570696
 O 2.372448 1.930381 -2.739502
 N 2.562235 3.629333 -1.178972
 H 2.662538 4.375267 -1.852110
 C 2.145021 1.521699 -0.308319
 H 2.710337 0.586737 -0.284587

Complex 3

H 5.791211 1.193580 -0.909510
 C 5.527752 -0.895805 -0.497671
 C 5.177878 0.453764 -0.402689
 H 5.018116 -2.868682 0.149995
 C 4.742335 -1.818497 0.195312
 C 4.073571 0.887634 0.339266
 C 3.625798 -1.442303 0.954207
 C 3.266870 -0.070022 1.003513
 P -0.015979 0.675735 -0.185884
 C 2.117774 0.357177 1.886763
 C 0.758910 0.537708 1.505645
 H 3.490867 0.415659 3.531155
 C 2.449283 0.528244 3.244657
 C -0.192678 0.789055 2.519454
 H -1.245271 0.880114 2.256551
 C 1.501385 0.820095 4.222668
 C 0.162440 0.929304 3.858952
 H 1.809325 0.941726 5.257736
 H -0.607530 1.124600 4.599481
 C 1.059150 -0.145915 -1.488712
 C 0.842231 -1.673251 -1.479365
 C 0.816425 0.404593 -2.911495
 H 2.098916 0.065841 -1.217928
 C 1.751927 -2.377993 -2.498924
 H -0.205705 -1.887248 -1.719715
 H 1.009904 -2.078536 -0.477549
 C 1.727517 -0.297444 -3.935107
 H -0.233831 0.245053 -3.194526
 H 1.000698 1.483502 -2.954098
 C 1.544436 -1.820438 -3.914004
 H 1.550235 -3.456785 -2.482890
 H 2.802661 -2.248890 -2.203267
 H 1.523062 0.100375 -4.937369
 H 2.775490 -0.053248 -3.707446
 H 2.237256 -2.296022 -4.619828
 H 0.528724 -2.067573 -4.256141
 C 0.046822 2.541703 -0.572590
 C -1.100284 2.910294 -1.546810
 C -0.035276 3.450770 0.672483
 H 1.008025 2.731707 -1.069753
 C -1.056809 4.395628 -1.944318
 H -2.065043 2.708283 -1.051358
 H -1.081315 2.285241 -2.443961

C 0.008698 4.939239 0.282486
 H -0.969359 3.246862 1.213984
 H 0.777275 3.230517 1.370760
 C -1.100394 5.307602 -0.712095
 H -1.893395 4.618576 -2.618124
 H -0.135302 4.589121 -2.513675
 H -0.070884 5.553399 1.188267
 H 0.988278 5.166968 -0.164170
 H -1.011388 6.359515 -1.011209
 H -2.078065 5.202056 -0.219958
 C 3.815786 2.388566 0.471281
 C 3.950926 3.157495 -0.856130
 C 4.740901 3.005873 1.541277
 H 2.788289 2.522213 0.822179
 H 3.352262 2.703055 -1.653619
 H 3.615906 4.193409 -0.726574
 H 4.989242 3.197355 -1.204613
 H 4.595652 2.529180 2.516125
 H 5.794472 2.885966 1.261859
 H 4.539999 4.078165 1.654817
 C 2.885390 -2.517381 1.758052
 C 3.595353 -2.776076 3.105826
 C 2.723044 -3.858914 1.016624
 H 1.880637 -2.142656 1.980013
 H 3.647155 -1.874573 3.721940
 H 3.060292 -3.544339 3.676983
 H 4.619810 -3.130981 2.939939
 H 2.311207 -3.733211 0.011824
 H 3.676548 -4.392134 0.924063
 H 2.043242 -4.508700 1.578990
 C 6.733669 -1.352019 -1.308920
 C 8.049980 -0.773583 -0.754879
 C 6.575625 -1.024926 -2.806227
 H 6.789689 -2.445117 -1.215359
 H 8.186071 -1.036931 0.299750
 H 8.908389 -1.160150 -1.317115
 H 8.067988 0.320197 -0.831288
 H 5.661846 -1.470191 -3.215401
 H 6.524755 0.057604 -2.973662
 H 7.428126 -1.410283 -3.378186
 Pd -2.333998 0.238590 -0.071139
 C -2.233292 -1.728530 0.263691
 C -2.702298 -2.597461 -0.725027
 C -1.769611 -2.228187 1.481564
 C -2.669664 -3.979236 -0.502753
 H -3.107236 -2.214781 -1.656477

C -1.747324 -3.612594 1.695005
 H -1.435815 -1.559962 2.267766
 C -2.188715 -4.490576 0.703979
 H -3.033830 -4.651483 -1.276214
 H -1.389103 -3.997578 2.647163
 H -2.170707 -5.563701 0.875116
 N -4.363642 0.283580 0.260172
 C -4.749513 0.456590 1.573640
 C -5.466131 -0.120510 -0.496708
 C -6.265317 0.188794 1.692048
 O -4.007492 0.774860 2.500956
 C -6.640457 -0.196555 0.286409
 C -5.508016 -0.399241 -1.864795
 H -6.773716 1.090827 2.055284
 H -6.441201 -0.598331 2.435571
 C -7.847888 -0.557789 -0.290918
 C -6.731680 -0.769533 -2.434893
 H -4.609449 -0.318874 -2.471289
 C -7.893320 -0.851919 -1.663066
 H -8.753145 -0.614450 0.310026
 H -6.776654 -0.991843 -3.498511
 H -8.833924 -1.139091 -2.124994

Complex 4

H 5.899073 0.721299 -0.868346
 C 5.412931 -1.325692 -0.445980
 C 5.204762 0.053722 -0.365704
 H 4.687366 -3.229602 0.201853
 C 4.523621 -2.155889 0.238360
 C 4.139910 0.606460 0.354260
 C 3.441402 -1.658581 0.977038
 C 3.228909 -0.255691 1.013564
 P 0.043953 0.835453 -0.207644
 C 2.124605 0.297817 1.883723
 C 0.796581 0.621397 1.488486
 H 3.484371 0.219412 3.538252
 C 2.462325 0.439620 3.243610
 C -0.129670 0.971320 2.495695
 H -1.163479 1.167893 2.218584
 C 1.543325 0.834343 4.213140
 C 0.225843 1.080439 3.837909
 H 1.854279 0.928027 5.250197
 H -0.525027 1.357378 4.572164
 C 1.029697 -0.122744 -1.490281
 C 0.623079 -1.610556 -1.454014

C 0.853436 0.428089 -2.922491
 H 2.088446 -0.037562 -1.224902
 C 1.433649 -2.441251 -2.462180
 H -0.444824 -1.694270 -1.688655
 H 0.742255 -2.015772 -0.444571
 C 1.667243 -0.399140 -3.934150
 H -0.209448 0.394056 -3.202170
 H 1.168667 1.475682 -2.983117
 C 1.293263 -1.886301 -3.886629
 H 1.100060 -3.486351 -2.427629
 H 2.493569 -2.437175 -2.170439
 H 1.513476 0.003917 -4.943468
 H 2.738124 -0.285634 -3.709757
 H 1.918125 -2.457656 -4.584938
 H 0.253214 -2.008774 -4.222794
 C 0.338422 2.675307 -0.611442
 C -0.749109 3.161853 -1.600633
 C 0.346001 3.602558 0.622722
 H 1.319132 2.751974 -1.100899
 C -0.536630 4.628622 -2.012534
 H -1.734372 3.072563 -1.111052
 H -0.792090 2.527362 -2.490313
 C 0.566724 5.071347 0.218759
 H -0.613206 3.515151 1.152105
 H 1.117227 3.298094 1.335885
 C -0.483300 5.554524 -0.790507
 H -1.337109 4.938365 -2.696166
 H 0.404867 4.709464 -2.575922
 H 0.551643 5.701961 1.116676
 H 1.569901 5.178025 -0.220712
 H -0.269824 6.585087 -1.100900
 H -1.470568 5.570923 -0.306031
 C 4.031357 2.127069 0.464441
 C 4.263972 2.858567 -0.870704
 C 4.995795 2.666317 1.541771
 H 3.015940 2.364418 0.795018
 H 3.633317 2.456153 -1.671516
 H 4.035912 3.925378 -0.760173
 H 5.305962 2.785852 -1.202607
 H 4.787423 2.223561 2.521069
 H 6.036586 2.436817 1.283591
 H 4.902004 3.755209 1.635203
 C 2.575744 -2.643910 1.770809
 C 3.222455 -2.963934 3.136957
 C 2.292018 -3.966897 1.032945
 H 1.610160 -2.165509 1.966673

H 3.349283 -2.067661 3.749618
 H 2.598135 -3.670093 3.697730
 H 4.209428 -3.421927 2.998725
 H 1.927077 -3.806477 0.015088
 H 3.184659 -4.600828 0.973743
 H 1.529327 -4.534440 1.577813
 C 6.578415 -1.911950 -1.232607
 C 7.937428 -1.498429 -0.635364
 C 6.501607 -1.554012 -2.728946
 H 6.503619 -3.005023 -1.151958
 H 8.011005 -1.786090 0.419138
 H 8.760322 -1.978072 -1.178845
 H 8.086007 -0.413643 -0.696822
 H 5.551754 -1.881293 -3.166343
 H 6.586490 -0.471937 -2.884620
 H 7.316332 -2.034504 -3.283743
 Pd -2.385129 0.619535 -0.133591
 C -2.578894 -1.339752 0.254365
 C -3.074141 -2.195757 -0.734056
 C -2.155452 -1.859078 1.481409
 C -3.105353 -3.576894 -0.505955
 H -3.452855 -1.800651 -1.671660
 C -2.202452 -3.240931 1.704822
 H -1.792997 -1.203290 2.266264
 C -2.668425 -4.103690 0.710879
 H -3.485307 -4.236693 -1.282756
 H -1.876130 -3.636960 2.664222
 H -2.701611 -5.175838 0.887225
 C -4.749135 0.696722 1.569124
 C -5.464612 0.106150 -0.607319
 O -4.262910 1.237158 2.557964
 C -6.164742 -0.669183 0.348336
 C -5.785094 -0.033620 -1.955569
 C -7.146951 -1.582008 -0.017277
 C -6.781823 -0.942043 -2.339360
 H -5.263320 0.556885 -2.705931
 C -7.447644 -1.710235 -1.380335
 H -7.673669 -2.172556 0.727784
 H -7.036557 -1.050592 -3.390226
 H -8.214900 -2.414869 -1.690412
 C -4.471903 0.930593 0.111107
 N -5.703952 -0.320564 1.617761
 H -6.030297 -0.706848 2.491768
 H -4.424527 1.995977 -0.155309

Complex 5

H 2.604766 1.727180 -2.962061
C 2.993218 2.542381 -1.018881
C 2.156225 2.083583 -2.040517
H 3.027436 3.409858 0.934682
C 2.391956 3.027390 0.140295
C 0.762912 2.078138 -1.922289
C 1.002359 3.054623 0.314907
C 0.173928 2.540470 -0.715291
P -1.999714 -0.014169 0.354419
C -1.322222 2.717374 -0.587899
C -2.274651 1.792374 -0.085694
H -1.057093 4.703314 -1.348911
C -1.782374 4.003330 -0.946709
C -3.600991 2.241251 0.103781
H -4.335310 1.574586 0.543616
C -3.101349 4.411188 -0.786706
C -4.020055 3.523470 -0.231963
H -3.400575 5.415180 -1.075048
H -5.051682 3.819287 -0.062516
C -3.445050 -0.787175 -0.601709
C -3.260793 -0.636339 -2.126183
C -3.774406 -2.245534 -0.220020
H -4.317799 -0.184514 -0.317745
C -4.479999 -1.170239 -2.898101
H -2.368713 -1.190284 -2.436957
H -3.097316 0.416536 -2.382074
C -4.991530 -2.763504 -1.009493
H -2.912769 -2.890049 -0.417127
H -3.992733 -2.319276 0.850894
C -4.791327 -2.625264 -2.523893
H -4.296240 -1.080913 -3.976420
H -5.355723 -0.541283 -2.677693
H -5.176413 -3.811047 -0.740171
H -5.888530 -2.200379 -0.709737
H -5.682663 -2.975310 -3.060087
H -3.957252 -3.268201 -2.839204
C -2.572145 -0.113828 2.162163
C -2.122227 -1.436066 2.827774
C -2.085501 1.075272 3.018752
H -3.672884 -0.094560 2.130909
C -2.663190 -1.549103 4.263331
H -1.024668 -1.454891 2.850840
H -2.435266 -2.305392 2.241689
C -2.608717 0.971887 4.462494
H -0.988165 1.082191 3.025626

H -2.411260 2.024422 2.582439
C -2.219687 -0.357865 5.122994
H -2.321152 -2.491572 4.709628
H -3.762486 -1.595875 4.238111
H -2.224984 1.816089 5.049303
H -3.705202 1.068158 4.457607
H -2.655930 -0.426760 6.127747
H -1.128108 -0.392581 5.249104
C -0.081229 1.654082 -3.126832
C 0.610197 0.618365 -4.033140
C -0.487040 2.869427 -3.990489
H -1.001423 1.197961 -2.745107
H 1.078730 -0.184347 -3.457080
H -0.119912 0.174425 -4.720043
H 1.389386 1.080120 -4.651081
H -1.091211 3.589007 -3.432735
H 0.405054 3.388847 -4.361123
H -1.071440 2.541771 -4.859368
C 0.443050 3.727669 1.572514
C 0.462684 5.265029 1.421175
C 1.176816 3.333111 2.868901
H -0.601579 3.421687 1.684799
H -0.126095 5.604588 0.563757
H 0.054604 5.742168 2.320891
H 1.489460 5.625924 1.286077
H 1.279460 2.249412 2.954393
H 2.180020 3.775171 2.914021
H 0.623037 3.715510 3.735513
C 4.508286 2.555803 -1.176171
C 4.953707 3.556727 -2.260686
C 5.083520 1.154267 -1.452296
H 4.926423 2.901773 -0.220549
H 4.584816 4.565741 -2.044993
H 6.047946 3.598346 -2.323779
H 4.573927 3.265933 -3.247592
H 4.797294 0.440340 -0.672889
H 4.727258 0.757148 -2.410154
H 6.178757 1.190673 -1.496771
Pd 0.173177 -0.929802 0.327336
C -0.257250 -2.561400 -0.746529
C -0.214314 -2.604183 -2.143167
C -0.446299 -3.756318 -0.035904
C -0.374870 -3.819677 -2.822118
H -0.051447 -1.697824 -2.713168
C -0.610165 -4.967581 -0.716643
H -0.458888 -3.751839 1.050250

C -0.578359 -5.004029 -2.112820
H -0.335042 -3.833635 -3.909151
H -0.756061 -5.884387 -0.149790
H -0.702757 -5.946119 -2.640322
N 2.143258 -1.518811 0.785745
C 2.335283 -0.615559 1.751840
C 3.292115 -2.303974 0.639693
C 3.729218 -0.745604 2.364441
O 1.417842 0.200563 2.050374
C 4.291131 -1.894283 1.555869
C 3.519118 -3.353586 -0.248001
H 3.659132 -0.950525 3.440137
H 4.285078 0.193438 2.251419
C 5.520563 -2.534236 1.581761
C 4.765860 -3.990974 -0.208611
H 2.747247 -3.663515 -0.945152
C 5.758323 -3.592765 0.690378
H 6.293332 -2.224200 2.281992
H 4.961765 -4.812680 -0.893207
H 6.717515 -4.102978 0.701579

Complex 6

C 0.284678 2.499120 0.298059
C 0.163307 2.965712 -1.045551
C -1.091640 3.365655 -1.509637
C -2.236559 3.326112 -0.710483
C -2.110523 2.827043 0.587319
C -0.878817 2.427408 1.118753
C 1.658292 2.469566 0.931236
C 2.514285 1.348129 1.026508
C 3.794568 1.514529 1.587158
C 4.230271 2.746389 2.069292
C 3.378730 3.847693 2.001292
C 2.114720 3.702479 1.435286
H -1.182502 3.738130 -2.526552
H -2.990403 2.772791 1.221611
H 4.473312 0.670847 1.645641
H 5.225650 2.841060 2.494330
H 3.697349 4.816242 2.376802
H 1.456267 4.563570 1.366420
P 1.924792 -0.324397 0.483921
Pd -0.064095 -0.064040 -0.694339
C 3.470492 -1.139049 -0.207324
C 3.300985 -2.645171 -0.508641
C 3.987622 -0.385376 -1.452630

H 4.231358 -1.053380 0.581184
C 4.618433 -3.249830 -1.024136
H 2.517670 -2.786622 -1.258325
H 2.979259 -3.183908 0.388844
C 5.292832 -1.006091 -1.979752
H 3.221612 -0.426721 -2.236347
H 4.148912 0.673451 -1.218547
C 5.134450 -2.506450 -2.264033
H 4.465325 -4.311970 -1.252084
H 5.379264 -3.205957 -0.229901
H 5.610389 -0.474712 -2.885916
H 6.090489 -0.858388 -1.236168
H 6.089602 -2.933098 -2.595584
H 4.421304 -2.646468 -3.088838
C 1.545111 -1.163247 2.142978
C 0.541564 -2.328251 2.004999
C 2.774071 -1.569013 2.984072
H 1.027135 -0.361002 2.686769
C 0.138547 -2.875932 3.384307
H 0.984527 -3.138054 1.410087
H -0.350048 -1.986316 1.469383
C 2.346289 -2.120316 4.357466
H 3.349407 -2.342104 2.457514
H 3.443078 -0.713621 3.130049
C 1.357893 -3.286730 4.220327
H -0.542366 -3.726095 3.253041
H -0.428619 -2.103650 3.924573
H 3.236725 -2.432541 4.918367
H 1.877832 -1.312664 4.938864
H 1.044216 -3.635261 5.212493
H 1.863550 -4.135133 3.735354
C 0.166607 -1.727245 -1.801862
C -0.378072 -2.953177 -1.411559
C 0.779411 -1.609772 -3.054812
C -0.282732 -4.061923 -2.261746
H -0.903209 -3.042363 -0.467790
C 0.866004 -2.721460 -3.902404
H 1.187184 -0.660382 -3.387502
C 0.343357 -3.953171 -3.504723
H -0.710676 -5.011284 -1.947488
H 1.340810 -2.615937 -4.875525
H 0.413545 -4.816266 -4.161680
C -0.805569 2.036177 2.594874
C -1.866695 0.992638 2.993896
C -0.907608 3.281319 3.501099
H 0.180490 1.593840 2.772856

H -1.890376 0.143786 2.303114
 H -1.663931 0.626497 4.008205
 H -2.872375 1.429394 3.007774
 H -0.108490 4.000968 3.294191
 H -1.867062 3.791966 3.356970
 H -0.837003 2.990905 4.556287
 C 1.377392 3.128751 -1.960519
 C 1.797180 4.609123 -2.073294
 C 1.147087 2.531914 -3.361591
 H 2.212279 2.583579 -1.508579
 H 2.044105 5.034281 -1.095223
 H 2.678923 4.709107 -2.717906
 H 0.991726 5.211874 -2.509519
 H 0.786536 1.500717 -3.297755
 H 0.409860 3.106006 -3.934382
 H 2.083104 2.541835 -3.932934
 C -3.566393 3.837231 -1.246806
 C -4.136425 4.975932 -0.379702
 C -4.588471 2.699026 -1.415113
 H -3.369719 4.251990 -2.244934
 H -3.421833 5.801262 -0.283689
 H -5.056962 5.371990 -0.824654
 H -4.381833 4.625942 0.629898
 H -4.182072 1.912152 -2.056442
 H -4.840553 2.246850 -0.448482
 H -5.515889 3.076762 -1.862598
 C -3.858727 -2.041465 0.578282
 C -4.800000 -2.002222 -0.477493
 N -2.701536 -1.291343 0.310871
 C -4.186628 -1.143699 -1.550705
 C -6.007323 -2.675704 -0.380248
 H -6.732336 -2.643786 -1.191289
 C -6.285173 -3.409306 0.785096
 H -7.225938 -3.946002 0.875309
 C -5.353940 -3.452074 1.826300
 H -5.580371 -4.023466 2.723816
 C -4.133577 -2.770854 1.736666
 H -3.413079 -2.801036 2.549818
 C -2.857557 -0.754115 -0.885663
 O -2.011939 0.001247 -1.497388
 H -3.982507 -1.679989 -2.486523
 H -4.780404 -0.260224 -1.811649

Complex 7

C 0.322192 2.499608 -0.033323

C -0.020168 2.699387 -1.403237
 C -1.353117 2.957770 -1.735404
 C -2.367039 3.031701 -0.780149
 C -2.016397 2.827826 0.558518
 C -0.700356 2.576634 0.957613
 C 1.775790 2.588152 0.376157
 C 2.664311 1.500807 0.549425
 C 4.008064 1.768686 0.872744
 C 4.477753 3.068348 1.047603
 C 3.597524 4.139299 0.903905
 C 2.268357 3.892775 0.569652
 H -1.614250 3.109797 -2.778807
 H -2.788618 2.900985 1.319943
 H 4.710566 0.950543 0.985317
 H 5.521896 3.238806 1.294848
 H 3.942766 5.160414 1.040806
 H 1.584373 4.726762 0.440697
 P 2.048875 -0.246487 0.408623
 Pd -0.047922 -0.213488 -0.615672
 C 3.512271 -1.169671 -0.328714
 C 3.356545 -2.707101 -0.303798
 C 3.805879 -0.670848 -1.760453
 H 4.379934 -0.925140 0.299908
 C 4.598699 -3.393324 -0.899862
 H 2.469990 -3.000611 -0.873408
 H 3.205121 -3.061380 0.721387
 C 5.036868 -1.373687 -2.358078
 H 2.931463 -0.871807 -2.390539
 H 3.960041 0.414667 -1.763094
 C 4.888797 -2.901217 -2.324323
 H 4.449938 -4.480208 -0.893789
 H 5.471970 -3.192551 -0.260459
 H 5.192708 -1.025520 -3.387048
 H 5.933578 -1.081358 -1.790998
 H 5.794801 -3.380030 -2.716841
 H 4.060960 -3.200468 -2.982673
 C 1.935270 -0.765079 2.229974
 C 0.982015 -1.960142 2.445648
 C 3.283588 -0.983108 2.949205
 H 1.459585 0.113281 2.688983
 C 0.794707 -2.266137 3.941078
 H 1.371859 -2.851647 1.938467
 H 0.014232 -1.742850 1.981774
 C 3.073509 -1.291827 4.443313
 H 3.823130 -1.820820 2.487701
 H 3.919718 -0.097141 2.847640

C 2.137365 -2.490213 4.650267
 H 0.147260 -3.144170 4.056537
 H 0.269444 -1.425960 4.419006
 H 4.045613 -1.476007 4.918326
 H 2.646820 -0.406917 4.937927
 H 1.978998 -2.667823 5.721333
 H 2.613720 -3.396989 4.249070
 C 0.002228 -2.096731 -1.334828
 C -0.550845 -3.167010 -0.626718
 C 0.493756 -2.308941 -2.628552
 C -0.576208 -4.446814 -1.194272
 H -0.987100 -3.015726 0.355056
 C 0.459171 -3.589169 -3.194653
 H 0.894582 -1.485049 -3.211832
 C -0.065924 -4.663997 -2.474681
 H -1.010150 -5.270389 -0.631953
 H 0.837648 -3.738685 -4.203662
 H -0.091118 -5.657817 -2.914083
 C -0.384702 2.500409 2.451940
 C -1.237221 1.452482 3.191190
 C -0.531466 3.883298 3.120009
 H 0.663855 2.204211 2.560378
 H -1.120124 0.457638 2.747089
 H -0.936665 1.389521 4.243929
 H -2.302933 1.709161 3.174655
 H 0.115426 4.626789 2.642541
 H -1.563704 4.246502 3.055584
 H -0.259405 3.828505 4.180993
 C 1.035657 2.726305 -2.509896
 C 1.317089 4.171714 -2.970764
 C 0.657757 1.843757 -3.714542
 H 1.967799 2.329205 -2.095319
 H 1.666734 4.798246 -2.143520
 H 2.087723 4.181018 -3.751016
 H 0.413676 4.634582 -3.385085
 H 0.412111 0.825581 -3.397432
 H -0.209726 2.239334 -4.254598
 H 1.493484 1.800359 -4.423394
 C -3.790548 3.386909 -1.187765
 C -4.171534 4.793391 -0.681254
 C -4.824183 2.338573 -0.739202
 H -3.809221 3.417072 -2.285375
 H -3.463699 5.552056 -1.034433
 H -5.172433 5.069548 -1.033496
 H -4.182889 4.830593 0.415000
 H -4.588970 1.347426 -1.136924

H -4.872549 2.261645 0.353757
 H -5.823489 2.622209 -1.090394
 C -4.336717 -1.555366 0.824766
 C -4.786832 -2.096286 -0.419594
 N -3.193744 -0.817000 0.558639
 C -3.896357 -1.622210 -1.436787
 C -5.922335 -2.924650 -0.412691
 H -6.287367 -3.359087 -1.340512
 C -6.580275 -3.177247 0.789613
 H -7.461667 -3.814155 0.794091
 C -6.126308 -2.621609 1.998779
 H -6.660281 -2.829819 2.922359
 C -4.993104 -1.805008 2.028021
 H -4.635757 -1.378072 2.962880
 C -2.946926 -0.813032 -0.827529
 O -1.986879 -0.090042 -1.335393
 H -2.807895 -0.103636 1.159576
 H -3.920612 -1.851958 -2.492751

Complex 8

H -1.988651 2.758101 -2.894183
 C -2.474623 3.361344 -0.894174
 C -2.259246 2.414641 -1.900509
 H -3.041294 3.617886 1.150888
 C -2.855839 2.894262 0.361524
 C -2.403046 1.041088 -1.678564
 C -3.012788 1.531746 0.643399
 C -2.756151 0.586702 -0.381230
 P -0.328711 -1.799439 0.412486
 C -3.084644 -0.866235 -0.122296
 C -2.202554 -1.899124 0.291720
 H -5.125215 -0.392112 -0.578104
 C -4.455704 -1.178912 -0.244566
 C -2.761382 -3.150104 0.633667
 H -2.118275 -3.940518 1.006436
 C -4.977935 -2.429948 0.063606
 C -4.120872 -3.423966 0.530071
 H -6.042847 -2.617739 -0.043603
 H -4.500231 -4.403546 0.807872
 C 0.120023 -3.377931 -0.546038
 C -0.236616 -3.237074 -2.040569
 C 1.577050 -3.851120 -0.361938
 H -0.521877 -4.165148 -0.129096
 C 0.052570 -4.531804 -2.819694
 H 0.347908 -2.418496 -2.474823

H -1.295545 -2.975963 -2.149010
C 1.845545 -5.144587 -1.154244
H 2.271444 -3.072540 -0.691362
H 1.782158 -4.039237 0.697714
C 1.507990 -4.983971 -2.641905
H -0.175467 -4.376608 -3.882084
H -0.621706 -5.327468 -2.468491
H 2.897017 -5.432257 -1.028302
H 1.243578 -5.963968 -0.732202
H 1.683241 -5.926431 -3.176646
H 2.179097 -4.235222 -3.085623
C 0.011588 -2.277617 2.219210
C 1.465314 -1.933005 2.617206
C -0.961103 -1.604425 3.210471
H -0.120672 -3.368752 2.286902
C 1.772400 -2.359361 4.063015
H 1.600883 -0.847119 2.520626
H 2.184138 -2.390482 1.931627
C -0.659186 -2.014807 4.663272
H -0.870055 -0.514811 3.110552
H -1.996793 -1.862151 2.968934
C 0.793998 -1.717684 5.055765
H 2.806264 -2.088381 4.313333
H 1.709333 -3.454959 4.143238
H -1.351275 -1.496719 5.339373
H -0.853869 -3.091368 4.782490
H 0.994436 -2.070861 6.075410
H 0.949739 -0.628788 5.062936
C -2.273283 0.078926 -2.860088
C -1.255351 0.532590 -3.921453
C -3.639829 -0.156169 -3.541093
H -1.929994 -0.883403 -2.467832
H -0.313149 0.853261 -3.468384
H -1.043972 -0.290114 -4.614569
H -1.637925 1.366488 -4.522018
H -4.368690 -0.596919 -2.855425
H -4.051317 0.790877 -3.910893
H -3.529635 -0.833822 -4.396973
C -3.532075 1.133358 2.027933
C -5.053556 1.376935 2.131601
C -2.814438 1.851237 3.187742
H -3.363675 0.060018 2.157658
H -5.612252 0.809099 1.380982
H -5.422177 1.081668 3.121912
H -5.286622 2.439160 1.989294
H -1.729038 1.780536 3.092285

H -3.078300 2.915106 3.228496
H -3.123955 1.408503 4.142907
C -2.332852 4.854428 -1.160694
C -3.373773 5.351718 -2.182799
C -0.906181 5.233878 -1.599881
H -2.531889 5.370286 -0.211411
H -4.393369 5.123819 -1.852518
H -3.293662 6.436847 -2.321248
H -3.226561 4.879328 -3.161557
H -0.166180 4.915770 -0.857416
H -0.645803 4.764948 -2.556547
H -0.816594 6.319537 -1.727998
Pd 0.875157 0.261034 0.006710
C 2.361879 -0.443117 -1.164039
C 2.256330 -0.568613 -2.555412
C 3.585832 -0.774077 -0.559824
C 3.332391 -1.039518 -3.319647
H 1.334246 -0.302299 -3.060125
C 4.658484 -1.249856 -1.321372
H 3.714826 -0.661801 0.513676
C 4.535687 -1.389693 -2.705655
H 3.224350 -1.127088 -4.398959
H 5.594055 -1.504684 -0.827895
H 5.370174 -1.756227 -3.298046
O 0.094198 1.845232 1.688028
C 1.235739 2.250004 1.345688
N 2.272892 2.553200 2.211072
C 3.453022 2.792888 1.494989
C 4.712481 3.146653 1.966385
C 3.171596 2.648101 0.113034
C 5.720205 3.367579 1.020876
H 4.908457 3.255634 3.029962
C 4.190464 2.887380 -0.810381
C 5.461379 3.244594 -0.349910
H 6.715663 3.642007 1.359418
H 3.999748 2.779090 -1.874452
H 6.260145 3.423339 -1.064438
C 1.761554 2.280218 -0.018655
H 2.205605 2.417188 3.209622
H 1.138670 2.653948 -0.827285

Complex 9

H 5.778881 1.384538 -0.628112
C 5.613832 -0.722011 -0.257721
C 5.180430 0.603543 -0.167839

H 5.185960 -2.729943 0.338692
C 4.845463 -1.698544 0.377949
C 4.010910 0.962171 0.511607
C 3.665652 -1.398976 1.072750
C 3.222519 -0.051116 1.112574
P -0.062896 0.584999 -0.220047
C 2.007388 0.297712 1.941505
C 0.658769 0.430015 1.504197
H 3.305288 0.368359 3.644436
C 2.272286 0.442903 3.317952
C -0.338077 0.612122 2.487745
H -1.375603 0.678279 2.169306
C 1.274787 0.661025 4.264056
C -0.050471 0.724863 3.845167
H 1.534025 0.763386 5.314346
H -0.857191 0.868191 4.558304
C 1.114108 -0.212798 -1.459354
C 0.979061 -1.748326 -1.472290
C 0.976991 0.337671 -2.896512
H 2.118250 0.044471 -1.104737
C 2.010349 -2.397222 -2.410164
H -0.027549 -2.018043 -1.807531
H 1.076510 -2.150601 -0.460093
C 1.996283 -0.322499 -3.843727
H -0.039860 0.152790 -3.270311
H 1.135980 1.419873 -2.916382
C 1.884378 -1.851442 -3.838674
H 1.871252 -3.485993 -2.405401
H 3.024705 -2.205290 -2.033130
H 1.854447 0.071972 -4.858103
H 3.010949 -0.032684 -3.533318
H 2.651856 -2.291196 -4.488469
H 0.910946 -2.146872 -4.256609
C 0.033177 2.449939 -0.589306
C -0.932180 2.856377 -1.732300
C -0.248148 3.333171 0.647125
H 1.067116 2.631579 -0.916379
C -0.775897 4.347035 -2.082417
H -1.960588 2.674377 -1.403851
H -0.771137 2.251818 -2.627897
C -0.116474 4.828732 0.305720
H -1.266081 3.132447 1.003802
H 0.434645 3.088296 1.466466
C -1.028820 5.235763 -0.858287
H -1.472178 4.603151 -2.891169
H 0.237410 4.534184 -2.470301

H -0.345413 5.424208 1.198901
H 0.929450 5.050311 0.042994
H -0.875151 6.292824 -1.111504
H -2.077740 5.129253 -0.549077
C 3.661058 2.443486 0.651995
C 3.860747 3.251094 -0.643907
C 4.462996 3.084113 1.804887
H 2.603040 2.513407 0.921864
H 3.365628 2.779266 -1.499994
H 3.447393 4.259437 -0.525636
H 4.920900 3.366447 -0.896411
H 4.267248 2.579371 2.756403
H 5.540475 3.027483 1.608875
H 4.194343 4.141132 1.920997
C 2.951280 -2.526558 1.826826
C 3.624197 -2.778716 3.194644
C 2.884120 -3.858763 1.054688
H 1.921485 -2.207144 2.017798
H 3.614984 -1.887843 3.828185
H 3.104673 -3.580642 3.733053
H 4.668570 -3.085154 3.059139
H 2.488121 -3.734753 0.043908
H 3.868700 -4.333876 0.974265
H 2.231766 -4.559435 1.588096
C 6.889987 -1.095918 -1.000402
C 8.136823 -0.462787 -0.353149
C 6.807699 -0.744195 -2.498129
H 6.998331 -2.186480 -0.924404
H 8.218437 -0.738890 0.703867
H 9.048103 -0.795185 -0.864539
H 8.103765 0.631759 -0.411311
H 5.942363 -1.222221 -2.970609
H 6.715639 0.338048 -2.648676
H 7.710606 -1.077228 -3.023694
Pd -2.359651 0.071136 -0.144856
C -2.097298 -1.905525 -0.153238
C -2.584574 -2.641428 -1.242353
C -1.578524 -2.584480 0.954984
C -2.541114 -4.040099 -1.223569
H -3.008381 -2.131746 -2.103357
C -1.545087 -3.984701 0.971529
H -1.196826 -2.033723 1.810153
C -2.020517 -4.716458 -0.117531
H -2.921445 -4.599200 -2.075690
H -1.144952 -4.500103 1.842063
H -1.990796 -5.802863 -0.103808

N -4.483273 0.104584 -0.017698
 C -4.572629 1.430284 0.111699
 C -5.766714 -0.455230 0.025002
 C -6.025011 1.883257 0.249863
 O -3.525208 2.143076 0.112528
 C -6.745366 0.555391 0.180901
 C -6.129781 -1.797282 -0.064181
 H -6.289463 2.576841 -0.558308
 H -6.171307 2.421256 1.194917
 C -8.089768 0.224210 0.244537
 C -7.491952 -2.116832 0.002335
 H -5.373502 -2.566679 -0.182120
 C -8.464820 -1.125805 0.153869
 H -8.847212 0.995996 0.363898
 H -7.794984 -3.158921 -0.065192
 H -9.515325 -1.398966 0.202784

Complex 10

C -3.366826 -0.921406 -0.936542
 C -3.383415 -2.215050 -0.360209
 C -4.474672 -2.582081 0.438298
 C -5.555704 -1.728760 0.670156
 C -5.526351 -0.465114 0.072854
 C -4.460396 -0.043301 -0.730188
 C -2.296719 -0.558545 -1.934805
 C -1.056451 0.088926 -1.687664
 C -0.206027 0.325789 -2.794410
 C -0.536302 -0.041469 -4.095692
 C -1.750652 -0.678004 -4.332093
 C -2.603814 -0.925074 -3.260509
 H -4.494369 -3.574633 0.881247
 H -6.365723 0.208222 0.224157
 H 0.750893 0.814071 -2.628843
 H 0.157909 0.161702 -4.905638
 H -2.033104 -0.985210 -5.335202
 H -3.552601 -1.422092 -3.440111
 P -0.280258 0.715343 -0.096630
 Pd 1.942741 0.062117 -0.514920
 C -0.790919 2.528494 0.008877
 C -0.136097 3.252776 1.207649
 C -0.501749 3.312596 -1.289303
 H -1.879413 2.511533 0.161518
 C -0.648580 4.698918 1.324058
 H 0.949456 3.264283 1.069010
 H -0.324323 2.720263 2.145470

C -0.993800 4.767209 -1.179622
 H 0.580724 3.307562 -1.476826
 H -0.977651 2.830944 -2.149349
 C -0.391195 5.488275 0.033647
 H -0.160927 5.189396 2.175741
 H -1.727198 4.691161 1.541639
 H -0.749668 5.303834 -2.105122
 H -2.090998 4.770263 -1.097472
 H -0.801472 6.502590 0.116255
 H 0.693364 5.596228 -0.110408
 C -1.012906 -0.145321 1.421120
 C 0.088510 -0.366896 2.487054
 C -2.255436 0.507662 2.062410
 H -1.307095 -1.129674 1.039007
 C -0.432676 -1.175316 3.687525
 H 0.452611 0.605993 2.843247
 H 0.948795 -0.873820 2.034311
 C -2.766578 -0.316548 3.259450
 H -2.003535 1.514294 2.417862
 H -3.056677 0.613801 1.328728
 C -1.673850 -0.527899 4.314395
 H 0.367248 -1.277435 4.431777
 H -0.682095 -2.194535 3.357980
 H -3.634465 0.190076 3.700792
 H -3.123589 -1.290380 2.898108
 H -2.051768 -1.146870 5.137830
 H -1.396407 0.442072 4.753423
 C 2.889826 1.582385 0.366581
 C 3.131701 1.613857 1.742658
 C 3.417624 2.578136 -0.461947
 C 3.890508 2.656039 2.290775
 H 2.740200 0.839547 2.393331
 C 4.169782 3.618426 0.096873
 H 3.266543 2.542994 -1.536335
 C 4.404891 3.662516 1.472447
 H 4.077551 2.673158 3.361933
 H 4.581217 4.386871 -0.553156
 H 4.993396 4.469098 1.901131
 C -4.542857 1.324514 -1.412405
 C -4.944500 2.462576 -0.454666
 C -5.507290 1.279119 -2.615997
 H -3.549133 1.565678 -1.804262
 H -4.291466 2.507174 0.423838
 H -4.882854 3.427247 -0.972134
 H -5.974367 2.353641 -0.096230
 H -5.194112 0.530943 -3.351216

H -6.524655 1.027466 -2.293408
 H -5.543311 2.253365 -3.118164
 C -2.288771 -3.246511 -0.649457
 C -2.741269 -4.228204 -1.751662
 C -1.833433 -4.036040 0.592583
 H -1.413479 -2.710573 -1.032909
 H -2.984063 -3.705848 -2.681938
 H -1.947369 -4.952615 -1.968707
 H -3.631298 -4.785229 -1.435270
 H -1.533450 -3.375821 1.413351
 H -2.620640 -4.698934 0.969353
 H -0.974492 -4.666631 0.336738
 C -6.732937 -2.179539 1.525621
 C -8.040144 -2.241188 0.712225
 C -6.905049 -1.301782 2.780078
 H -6.510360 -3.199905 1.866399
 H -7.931415 -2.888475 -0.164846
 H -8.858706 -2.633660 1.327099
 H -8.337376 -1.246394 0.359433
 H -5.990106 -1.285905 3.382298
 H -7.146902 -0.266282 2.511906
 H -7.720312 -1.681084 3.407593
 C 6.781276 -1.901018 -0.772783
 C 6.369632 -2.029778 0.575466
 N 5.778106 -1.396654 -1.613903
 C 4.939155 -1.565620 0.613660
 C 7.241857 -2.496692 1.545670
 H 6.928020 -2.593203 2.583487
 C 8.547854 -2.850549 1.168287
 H 9.244114 -3.222786 1.915443
 C 8.954223 -2.727603 -0.164110
 H 9.968696 -3.005500 -0.441171
 C 8.079297 -2.252937 -1.148125
 H 8.391630 -2.154127 -2.183633
 C 4.720257 -1.206062 -0.864937
 O 3.581946 -0.798705 -1.340070
 H 4.226559 -2.340218 0.927656
 H 4.775288 -0.692385 1.257199

Complex 11

C 3.406345 -0.730628 0.973803
 C 3.381402 -2.110568 0.655240
 C 4.393057 -2.632219 -0.161909
 C 5.436233 -1.847009 -0.657284
 C 5.452717 -0.493239 -0.309311

C 4.465656 0.082745 0.498568
 C 2.426972 -0.176606 1.977389
 C 1.156737 0.406374 1.721549
 C 0.396331 0.839112 2.833412
 C 0.845526 0.730440 4.146346
 C 2.092101 0.162642 4.391779
 C 2.855654 -0.280875 3.315876
 H 4.380575 -3.691035 -0.408123
 H 6.266043 0.131849 -0.667522
 H -0.585454 1.273362 2.660341
 H 0.218611 1.079210 4.961799
 H 2.467201 0.057446 5.406047
 H 3.826881 -0.730131 3.501851
 P 0.243580 0.742654 0.113565
 Pd -1.976294 0.252960 0.762542
 C 0.787672 2.479102 -0.383855
 C 0.041364 2.985058 -1.640348
 C 0.635065 3.504679 0.759712
 H 1.856860 2.391203 -0.622303
 C 0.565019 4.365137 -2.074005
 H -1.027399 3.057696 -1.416920
 H 0.137855 2.278785 -2.470963
 C 1.136986 4.895325 0.330911
 H -0.424539 3.571956 1.039996
 H 1.181056 3.177393 1.650366
 C 0.436065 5.391976 -0.941127
 H 0.011589 4.701616 -2.959531
 H 1.620042 4.281328 -2.375404
 H 0.987284 5.605604 1.153985
 H 2.221812 4.847798 0.153271
 H 0.850716 6.359548 -1.251065
 H -0.629609 5.557523 -0.727667
 C 0.820612 -0.414411 -1.271483
 C -0.383890 -0.793766 -2.168225
 C 2.007027 0.058174 -2.138775
 H 1.133945 -1.319057 -0.737205
 C 0.000145 -1.833229 -3.234660
 H -0.768383 0.105847 -2.667061
 H -1.204032 -1.171746 -1.546495
 C 2.381193 -0.995462 -3.198679
 H 1.741830 0.988113 -2.655706
 H 2.878215 0.270862 -1.516443
 C 1.185871 -1.362315 -4.086704
 H -0.870701 -2.043326 -3.868492
 H 0.262057 -2.781161 -2.741579
 H 3.210371 -0.614328 -3.808750

H 2.753853 -1.896489 -2.693117
H 1.469534 -2.139363 -4.807725
H 0.884121 -0.483480 -4.675742
C -2.957511 1.646995 -0.293585
C -3.434580 1.373685 -1.577868
C -3.264749 2.864372 0.323255
C -4.202066 2.331288 -2.252548
H -3.226735 0.422142 -2.056430
C -4.032832 3.816050 -0.358626
H -2.923824 3.075403 1.332599
C -4.497624 3.554637 -1.649033
H -4.572762 2.111046 -3.250954
H -4.272276 4.758611 0.128594
H -5.095287 4.294046 -2.175445
C 4.598807 1.555496 0.894474
C 4.918100 2.481840 -0.294475
C 5.658883 1.731698 2.001999
H 3.639354 1.880548 1.310574
H 4.199238 2.359365 -1.111891
H 4.889518 3.529312 0.028175
H 5.918419 2.297029 -0.702324
H 5.407812 1.148391 2.893640
H 6.646014 1.404820 1.653823
H 5.736417 2.785069 2.297179
C 2.333581 -3.060481 1.242697
C 2.904775 -3.811506 2.464657
C 1.772406 -4.074081 0.227394
H 1.491758 -2.456238 1.598056
H 3.238733 -3.118649 3.242957
H 2.143564 -4.469072 2.901281
H 3.761547 -4.431481 2.174329
H 1.385519 -3.584012 -0.672427
H 2.529554 -4.800435 -0.088768
H 0.951943 -4.640168 0.682978
C 6.531515 -2.461492 -1.520127
C 7.892367 -2.453805 -0.796219
C 6.636716 -1.784193 -2.899093
H 6.256326 -3.511489 -1.689670
H 7.831885 -2.971406 0.167416
H 8.656454 -2.952377 -1.404502
H 8.234716 -1.429785 -0.604519
H 5.679678 -1.815876 -3.431088
H 6.933898 -0.732751 -2.806739
H 7.388690 -2.287302 -3.518410
C -5.926640 -2.440514 -0.099337
C -6.833473 -1.615396 0.637825

N -4.647781 -2.022212 0.218896
C -6.046827 -0.714642 1.420541
C -8.213788 -1.827524 0.470354
H -8.929977 -1.214332 1.012271
C -8.653416 -2.830457 -0.389374
H -9.720131 -2.997526 -0.517332
C -7.740630 -3.635246 -1.096273
H -8.110096 -4.413904 -1.758505
C -6.364371 -3.446289 -0.959490
H -5.657426 -4.065685 -1.507224
C -4.708634 -0.991405 1.168546
O -3.629165 -0.480870 1.692645
H -3.792963 -2.508627 -0.004978
H -6.397502 0.057997 2.090129

Complex 12

H 5.712383 -0.095514 -1.201419
C 5.006686 -1.949416 -0.382436
C 4.986332 -0.561039 -0.540696
H 4.109898 -3.589372 0.654878
C 4.086369 -2.513481 0.502440
C 4.070472 0.253247 0.134789
C 3.148658 -1.747447 1.208333
C 3.117901 -0.344372 0.997763
P -0.008304 0.981211 -0.175548
C 2.178752 0.504801 1.822919
C 0.875564 0.957052 1.470253
H 3.667393 0.497075 3.363469
C 2.663514 0.822381 3.106860
C 0.117221 1.621878 2.456074
H -0.897151 1.921545 2.221834
C 1.909734 1.516334 4.049767
C 0.612928 1.902656 3.726056
H 2.329371 1.733730 5.028360
H -0.015763 2.414756 4.448664
C 0.775713 -0.275501 -1.338361
C 0.223104 -1.680859 -1.019326
C 0.546515 0.047950 -2.831874
H 1.853510 -0.270685 -1.148716
C 0.850148 -2.758541 -1.918661
H -0.866589 -1.670989 -1.164576
H 0.389606 -1.924073 0.034892
C 1.185425 -1.027005 -3.730209
H -0.530042 0.104125 -3.037639
H 0.974896 1.023413 -3.087913

C 0.656714 -2.430445 -3.405416
 H 0.409851 -3.736724 -1.684010
 H 1.923872 -2.835119 -1.696970
 H 0.994954 -0.781048 -4.782822
 H 2.277335 -1.011819 -3.596520
 H 1.155944 -3.181533 -4.031075
 H -0.414588 -2.478359 -3.651995
 C 0.454686 2.681380 -0.901148
 C -0.631167 3.154566 -1.895502
 C 0.701221 3.789385 0.144248
 H 1.394765 2.524110 -1.449270
 C -0.231463 4.470895 -2.582626
 H -1.566841 3.302647 -1.338440
 H -0.853756 2.393296 -2.645803
 C 1.102864 5.112229 -0.533903
 H -0.214697 3.948750 0.730286
 H 1.475957 3.494727 0.857985
 C 0.060022 5.576169 -1.559674
 H -1.030917 4.782074 -3.266723
 H 0.661780 4.302269 -3.203015
 H 1.256314 5.882506 0.233010
 H 2.071975 4.977366 -1.037624
 H 0.402046 6.488933 -2.064191
 H -0.871184 5.837500 -1.035658
 C 4.171456 1.770344 -0.025849
 C 4.364720 2.223158 -1.484866
 C 5.298909 2.336169 0.863055
 H 3.233824 2.207390 0.330190
 H 3.607191 1.791790 -2.148575
 H 4.294392 3.315263 -1.552461
 H 5.348465 1.939729 -1.876343
 H 5.132408 2.095484 1.918060
 H 6.271194 1.920456 0.572464
 H 5.355168 3.427528 0.768867
 C 2.249429 -2.445757 2.235086
 C 2.994175 -2.630284 3.576110
 C 1.712459 -3.815344 1.774418
 H 1.385096 -1.800250 2.423736
 H 3.313739 -1.675391 4.001364
 H 2.344502 -3.124872 4.308338
 H 3.885310 -3.254816 3.438683
 H 1.244114 -3.770765 0.787298
 H 2.504749 -4.571869 1.734402
 H 0.963099 -4.175196 2.488871
 C 6.006807 -2.823486 -1.128133
 C 7.459671 -2.504894 -0.725925

C 5.824541 -2.730531 -2.655118
 H 5.806023 -3.863176 -0.835420
 H 7.602928 -2.607461 0.355344
 H 8.157802 -3.184550 -1.229168
 H 7.734925 -1.480334 -1.003585
 H 4.800844 -2.987900 -2.949132
 H 6.032175 -1.717299 -3.019489
 H 6.509702 -3.415425 -3.168929
 H -7.286039 -4.197359 -0.694443
 C -6.749620 -3.252457 -0.680815
 C -5.842998 -2.965106 -1.707155
 C -6.976457 -2.339116 0.356580
 C -5.171611 -1.748817 -1.651786
 H -5.675243 -3.667390 -2.519626
 C -6.296020 -1.118800 0.400116
 H -7.687466 -2.584747 1.140659
 C -5.373596 -0.816258 -0.603127
 N -4.246468 -1.203059 -2.552158
 H -6.465862 -0.420758 1.215193
 C -4.514948 0.338733 -0.865037
 C -3.830472 0.041871 -2.118280
 H -3.765157 -1.710762 -3.280763
 H -4.823439 1.355457 -0.637038
 O -2.874900 0.706932 -2.612262
 Pd -2.390150 0.590527 -0.275689
 C -2.756367 0.191186 1.657865
 C -3.469799 1.100572 2.454479
 C -2.348923 -1.022170 2.230173
 C -3.751242 0.810075 3.794818
 H -3.812995 2.044174 2.036040
 C -2.638348 -1.314745 3.567577
 H -1.801297 -1.749065 1.635765
 C -3.336068 -0.398636 4.356986
 H -4.302964 1.530381 4.395801
 H -2.315122 -2.263365 3.991416
 H -3.558128 -0.626092 5.396563

Transition State 1-TS

C -0.556715 2.567021 -0.425372
 C -1.190641 2.211590 -1.643748
 C -2.567920 1.959315 -1.637623
 C -3.345179 2.063346 -0.481732
 C -2.699973 2.419507 0.705432
 C -1.324750 2.673481 0.759965
 C 0.876878 3.037191 -0.449920

C 2.028435 2.226000 -0.284154
C 3.293061 2.831300 -0.422752
C 3.444769 4.191457 -0.682692
C 2.312860 4.993403 -0.808418
C 1.052776 4.412391 -0.696435
H -3.054941 1.684958 -2.569824
H -3.284514 2.518566 1.616035
H 4.190214 2.229837 -0.333557
H 4.440053 4.616164 -0.782677
H 2.406384 6.058446 -1.003116
H 0.166236 5.029259 -0.813225
P 1.914471 0.415689 0.168575
Pd -0.130341 -0.699601 -0.225750
C 3.398505 -0.333811 -0.718683
C 3.659348 -1.795353 -0.295916
C 3.204242 -0.245144 -2.248138
H 4.290393 0.248070 -0.449735
C 4.858272 -2.390391 -1.056150
H 2.768183 -2.399905 -0.493708
H 3.850645 -1.856250 0.780995
C 4.401183 -0.844334 -3.005873
H 2.290866 -0.791477 -2.518865
H 3.054163 0.796810 -2.554908
C 4.673214 -2.292715 -2.576412
H 4.994580 -3.436848 -0.755313
H 5.777032 -1.857818 -0.766170
H 4.214444 -0.793518 -4.086287
H 5.296273 -0.232886 -2.815088
H 5.557545 -2.685191 -3.094915
H 3.824077 -2.923793 -2.874165
C 2.372349 0.487037 2.014228
C 1.897623 -0.767033 2.780641
C 3.842362 0.810394 2.351279
H 1.761100 1.329507 2.368820
C 2.117116 -0.618648 4.295679
H 2.434967 -1.653979 2.421150
H 0.838335 -0.945088 2.564800
C 4.052904 0.951690 3.870672
H 4.494680 0.009543 1.977044
H 4.156064 1.735969 1.857784
C 3.579909 -0.295375 4.629810
H 1.802064 -1.537592 4.806915
H 1.472553 0.187816 4.675765
H 5.112658 1.148801 4.078271
H 3.495602 1.829097 4.230722
H 3.702744 -0.152453 5.711022

H 4.213635 -1.151055 4.352882
C -0.111479 -2.814364 -0.492306
C 0.212769 -3.629243 0.608937
C 0.308812 -3.199526 -1.782538
C 0.988344 -4.774786 0.422419
H -0.123076 -3.375288 1.605360
C 1.079880 -4.351823 -1.943306
H 0.025370 -2.607131 -2.641100
C 1.431337 -5.146964 -0.848808
H 1.243749 -5.380460 1.289103
H 1.405203 -4.626406 -2.944349
H 2.028864 -6.043745 -0.985301
C -0.711563 3.119101 2.087472
C -1.038800 2.154537 3.243054
C -1.138436 4.557453 2.444911
H 0.377190 3.129894 1.968443
H -0.756825 1.126085 2.993586
H -0.499943 2.451223 4.151405
H -2.108237 2.155069 3.482946
H -0.845205 5.265588 1.662447
H -2.225701 4.627153 2.568415
H -0.671629 4.877749 3.384548
C -0.434188 2.185431 -2.973246
C -0.672324 3.492392 -3.759615
C -0.777978 0.968999 -3.850876
H 0.635654 2.132943 -2.747748
H -0.351182 4.372343 -3.192622
H -0.116135 3.477515 -4.705046
H -1.736103 3.614515 -3.997137
H -0.716444 0.029808 -3.294576
H -1.791911 1.035852 -4.262661
H -0.088257 0.921153 -4.702735
C -4.854464 1.863554 -0.548763
C -5.584917 3.222227 -0.536685
C -5.398102 0.941356 0.556132
H -5.070816 1.385058 -1.514093
H -5.238026 3.866284 -1.352354
H -6.667584 3.083904 -0.646611
H -5.407908 3.753429 0.406639
H -4.892708 -0.029829 0.556438
H -5.269614 1.383171 1.551371
H -6.471784 0.768898 0.413300
C -2.615093 -2.351825 0.688948
C -3.870003 -2.818647 0.257077
N -1.777782 -2.029020 -0.412508
C -3.898586 -2.761940 -1.242375

H -3.999626 -3.742064 -1.726773
 C -4.844112 -3.177612 1.179319
 H -5.815984 -3.531240 0.843298
 C -4.563560 -3.072525 2.548168
 H -5.315432 -3.355778 3.279200
 C -3.325720 -2.583753 2.971340
 H -3.121343 -2.480992 4.033883
 C -2.342963 -2.205867 2.049224
 H -1.402263 -1.782397 2.384492
 C -2.523930 -2.177703 -1.594175
 O -2.129745 -1.922675 -2.718677
 H -4.690584 -2.121188 -1.647567

Transition State 2-TS

C 0.454677 2.617400 -0.576890
 C -0.501793 2.451653 -1.609330
 C -1.845022 2.744718 -1.341347
 C -2.278942 3.199395 -0.094054
 C -1.317991 3.349349 0.910836
 C 0.037917 3.076194 0.696796
 C 1.922144 2.503340 -0.911362
 C 2.711659 1.328680 -0.818920
 C 4.048970 1.390614 -1.257536
 C 4.618765 2.563419 -1.748420
 C 3.849799 3.723408 -1.809925
 C 2.520297 3.681283 -1.398423
 H -2.578079 2.634692 -2.137335
 H -1.628667 3.710502 1.887642
 H 4.666445 0.500082 -1.224146
 H 5.654622 2.566568 -2.077053
 H 4.274886 4.651052 -2.183847
 H 1.911088 4.578828 -1.461957
 P 2.045433 -0.258813 -0.092674
 Pd -0.308609 -0.566927 0.113855
 C 2.897373 -1.586478 -1.123315
 C 2.656453 -2.998203 -0.545250
 C 2.405155 -1.513225 -2.585653
 H 3.980627 -1.403807 -1.112979
 C 3.298134 -4.085237 -1.425239
 H 1.579059 -3.182647 -0.465719
 H 3.061759 -3.070389 0.470046
 C 3.043755 -2.606290 -3.459221
 H 1.312963 -1.633261 -2.594975
 H 2.619228 -0.525046 -3.010308
 C 2.803773 -4.005634 -2.875437

H 3.077668 -5.072716 -1.000568
 H 4.393028 -3.973060 -1.407620
 H 2.643009 -2.541843 -4.479194
 H 4.126343 -2.424668 -3.537435
 H 3.300177 -4.766665 -3.491380
 H 1.727551 -4.229004 -2.899663
 C 2.887126 -0.254877 1.612862
 C 2.144649 -1.150295 2.630169
 C 4.402858 -0.533835 1.632917
 H 2.739270 0.785556 1.936826
 C 2.735470 -0.997760 4.042451
 H 2.214048 -2.202088 2.322773
 H 1.076951 -0.902416 2.638065
 C 4.981336 -0.385130 3.052836
 H 4.597180 -1.554857 1.276802
 H 4.929308 0.147109 0.955768
 C 4.245239 -1.274995 4.063640
 H 2.211291 -1.669155 4.734102
 H 2.549723 0.025421 4.401133
 H 6.053315 -0.622118 3.040122
 H 4.897631 0.666064 3.365892
 H 4.649906 -1.119623 5.072021
 H 4.423949 -2.331525 3.813429
 C -1.229510 -2.430255 0.142046
 C -0.862470 -3.323999 1.162816
 C -1.526638 -2.939759 -1.134326
 C -0.732997 -4.688212 0.888287
 H -0.679773 -2.954179 2.166137
 C -1.379195 -4.303298 -1.401791
 H -1.870510 -2.277909 -1.922095
 C -0.980536 -5.184955 -0.393919
 H -0.437753 -5.364605 1.687516
 H -1.592653 -4.676087 -2.401161
 H -0.882917 -6.247399 -0.600560
 C 1.031371 3.345221 1.826752
 C 0.619664 2.682004 3.154762
 C 1.250257 4.859845 2.020434
 H 1.996537 2.918815 1.533198
 H 0.424961 1.611971 3.028708
 H 1.415199 2.804041 3.900073
 H -0.286964 3.134418 3.572940
 H 1.615245 5.331264 1.101394
 H 0.316185 5.358990 2.304873
 H 1.985880 5.045603 2.812591
 C -0.104946 2.030588 -3.024761
 C -0.207325 3.218114 -4.003295

C -0.917112 0.827603 -3.537771
 H 0.943336 1.718706 -3.001852
 H 0.427343 4.051947 -3.684068
 H 0.108359 2.917206 -5.009732
 H -1.237344 3.588520 -4.070448
 H -0.836260 -0.016773 -2.844154
 H -1.979405 1.072184 -3.658215
 H -0.542709 0.506806 -4.517625
 C -3.739392 3.569541 0.136597
 C -3.899708 5.085521 0.367595
 C -4.381659 2.767591 1.283349
 H -4.284049 3.318285 -0.783781
 H -3.478962 5.660860 -0.464629
 H -4.959057 5.351567 0.466449
 H -3.388973 5.402808 1.284749
 H -4.338773 1.691604 1.085749
 H -3.877106 2.957024 2.238219
 H -5.435118 3.047911 1.403225
 C -3.695761 -1.082915 0.002711
 C -4.600366 -1.694269 0.899012
 C -5.890566 -2.045312 0.520690
 H -6.575569 -2.515680 1.220861
 C -6.285210 -1.761657 -0.793718
 H -7.289173 -2.026431 -1.114392
 C -5.413140 -1.137287 -1.688349
 H -5.743728 -0.916537 -2.699440
 C -4.112656 -0.793513 -1.292106
 H -3.436131 -0.304168 -1.987146
 C -2.703296 -1.267701 2.151211
 O -1.987440 -1.166588 3.137484
 N -3.978479 -1.819348 2.144435
 H -4.408141 -2.178566 2.984962
 C -2.418938 -0.845931 0.727239
 H -2.122889 0.229057 0.725203

Transition State 3-TS

H -5.828729 1.011747 1.035861
 C -5.462191 -1.079481 0.728094
 C -5.198901 0.279599 0.538444
 H -4.875615 -3.054359 0.158211
 C -4.662307 -1.994954 0.042811
 C -4.159499 0.730826 -0.282759
 C -3.609967 -1.601325 -0.794863
 C -3.329773 -0.216149 -0.933644
 P -0.027855 0.806681 0.057154

C -2.243134 0.216794 -1.891400
 C -0.879849 0.488934 -1.582007
 H -3.684119 0.083048 -3.471771
 C -2.638435 0.266562 -3.242113
 C 0.013729 0.688580 -2.656320
 H 1.067296 0.839397 -2.432365
 C -1.746611 0.521144 -4.281533
 C -0.399765 0.709347 -3.986247
 H -2.101925 0.548507 -5.308253
 H 0.328318 0.874207 -4.775536
 C -0.981933 -0.061807 1.426858
 C -0.609550 -1.558461 1.426516
 C -0.726367 0.541541 2.824268
 H -2.049839 0.037874 1.208509
 C -1.369905 -2.334870 2.513595
 H 0.470770 -1.653701 1.595551
 H -0.801060 -1.996126 0.441530
 C -1.487082 -0.235453 3.914144
 H 0.350598 0.514302 3.045438
 H -1.034012 1.592586 2.856508
 C -1.133602 -1.728387 3.903644
 H -1.059232 -3.387785 2.500183
 H -2.445669 -2.319536 2.287536
 H -1.270366 0.204333 4.896316
 H -2.568226 -0.118260 3.748690
 H -1.720365 -2.263724 4.661217
 H -0.075996 -1.852695 4.179901
 C -0.295338 2.670991 0.345498
 C 0.789268 3.220144 1.303701
 C -0.277266 3.498141 -0.957938
 H -1.279733 2.792363 0.818234
 C 0.595629 4.719251 1.590685
 H 1.773700 3.060636 0.838615
 H 0.806180 2.665526 2.245863
 C -0.469278 4.999962 -0.681856
 H 0.685485 3.345019 -1.466136
 H -1.048560 3.153196 -1.652559
 C 0.579187 5.543442 0.297112
 H 1.392782 5.069479 2.258916
 H -0.351839 4.867110 2.130534
 H -0.430729 5.551892 -1.629810
 H -1.474587 5.165415 -0.265904
 H 0.385654 6.601048 0.517553
 H 1.572274 5.496454 -0.173167
 C -3.997483 2.232787 -0.513738
 C -4.154578 3.075871 0.765407

C -4.980234 2.725420 -1.597156
 H -2.987224 2.403229 -0.896684
 H -3.522819 2.703804 1.579764
 H -3.875352 4.117123 0.565882
 H -5.189405 3.084882 1.126653
 H -4.823824 2.201597 -2.545568
 H -6.018597 2.557638 -1.286750
 H -4.849550 3.799470 -1.777749
 C -2.859016 -2.679374 -1.585302
 C -3.638204 -3.059051 -2.864150
 C -2.567700 -3.962820 -0.783121
 H -1.895820 -2.262528 -1.896942
 H -3.792098 -2.198638 -3.520460
 H -3.091363 -3.822261 -3.431113
 H -4.622736 -3.469472 -2.608374
 H -2.084898 -3.754297 0.174885
 H -3.481011 -4.534924 -0.581373
 H -1.902055 -4.613332 -1.361863
 C -6.589027 -1.555720 1.635674
 C -7.967027 -1.062501 1.154940
 C -6.343644 -1.159986 3.104633
 H -6.598411 -2.653276 1.587954
 H -8.158658 -1.368122 0.120519
 H -8.765151 -1.471951 1.785700
 H -8.037613 0.030867 1.199191
 H -5.381940 -1.543783 3.463269
 H -6.334621 -0.070058 3.225753
 H -7.133471 -1.560703 3.751408
 Pd 2.284564 0.326796 -0.077386
 C 3.081495 -1.589832 -0.498035
 C 3.144125 -2.509269 0.561432
 C 2.805934 -2.036352 -1.802740
 C 2.867953 -3.857137 0.319596
 H 3.393039 -2.188409 1.564170
 C 2.533548 -3.388500 -2.017679
 H 2.809062 -1.336513 -2.627122
 C 2.557958 -4.307010 -0.964925
 H 2.900980 -4.556684 1.151659
 H 2.299901 -3.720272 -3.026688
 H 2.349237 -5.357784 -1.145059
 N 4.308175 -0.169580 -0.355043
 C 4.960217 0.107098 -1.567733
 C 5.274831 -0.214266 0.681080
 C 6.476044 0.103055 -1.320896
 O 4.410383 0.288779 -2.640164
 C 6.577722 -0.083752 0.166161

C 5.056406 -0.298824 2.055979
 H 6.915506 1.039887 -1.682740
 H 6.926387 -0.709667 -1.906107
 C 7.672294 -0.077418 1.019486
 C 6.167968 -0.306632 2.906635
 H 4.048118 -0.323428 2.456941
 C 7.465506 -0.205592 2.399797
 H 8.678945 0.032367 0.623037
 H 6.012806 -0.378292 3.979996
 H 8.314891 -0.207824 3.076993

Transition State 4-TS

H 5.933380 0.743906 -1.106226
 C 5.480569 -1.315969 -0.713537
 C 5.280532 0.059730 -0.571741
 H 4.817044 -3.240235 -0.061124
 C 4.652153 -2.168773 0.017265
 C 4.275282 0.587346 0.246350
 C 3.631181 -1.697401 0.853839
 C 3.414412 -0.296985 0.943229
 P 0.149415 0.831778 -0.052165
 C 2.360756 0.220600 1.895751
 C 1.008537 0.544615 1.588316
 H 3.810456 0.079025 3.467678
 C 2.772366 0.303392 3.240004
 C 0.138095 0.830479 2.661963
 H -0.908870 1.022974 2.440207
 C 1.905095 0.640682 4.276609
 C 0.565940 0.883569 3.986280
 H 2.272339 0.690231 5.298247
 H -0.144272 1.114931 4.775172
 C 1.050415 -0.131182 -1.395346
 C 0.602404 -1.606433 -1.340199
 C 0.818412 0.434619 -2.812714
 H 2.123533 -0.078713 -1.186829
 C 1.313334 -2.459701 -2.403112
 H -0.483680 -1.652093 -1.497484
 H 0.780980 -2.017466 -0.341177
 C 1.533588 -0.418501 -3.875946
 H -0.259199 0.454191 -3.031391
 H 1.178832 1.466888 -2.883433
 C 1.102497 -1.889361 -3.812623
 H 0.946691 -3.493281 -2.352110
 H 2.389534 -2.494521 -2.181169
 H 1.335863 -0.002772 -4.872518

H 2.620093 -0.351779 -3.717425
H 1.656735 -2.480722 -4.552818
H 0.038529 -1.967430 -4.081147
C 0.500967 2.668121 -0.422233
C -0.561466 3.230731 -1.396267
C 0.536699 3.550587 0.844021
H 1.485540 2.718671 -0.906997
C -0.288163 4.702115 -1.753462
H -1.547426 3.148885 -0.916081
H -0.618651 2.632835 -2.309997
C 0.805782 5.026581 0.500100
H -0.428553 3.470564 1.364174
H 1.294682 3.196215 1.548576
C -0.218327 5.581255 -0.498228
H -1.069597 5.065226 -2.433353
H 0.662213 4.773691 -2.303403
H 0.803135 5.622044 1.422125
H 1.815604 5.118968 0.072607
H 0.030749 6.615817 -0.767000
H -1.209352 5.610039 -0.022146
C 4.183325 2.102751 0.421756
C 4.368011 2.889504 -0.889242
C 5.196353 2.590534 1.479243
H 3.184961 2.333966 0.804078
H 3.714662 2.515449 -1.685485
H 4.136189 3.948819 -0.727701
H 5.399586 2.839800 -1.256492
H 5.024830 2.110267 2.447848
H 6.223476 2.364653 1.168301
H 5.115526 3.675402 1.620073
C 2.847430 -2.709051 1.698009
C 3.636097 -3.076259 2.974704
C 2.479552 -4.006467 0.951938
H 1.911554 -2.235737 2.012394
H 3.849317 -2.198564 3.590347
H 3.065051 -3.786244 3.585179
H 4.592318 -3.546849 2.715052
H 1.981118 -3.811848 -0.001052
H 3.361275 -4.625621 0.749516
H 1.802058 -4.605696 1.570979
C 6.570574 -1.875260 -1.618724
C 7.976385 -1.424774 -1.178249
C 6.318306 -1.525453 -3.098205
H 6.533287 -2.969554 -1.528708
H 8.172005 -1.698821 -0.135766
H 8.745336 -1.892483 -1.804719

H 8.093325 -0.337995 -1.265944
H 5.335106 -1.879994 -3.427418
H 6.354601 -0.441651 -3.261426
H 7.079231 -1.984900 -3.740540
Pd -2.215974 0.382362 0.106931
C -3.317859 -1.290738 0.594708
C -3.451577 -2.261578 -0.407905
C -3.235904 -1.682757 1.939204
C -3.429927 -3.617898 -0.069800
H -3.575157 -1.967470 -1.444753
C -3.219215 -3.042188 2.264296
H -3.208948 -0.933971 2.723541
C -3.311286 -4.013144 1.264350
H -3.516462 -4.364799 -0.855650
H -3.143665 -3.338275 3.308078
H -3.308004 -5.068529 1.524109
C -5.222490 0.461021 1.478173
C -5.368156 0.093388 -0.862684
O -4.898728 0.821363 2.599509
C -6.595927 -0.238449 -0.247806
C -5.259057 0.029347 -2.247562
C -7.700485 -0.648893 -0.984479
C -6.366307 -0.377447 -3.005726
H -4.321668 0.290186 -2.733202
C -7.567218 -0.717378 -2.378038
H -8.639954 -0.901277 -0.500280
H -6.288738 -0.429642 -4.088040
H -8.417192 -1.035018 -2.976036
C -4.412115 0.484655 0.201814
N -6.470835 -0.046189 1.129963
H -7.210617 -0.149624 1.809652
H -3.988907 1.505528 0.068400

Complex 13

C 2.770923 -0.864727 0.279571
C 2.567312 0.629174 -0.094172
C 3.833984 1.450660 0.210349
C 5.096440 0.849354 -0.422081
C 5.287739 -0.604976 0.026126
C 4.054309 -1.446958 -0.333124
H 3.679313 2.480923 -0.133060
H 2.390902 0.675205 -1.178398
H 2.860836 -0.913666 1.373513
H 5.018499 0.885235 -1.518466
H 5.972426 1.451735 -0.152290

H 6.179882 -1.040272 -0.439986
 H 5.455260 -0.634974 1.112612
 H 3.964079 -1.472648 -1.426720
 H 4.186914 -2.486265 -0.002460
 H 3.981108 1.501684 1.297571
 N 1.333257 1.125997 0.529613
 N 1.523234 -1.643577 -0.031147
 Cu -0.014737 -0.460999 0.220787
 N -1.690797 0.260903 -0.109839
 C -1.759902 1.512613 -0.652350
 C -3.231304 1.904106 -0.882604
 H -3.395563 2.105974 -1.948753
 O -0.802091 2.251520 -0.938959
 H -3.454724 2.835617 -0.347532
 C -3.971468 0.702971 -0.365262
 C -5.320885 0.401851 -0.268619
 C -2.995602 -0.216674 0.075119
 C -5.711241 -0.832129 0.275075
 H -6.072334 1.111510 -0.609170
 C -3.378171 -1.443161 0.618305
 C -4.742812 -1.738999 0.712192
 H -6.766157 -1.079457 0.357712
 H -2.625193 -2.146483 0.965442
 H -5.052023 -2.692166 1.135287
 C 1.397073 1.644725 1.896421
 H 2.027156 2.538629 2.011325
 H 0.378145 1.900860 2.200286
 H 1.763617 0.876946 2.588195
 H 0.824751 1.784174 -0.074494
 C 1.403505 -2.154812 -1.421202
 H 2.207740 -2.850197 -1.692480
 H 0.441907 -2.661825 -1.512149
 H 1.407100 -1.318424 -2.123317
 H 1.511217 -2.456674 0.583315

Complex 14

C 2.671791 0.713641 -0.621858
 C 2.472456 -0.628174 0.129375
 C 3.645551 -1.592035 -0.123532
 C 5.005378 -0.949755 0.183982
 C 5.192629 0.336708 -0.630219
 C 4.054978 1.327094 -0.343378
 H 3.500055 -2.498395 0.477490
 H 2.445970 -0.404108 1.204298
 H 2.605427 0.497052 -1.697237

H 5.072475 -0.715662 1.256176
 H 5.810849 -1.662015 -0.031753
 H 6.157210 0.804142 -0.398476
 H 5.212468 0.092371 -1.702311
 H 4.117301 1.627626 0.710421
 H 4.178594 2.241155 -0.939572
 H 3.641815 -1.907620 -1.175418
 N 1.131123 -1.179603 -0.179777
 N 1.519577 1.624896 -0.340879
 Cu -0.123320 0.442428 -0.004193
 N -2.461832 -1.562571 0.664594
 C -1.499264 -0.764899 1.317235
 C -1.809023 0.623782 0.960927
 O -0.629356 -1.262065 2.075343
 C -3.098650 0.579395 0.261598
 C -3.963607 1.562293 -0.220198
 C -3.455783 -0.783155 0.079523
 C -5.144650 1.190224 -0.873150
 H -3.720916 2.614529 -0.086878
 C -4.616912 -1.166345 -0.583551
 C -5.465394 -0.158788 -1.058496
 H -5.818704 1.959103 -1.242685
 H -4.868464 -2.216192 -0.715860
 H -6.384228 -0.432165 -1.570916
 H -2.517009 -2.556279 0.834597
 H -1.629490 1.387347 1.719354
 C 0.998318 -2.025850 -1.374747
 H 1.592789 -2.949064 -1.335707
 H -0.056253 -2.294652 -1.476245
 H 1.287110 -1.467362 -2.271443
 H 0.771122 -1.676992 0.642234
 C 1.616545 2.464652 0.874112
 H 2.449147 3.179406 0.846964
 H 0.677924 3.012448 0.979232
 H 1.727362 1.828943 1.755965
 H 1.410333 2.250714 -1.136675

Complex 15

C 3.085366 -0.214017 0.010453
 C 1.973628 0.862989 0.136835
 C 2.562609 2.231224 0.529667
 C 3.720946 2.664870 -0.378134
 C 4.824877 1.600716 -0.389516
 C 4.262957 0.251678 -0.860364
 H 1.759171 2.978153 0.519571

H 1.507052 0.968441 -0.852959
 H 3.462733 -0.407615 1.023780
 H 3.355392 2.821629 -1.403414
 H 4.119970 3.628389 -0.038402
 H 5.650569 1.904865 -1.044082
 H 5.246866 1.498541 0.620926
 H 3.931061 0.366683 -1.899950
 H 5.049116 -0.515721 -0.863148
 H 2.933149 2.185658 1.562514
 N 0.906846 0.367185 1.020706
 N 2.474753 -1.518649 -0.423079
 Cu 0.673369 -1.604612 0.284495
 C 1.031879 0.589107 2.461205
 H 1.057683 1.648159 2.757345
 H 0.170678 0.119431 2.945323
 H 1.933685 0.103320 2.852920
 H -0.022194 0.657072 0.685043
 O -1.088416 -2.188215 0.350490
 C -1.972739 -1.279927 0.158481
 C -4.075200 -0.276036 -0.107135
 H -3.754575 -2.069203 1.119910
 C -2.992917 0.626873 -0.224958
 C -5.383564 0.161037 -0.236098
 C -3.232178 1.978467 -0.475532
 C -5.625588 1.521322 -0.487438
 H -6.215807 -0.534222 -0.144682
 C -4.556838 2.413285 -0.604240
 H -2.402733 2.674672 -0.569237
 H -6.646376 1.879565 -0.590931
 H -4.755471 3.464803 -0.799317
 N -1.743168 0.007502 -0.067024
 C -3.465195 -1.625802 0.158511
 H 3.071685 -2.266525 -0.071473
 C 2.350110 -1.726623 -1.889599
 H 3.318707 -1.729197 -2.405552
 H 1.851992 -2.683570 -2.051199
 H 1.721087 -0.945341 -2.321388
 H -3.681769 -2.375782 -0.612929

Complex 16

C -3.121557 -0.139537 -0.187302
 C -2.077413 0.977912 0.075451
 C -2.587887 2.333268 -0.449570
 C -3.975500 2.692496 0.100891
 C -4.989068 1.583602 -0.209313

C -4.509740 0.237917 0.355383
 H -1.857340 3.111538 -0.196019
 H -1.955158 1.064664 1.164506
 H -3.205142 -0.258267 -1.275953
 H -3.917349 2.838406 1.189365
 H -4.309925 3.646709 -0.323545
 H -5.972070 1.830039 0.209227
 H -5.122848 1.502592 -1.297650
 H -4.474047 0.316026 1.449700
 H -5.228951 -0.557886 0.117842
 H -2.643253 2.300749 -1.545765
 N -0.767521 0.557407 -0.439350
 N -2.604220 -1.466119 0.291120
 Cu -0.740569 -1.581931 -0.145960
 C -0.495380 0.722654 -1.870437
 H -0.502640 1.766265 -2.213195
 H 0.489541 0.295111 -2.071742
 H -1.226241 0.160301 -2.462361
 H 0.003685 0.953799 0.095295
 O 0.999440 -2.097307 -0.382943
 C 1.908894 -1.208849 -0.092010
 C 3.287003 0.406449 0.764952
 H 1.328953 -0.147095 1.747330
 C 3.919819 -0.162755 -0.382865
 H 3.232766 -1.756364 -1.648523
 C 3.964710 1.423850 1.455707
 C 5.168373 0.255212 -0.833884
 C 5.217397 1.844537 1.008590
 H 3.517653 1.878807 2.337342
 C 5.816173 1.270159 -0.123913
 H 5.628316 -0.195166 -1.710892
 H 5.740575 2.631082 1.547578
 H 6.792967 1.614725 -0.453173
 N 3.056380 -1.125016 -0.882071
 C 2.023984 -0.256421 0.923963
 H -3.140830 -2.186425 -0.192182
 C -2.748850 -1.731179 1.746628
 H -3.794212 -1.721406 2.077548
 H -2.312348 -2.708805 1.956202
 H -2.189342 -0.984764 2.313932

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