

Sterically Demanding, Sulfonated, Triarylphosphines: Application to Palladium- Catalyzed Cross-Coupling, Steric and Electronic Properties, and Coordination Chemistry

Lucas R. Moore, Elizabeth C. Western, Raluca Craciun, Jason M. Spruell, David A. Dixon,
Kevin P. O'Halloran, Kevin H. Shaughnessy**

Department of Chemistry and Center for Green Manufacturing, The University of Alabama,
Tuscaloosa, Alabama 35487-0336

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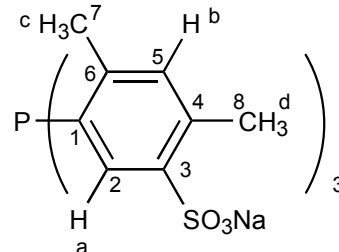
Synthetic Details and Characterization Data

General Information. TXPTS•Na₃ and TMAPTS•Na₃ were prepared as previously described.^{1,2} All other materials were obtained from commercial suppliers and used as received. Water (deionized) and aqueous acetonitrile solutions were deoxygenated by sparging with nitrogen for at least 15 minutes before each use.

Tri(2,4-dimethyl-5-sulfonatophenyl)phosphine (TXPTS•Na₃). ¹H NMR (360 MHz, CD₃OD): δ 7.32 (d, *J* = 4.93 Hz, 3H), 7.25 (d, *J* = 4.93 Hz, 3H), 2.59 (s, 9H), 2.31 (s, 9H). ¹³C NMR (90.5 MHz, 2:1 D₂O/CD₃CN): δ 145.9 (d, *J*_{C-P} = 26.0 Hz), 140.7, 138.0, 134.4, 131.8, 130.7 (d, *J*_{C-P} = 8.1 Hz), 20.6 (d, *J*_{C-P} = 21.5 Hz), 19.8, ³¹P NMR (202.5 MHz, CD₃OD): δ -30.3.

Table S1. ¹H and ¹³C peak assignments for TXPTS•Na₃

¹ H (2:1 D ₂ O/CD ₃ CN)			¹³ C (2:1 D ₂ O/CD ₃ CN)	
	δ (ppm)	<i>J</i> _{H,P} (Hz)	δ (ppm)	<i>J</i> _{C,P} (Hz)
H ^a	7.19	4.6	C ¹	145.9
H ^b	7.16	4.3	C ²	131.8
H ^c	2.48		C ³	138.0
H ^d	2.26		C ⁴	140.7
			C ⁵	134.4
			C ⁶	130.7
			C ⁷	20.6
			C ⁸	19.8



Complete assignments of the proton and carbon resonances of TXPTS•Na₃ (Table S1) were made using HSQC/HMBC spectra (Table S2). The assignment was started by observing that H^a should not be coupled to either methyl group carbon. The cross peaks for the two aromatic protons show that the 7.16 ppm peak is not coupled to the upfield carbon resonances, while the 7.19 ppm peak is coupled to the 20 ppm ¹³C NMR resonances. Since the 7.16 ppm peak shows a ¹*J* coupling to the peak at 131.8 (HSQC singlet), this carbon peak must be C². The ¹H resonance at 7.19 ppm, which must be H^b, has a 1 bond coupling to the ¹³C NMR resonance at 134.4 ppm. Therefore, the 134.4 ppm peak must be C⁵. The two methyl carbons could not be resolved in the HSQC and HMBC experiments, thus the assignments for H^c, H^d, C¹, C³, C⁴, and C⁶ cannot be unambiguously determined. H^c would be coupled to C¹, C⁵, and C⁶ by two- and three-bond couplings, but not to C³ and C⁴. Conversely, H^d would be coupled to C³, C⁴, and C⁵ by two- and three-bond couplings, but not to C¹ and C⁶. Both the 2.48 and 2.26 ppm peaks are coupled to the 134.4 peak, which has already been assigned to C⁵. Therefore, if the 2.26 ppm resonance is H^c, then the C¹ peak would be at 145.9 or 130.7 ppm, with C⁶ being the other peak. Alternatively, if the 2.26 resonance is H^d, the C¹ peak would be at 140.7 or 138 ppm. The ¹³C resonances at 145.9 and 138 ppm correspond to C¹ and C³ based on their coupling to H^a. Assuming that the ¹*J*_{C,P} coupling would be larger than the three bond coupling, C¹ has been assigned to the doublet at 145.9 ppm and C³ to the singlet at 138 ppm. Therefore, the ¹H NMR resonance at 2.26 ppm corresponds to H^c and the 2.48 ppm resonance is H^d. The other assignments can be obtained by a process of elimination: 140.7 = C⁴; 130.7 = C⁶. The peak at 20.6 ppm was assigned to C⁷, since it has a ²*J* coupling to the phosphorus. C⁸, which would not be expected to couple to the P, was assigned to the singlet at 19.8 ppm.

Table S2. ^1H - ^{13}C coupling determined by HSQC/HMBC tests.

^1H (δ)	Coupled ^{13}C resonances ^a
7.19 ppm	134.4 (1J), 140.3 ($^{\gamma^1}J$), and 20 ($^{\gamma^1}J$) ppm
7.16 ppm	131.8 (1J), 138.0 ($^{\gamma^1}J$), and 145.9 ($^{\gamma^1}J$) ppm
2.48 ppm	20 (1J), 140.7 ($^{\gamma^1}J$), 138 ($^{\gamma^1}J$), and 134.4 ($^{\gamma^1}J$) ppm
2.26 ppm	20 (1J), 145.9 ($^{\gamma^1}J$), 134.4 ($^{\gamma^1}J$), and 130.7 ($^{\gamma^1}J$) ppm

^aHMBC spectra gave all ^1H - ^{13}C couplings, while the HSQC experiment gave only $^1J_{\text{H,C}}$ couplings.

Tri(4-methoxy-2-methyl-5-sulfonatophenyl)phosphine trisodium (TMPTS•Na₃). ^1H NMR (360MHz, CD₃OD): δ 6.82 (d, J = 4.32 Hz, 3H), 6.39 (d, J = 3.69 Hz, 3H), 3.31 (s, 9H), 1.75 (s, 9H). ^{13}C NMR (90.5 MHz, CD₃OD): δ 158.9, 149.5 (d, $J_{\text{C-P}}$ = 26.36 Hz), 134.6, 131.2, 125.0 (d, $J_{\text{C-P}}$ = 8.32 Hz), 115.9 (d, $J_{\text{C-P}}$ = 4.16Hz), 57.0, 22.0 (d, $J_{\text{C-P}}$ = 20.81 Hz). ^{31}P NMR (202.5 MHz, CD₃OD): δ -29.5 (s).

Representative Procedure for the Suzuki Cross-Coupling Reactions. Pd(OAc)₂ (5.60 mg, 0.025 mmol), ligand (0.063 mmol), arylboronic acid (1.20 mmol) and Na₂CO₃ (0.210 g, 2.00 mmol) were added to a 50 mL round bottom equipped with a stir bar and rubber septum while in the dry box. Upon removing the flask from the dry box, the aryl bromide (1.00 mmol) and deoxygenated 1:1 CH₃CN:H₂O (10 mL) were added via syringe. The reaction was placed in a pre-heated oil bath at 50 or 80 °C and allowed to stir until determined to be complete by GC (typically 2-4 hours). The reaction mixture was poured into saturated sodium carbonate (50ml), extracted with ethyl acetate (3 × 30 mL), and dried with MgSO₄. The crude products were purified by flash chromatography (SiO₂).

4-Acetylbiphenyl (Table 1, entry 1)³ Using the general procedure, 4-bromoacetophenone (203 mg, 1.00 mmol) was coupled with phenylboronic acid. The crude product was chromatographed eluting with hexane:MeCl₂:EtOAc (75:20:5) to give 4-acetylbiphenyl (182 mg, 91 % yield) as a white solid. ^1H NMR (360 MHz, CDCl₃): δ 8.03 (d, J = 8.63 Hz, 2H), 7.68 (d, J = 8.63 Hz, 2H), 7.62 (d, J = 7.39 Hz, 2H), 7.51 (m, 3H), 2.69 (s, 3H). ^{13}C NMR (90.6 MHz, CDCl₃): δ 197.7, 145.8, 139.9, 135.8, 128.9, 128.8, 128.2, 127.3, 127.2, 26.6. mp 115-117 °C (lit. mp 119-120°)

4-Acetyl-4'-methoxybiphenyl (Table 1, entry 2)⁴ Using the general procedure, 4-bromoacetophenone (210 mg, 1.00 mmol) was coupled with 4-methoxyphenylboronic acid. The crude product was chromatographed eluting with hexane:MeCl₂:EtOAc (75:20:5) to give 4-acetyl-4'-methoxybiphenyl (223 mg, 93 %) yield as a white solid. ^1H NMR (360 MHz, CDCl₃): δ 8.03 (d, J = 8.63 Hz, 2H), 7.65 (d, J = 8.63 Hz, 2H), 7.58 (d, J = 9.25 Hz, 2H), 6.99 (d, J = 8.63 Hz, 2H), 3.87 (s, 3H), 2.63 (s, 3H). mp 149-151 °C (lit mp 153.5-155)³.

4-Methylbiphenyl (Table 1, entry 3)⁴ Using the general procedure, 4-bromotoluene (181 mg, 1.06 mmol) was coupled with phenylboronic acid. The crude product was chromatographed eluting with hexane:MeCl₂:EtOAc (75:20:5) to give 4-methylbiphenyl (169 mg, 95 % yield) as a colorless solid. ^1H NMR (360 MHz, CDCl₃): δ 7.56 (d, J = 1.23 Hz, 2H), 7.46 (d, J = 8.02 Hz, 2H), 7.39 (m, 1H), 7.37 (m, 2H), 7.25 (d, J = 8.02, 2H), 2.36 (s, 3H).

4-Fluoro-4'-methylbiphenyl (Table 1, entry 4)⁵ Using the general procedure, 4-bromotoluene (171 mg, 1.00 mmol) was coupled with 4-fluorophenylboronic acid. The crude product was chromatographed eluting with hexane:MeCl₂:EtOAc (75:20:5) to give 4-methyl-4'-fluorobiphenyl (177 mg, 94 % yield) as a white solid. ¹H NMR (360 MHz, CDCl₃): δ 7.52 (d, *J* = 8.63 Hz, 2H), 7.43 (d, 8.02 Hz, 2H), 7.23 (d, *J* = 8.02 Hz, 2H), 7.10 (d, *J* = 8.64 Hz, 2H), 2.39 (s, 3H). m.p. 74-77 °C.

4-Methoxy-4'-methylbiphenyl (Table 1, entry 5).⁶ Using the general procedure, 4-bromotoluene (174 mg, 1.00 mmol) was coupled with 4-methoxyphenylboronic acid. The crude product was chromatographed eluting with hexane:MeCl₂:EtOAc (75:20:5) to give 4-methoxy-4'-methylbiphenyl (186 mg, 92 % yield) as a white solid. ¹H NMR (360 MHz, CDCl₃): δ 7.49 (d, *J* = 8.63 Hz, 2H), 7.44 (d, *J* = 8.02 Hz, 2H), 7.22 (d, *J* = 8.02 Hz, 2H), 6.96 (d, *J* = 8.63 Hz, 2H), 3.83 (s, 3H), 2.38 (s, 3H). ¹³C NMR (90.6 MHz, CDCl₃): δ 159.6, 138.0, 136.3, 129.4, 127.9, 127.7, 126.6, 114.1, 55.3, 21.2. m.p. 106-108 °C.

4-Methoxybiphenyl (Table 1, entry 6).⁴ Using the general procedure, 4-bromoanisole (188 mg, 1.01 mmol) was coupled with phenylboronic acid. The crude product was chromatographed eluting with hexane:MeCl₂:EtOAc (75:20:5) to give 4-methoxybiphenyl (183 mg, 99 % yield) as a white solid. ¹H NMR (360 MHz, CDCl₃): δ 7.54 (m, H), 7.44 (m, 2H), 7.29 (m, 2H), 6.97 (d, *J* = 8.63 Hz, 2H), 3.85 (s, 3H). m.p. 84-86 °C (lit.⁷ m.p. 86-90 °C).

4-Fluoro-4'-methoxybiphenyl (Table 1, entry 7).⁸ Using the general procedure, 4-bromoanisole (187 mg, 1.00 mmol) was coupled with 4-fluorophenylboronic acid. The crude product was chromatographed eluting with hexane:MeCl₂:EtOAc (75:20:5) to give 4-methoxy-4'-fluorobiphenyl (195 mg, 97.0 % yield) as a white solid. ¹H NMR (360 MHz, CDCl₃): δ 7.49 (m, 4H), 7.12 (d, *J* = 8.63 Hz, 2H), 6.96 (d, *J* = 6.78 Hz, 2H), 3.84 (s, 3H). mp 86-88 °C (lit mp 87-88 °C).

4-Methoxy-2-methylbiphenyl (Table 1, entry 8).⁹ Using the general procedure, 1-methoxy-3-methyl-4-bromobenzene (199 mg, 1.00 mmol) was coupled with phenylboronic acid. The crude product was chromatographed eluting with hexane:MeCl₂:EtOAc (75:20:5) to give 4-methoxy-2-methylbiphenyl (175 mg, 88 % yield) as a pale yellow oil. ¹H NMR (360 MHz, CDCl₃): δ 7.30 (m, 5H), 7.15 (d, 1H, *J* = 8.63 Hz), 6.69 (m, 2H), 3.67 (s, 3H), 2.15 (s, 3H). ¹³C NMR (90.6 MHz, CDCl₃): δ 158.8, 141.6, 136.4, 134.5, 130.6, 129.2, 127.9, 126.3, 115.6, 111.0, 60.0, 13.9.

2,4'-dimethylbiphenyl (Table 1, entry 9).¹⁰ Using the general procedure, 4-bromotoluene (174 mg, 1.00 mmol) was coupled with 2-tolylboronic acid. The crude product was chromatographed eluting with hexane:MeCl₂:EtOAc (75:20:5) to give 2,4'-dimethylbiphenyl (146.6 mg, 86 %) yield as a pale yellow oil. ¹H NMR (360 MHz, CDCl₃): δ 7.07 (m, 8H), 2.23 (s, 3H), 2.13 (s, 3H). ¹³C NMR (90.6 MHz, CDCl₃): δ 142.1, 139.4, 136.6, 135.6, 130.6, 130.2, 129.4, 129.1, 127.4, 126.1, 21.4, 20.8.

4-Methoxy-2,2'-dimethylbiphenyl (Table 1, entries 10-12).² Using the general procedure, 1-methoxy-3-methyl-4-bromobenzene (199 mg, 1.00 mmol) was coupled with 2-tolylboronic acid. The crude product was chromatographed eluting with hexane:MeCl₂:EtOAc (75:20:5) to give 4-methoxy-2,2'-dimethylbiphenyl (157 mg, 75 % yield) as a pale yellow oil. ¹H NMR (360 MHz, CDCl₃): δ 7.13 (m, 3H), 6.98 (d, *J* = 7.4 Hz, 1H), 6.88 (d, *J* = 8.63 Hz, 1H), 6.69 (m, 2H), 3.69

(s, 3H), 2.02 (s, 3H), 1.85 (s, 3H). ^{13}C NMR (90.6 MHz, CDCl_3): δ 158.6, 141.2, 137.1, 136.2, 134.1, 130.2, 129.8, 129.7, 127.0, 125.4, 115.2, 110.8, 55.0, 20.0, 19.8.

2,6-Dimethylbiphenyl (Table 1, entry 13).¹¹ Using the general procedure, 2-bromo-*m*-xylene (188 mg, 1.00 mmol) was coupled with phenylboronic acid. The crude product was chromatographed eluting with hexane: MeCl_2 :EtOAc (75:20:5) to give 2,6-dimethylbiphenyl (145 mg, 78 % yield) as a pale yellow oil. ^1H NMR (360 MHz, CDCl_3): δ 7.71 (m, 2H), 7.62 (m, 1H), 7.43 (m, 5H), 2.36 (s, 6H).

4-Fluoro-2',6'-dimethylbiphenyl (Table 1, entry 14).² Using the general procedure, 2-bromo-*m*-xylene (188 mg, 1.00 mmol) was coupled with 4-fluorophenylboronic acid. The crude product was chromatographed eluting with hexane: MeCl_2 :EtOAc (75:20:5) to give 4-fluoro-2,6-dimethylbiphenyl (176 mg, 87 % yield) as a pale yellow oil. ^1H NMR (360 MHz, CDCl_3): δ 7.12 (m, 7H), 2.05 (s, 6H). ^{13}C NMR (90.6 MHz, CDCl_3): δ 163.1, 160.4, 140.8, 136.9, 136.2, 130.6 (d, $J_{\text{C-F}}$ = 8.34 Hz), 127.2 (d, $J_{\text{C-F}}$ = 11.14 Hz), 115.5 (d, $J_{\text{C-F}}$ = 20.84 Hz), 20.8.

Representative procedure for the Sonogashira cross-coupling reactions. $\text{Pd}(\text{OAc})_2$ (8.8 mg, 0.03 mmol) and ligand (0.08 mmol) were added to a 50 mL round bottom equipped with a stir bar and rubber septum while in the dry box. Upon removing from dry box, the aryl bromide (1.00 mmol), diisopropylamine (242 mg, 2.40 mmol), degassed 1:1 $\text{CH}_3\text{CN}:\text{H}_2\text{O}$ (10 mL), and alkyne (1.20 mmol), were added via syringe. For the best conversion the alkyne should be added last. The reaction was placed in a pre-heated oil bath and allowed to stir until determined to be complete by GC. The reaction was poured into saturated sodium carbonate (50ml), extracted with ethyl acetate (3×30 mL), and dried with MgSO_4 . The crude products were purified by flash chromatography (SiO_2).

4-(Phenylethynyl)acetophenone (Table 2, entries 1-2).¹² Using the general procedure, 4-bromoacetophenone (204 mg, 1.00 mmol) was coupled with phenylacetylene. The crude material was chromatographed eluting with hexane:EtOAc. The crude product was then recrystallized with hexane:toluene to give 4-(phenylethynyl)acetophenone (TXPTS: 218 mg, 97 % yield; TMAPTS: 208 mg, 94 %) as a tan solid. ^1H NMR (360 MHz, CDCl_3): δ 7.94 (d, J = 8.02 Hz, 2H), 7.56 (m, 4H), 7.37 (m, 3H), 2.61 (s, 3H). ^{13}C NMR (90.6 MHz, CDCl_3): δ 197.6, 136.5, 132.1, 132.0, 129.1, 128.7, 128.5, 122.9, 93.0, 88.8, 26.8. m.p. 94-96 °C (lit. m.p. 95-97 °C). Predicted for $\text{C}_{16}\text{H}_{12}\text{O}$: C, 87.25; H, 5.49. Found: C, 87.06; H, 5.64.

4-(Phenylethynyl)benzoic acid (Table 2, entries 3-4).¹² Using the general procedure, 4-bromobenzoic acid (201 mg, 1.00 mmol) was coupled with phenylacetylene. At the completion of the reaction, the reaction mixture was made strongly acidic (pH = 1) with concentrated HCl prior to extraction with ethyl acetate. The crude material recrystallized from water and a minimal amount of methanol to give 4-(phenylethynyl)benzoic acid (TXPTS: 240 mg, 99 % yield; TMAPTS: 221 mg, 99 %) as a tan solid. ^1H NMR (360 MHz, CDCl_3): δ 8.09 (d, J = 8.32 Hz, 2H), 7.62 (m, 4H), 7.38 (m, 3H). ^{13}C NMR (90.6 MHz, CDCl_3): δ 167.2, 143.1, 131.7, 131.3, 130.4, 130.0, 129.5, 127.1, 81.3, 79.9. One aromatic carbon was masked by solvent. Predicted for $\text{C}_{15}\text{H}_{10}\text{O}_2$: C, 81.07; H, 4.54. Found: C, 80.67; H, 4.83.

4-(Phenylethynyl)toluene (Table 2, entries 5-6).¹² Using the general procedure, 4-bromotoluene (171 mg, 1.00 mmol) was coupled with phenylacetylene. The crude product was

chromatographed eluting with hexane to give 4-(phenylethynyl)toluene (TXPTS: 138 mg, 74 % yield; TMAPTS: 139 mg, 74 % yield) as a white solid. ¹H NMR (360 MHz, CDCl₃): δ 7.51 (m, 2H), 7.42 (d, *J* = 8.32 Hz, 2H), 7.32 (m, 3H), 7.15 (d, *J* = 7.77 Hz, 2H), 2.37 (s, 3H). ¹³CNMR (90.6 MHz, CDCl₃): δ 138.6, 131.8, 131.7, 129.3, 128.5, 128.3, 123.7, 120.4, 89.8, 88.9, 21.7.

2-(Phenylethynyl)toluene (Table 2, entries 7-8).¹³ Using the general procedure, 2-bromotoluene (171 mg, 1.00 mmol) was coupled with phenylacetylene. The crude product was chromatographed eluting with hexane to give 2-phenylethynyl)toluene (TXPTS: 140 mg, 73 %; TMAPTS: 155 mg, 81 %) yield as a light yellow oil. ¹H NMR (360 MHz, CDCl₃): δ 7.39 (m, 3H), 7.18 (m, 3H), 7.07 (d, *J* = 3.70 Hz, 2H), 7.08 (m, 1H), 2.38 (s, 3H). ¹³CNMR (90.6 MHz, CDCl₃): δ 140.5, 132.1, 131.8, 129.8, 128.7, 128.6, 128.5, 125.9, 123.9, 123.4, 93.7, 88.7, 21.03. Calculated for C₁₅H₁₂ found C, 93.71; H, 6.29. Analysis found C, 93.48; H, 6.50.

Representative procedure for the Heck coupling reactions with styrene. Pd(OAc)₂ (5.60 mg, 0.025 mmol), TXPTS•Na₃ (43.7 mg, 0.075 mmol), and Na₂CO₃ (212 mg, 2.00 mmol) were added to a 50mL round bottom flask equipped with a stir bar and rubber septum while in the dry box. Upon removing from dry box, the aryl halide (1.00 mmol), styrene (156 mg, 1.50 mmol), and degassed 1:1 CH₃CN:H₂O (10 mL) were added via syringe. The round-bottom flask was placed in an oil bath at 80 °C, and allowed to stir until complete (GC). The reaction mixture was poured into saturated sodium carbonate (50mL), extracted with ethyl acetate (3 × 30 mL), and dried with MgSO₄. The crude products were purified by flash chromatography (SiO₂).

***E*-4-Acetylstilbene** (Table 3, entry 1).¹⁴ Using the general procedure, 4-bromoacetophenone (214 mg, 1.00 mmol) was coupled with styrene. The crude product was chromatographed eluting with hexane:MeCl₂:EtOAc (70:20:10) to give *E*-4-acetylstilbene (224 mg, 94 % yield) as a white solid. ¹H NMR (360 MHz, CDCl₃): δ 7.95 (d, *J* = 8.02, 2H), 7.58 (d, *J* = 8.02 Hz, 2H), 7.54 (d, *J* = 7.4 Hz, 2H), 7.26 (m, 5H), 2.60 (s, 3H). ¹³C NMR (90.6 MHz, CDCl₃): δ 197.8, 142.3, 137.0, 136.3, 131.8, 129.2, 129.1, 128.6, 127.8, 127.1, 126.8, 26.9. mp 134-137 °C.

***E*-4-Methylstilbene** (Table 3, entry 2).¹⁵ Using the general procedure, 4-bromotoluene (173.8 mg, 1.00 mmol) was coupled with styrene. The crude product was chromatographed eluting with hexane:MeCl₂:EtOAc (70:20:10) to give *E*-4-methylstilbene (177 mg, 90 % yield) as a white solid. ¹H NMR (360 MHz, CDCl₃): δ 7.46 (d, *J* = 7.40 Hz, 2H), 7.42 (d, *J* = 8.02 Hz, 2H), 7.35 (m, 2H), 7.25 (m, 1H), 7.17 (m, 2H), 7.07 (d, *J* = 1.85 Hz, 2H), 2.36 (s, 3H). ¹³C NMR (90.6 MHz, CDCl₃): δ 138.1, 135.1, 130.0, 129.4, 129.1, 129.0, 128.3, 127.8, 127.0, 126.8, 21.0. mp 112-115 °C (lit. mp 119-120 °C)¹⁶.

***E*-4-Methoxy-2-methylstilbene** (Table 3, entry 5).² Using the general procedure, 1-methoxy-3-methyl-4-bromobenzene (199 mg, 1.00 mmol) was coupled with styrene. The crude product was chromatographed eluting with hexane:MeCl₂:EtOAc (70:20:10) to give *E*-4-methoxy-2-methylstilbene (173 mg, 78% yield) as a white solid. ¹H NMR (360 MHz, CDCl₃): δ 7.52 (m, 3H), 7.30 (m, 4H), 6.90 (m, 1H), 6.80 (m, 2H), 3.38 (s, 3H), 2.40 (s, 3H). ¹³C NMR (90.6 MHz, CDCl₃): δ 159.4, 138.3, 137.6, 133.1, 128.9, 128.4, 127.5, 126.9, 126.6, 126.4, 116.0, 112.0, 54.6, 20.1. m.p. 67-70 °C.

Representative procedure for the Heck coupling reactions with sodium acrylate. The coupling was carried out as described above for styrene, but using sodium acrylate (141 mg, 1.50

mmol) as the alkene. Upon consumption of the starting materials, the reaction mixture was added to saturated solution of sodium carbonate (50 mL). The residual aryl bromide was extracted with ethyl acetate (3 × 30 mL). The pH of the aqueous phase was then brought to ca. 1 using concentrated H₂SO₄. The cinnamic acid product was extracted with CH₂Cl₂ (3 × 30 mL) and the combined organic extracts were dried over MgSO₄. Removal of solvent under reduced pressure gave the crude product, which was recrystallized from H₂O/ethanol.

***E*-4-Methylcinnamic acid** (Table 3, entry 3).² Using the general procedure, 4-bromotoluene (174 mg, 1.00 mmol) was coupled with styrene. Using the general work-up procedure gave *E*-4-methylcinnamic acid (134 mg, 81 % yield) as a white solid. ¹H NMR (360 MHz, CDCl₃): δ 10.13 (brs, 1H), 7.57 (m, 3H), 7.23 (d, *J* = 8.01 Hz, 2H), 6.47 (d, *J* = 16.03 Hz, 1H), 2.32 (s, 3H). ¹³C NMR (90.6 MHz, CDCl₃): δ 168.6, 144.8, 141.1, 132.4, 130.4, 129.1, 119.0, 21.9. m.p. 197-199 °C (lit.⁷ m.p. 198-200 °C).

***E*-4-Methoxycinnamic acid** (Table 3, entry 4).¹⁷ Using the general procedure, 4-bromoanisole (187 mg, 1.00 mmol) was coupled with styrene. Using the general work-up procedure gave *E*-4-methoxycinnamic acid (141 mg, 79 % yield) as a white solid. ¹H NMR (360 MHz, CDCl₃): δ 10.22 (brs, 1H), 7.67 (d, *J* = 8.63 Hz, 2H), 7.57 (d, *J* = 16.03 Hz, 1H), 6.99 (d, *J* = 8.63 Hz, 2H), 6.41 (d, *J* = 16.03 Hz, 1H), 3.84 (s, 3H). ¹³C NMR (90.6 MHz, CDCl₃): δ 168.7, 161.9, 144.6, 130.8, 127.8, 117.4, 115.3, 56.2. m.p. 173-174 °C (lit.⁷ m.p. 174 °C).

***E*-2-Methylcinnamic acid** (Table 3, entry 6).¹⁸ Using the general procedure, 2-bromotoluene (171 mg, 1.00 mmol) was coupled with styrene. Using the general work-up procedure gave *E*-2-methylcinnamic acid (156 mg, 82 % yield) as a white solid. ¹H NMR (360 MHz, CDCl₃): δ 10.00 (brs, 1H), 7.86 (d, *J* = 15.42 Hz, 1H), 7.72 (d, *J* = 7.4 Hz, 1H), 7.30 (m, 3H), 6.45 (d, *J* = 15.41 Hz, 1H), 2.42 (s, 3H). ¹³C NMR (90.6 MHz, CDCl₃): δ 168.4, 142.1, 138.1, 131.6, 130.9, 127.4, 127.3, 121.1, 20.2. One peak was not observed in the ¹³C NMR. mp 169-171 °C (lit mp 175-176 °C).

General procedure for synthesis of ligand TBA salts. The sodium salt of the trisulfonated ligand (0.17 mmol) was placed in a flask with tetrabutylammonium chloride (167 mg, 0.60 mmol). Water (4 mL) was added and the clear solution allowed to stir for 1 hour. The mixture was extracted with methylene chloride. Removal of solvent gave viscous oils that solidified after drying under vacuum (0.1 torr). The products were used without further purification.

General procedure for measurement of ligand electronic parameters. Solutions of L₂Rh(CO)Cl complexes were synthesized according to the procedure reported by Vastag.¹⁹ The phosphine (0.050 mmol), trimethylamine *N*-oxide (0.020 mmol), and [Rh(CO)₂μ-Cl]₂ (0.010 mmol) were added to a vial equipped with stir bar and septa while in the drybox. Upon removing from the drybox 1 mL of distilled methylene chloride was added to the reaction vessel via a syringe and the reaction mixture was allowed to stir for one hour. At this time a sample of the reaction solution was transferred to an air-free solution cell (NaCl windows) via a disposable syringe. Rh(PPh₃)₂(CO)Cl: 1979 cm⁻¹, Rh(TXPTS•(TBA)₃)₂(CO)Cl: 1993 cm⁻¹; Rh(TMAPTS•(TBA)₃)₂(CO)Cl: 1993 cm⁻¹; Rh(TPPTS•(TBA)₃)₂(CO)Cl: 1993 cm⁻¹.

General procedure for ligand complexation studies. Pd(OAc)₂ (2.2 mg, 0.01 mmol), ligand (0.025 – 0.05 mmol), Na₂CO₃ (0 – 1 mmol), and PhB(OH)₂ (0 – 0.05 mmol) were combined in a

small, septum-sealed vial in the drybox. The vial was removed from the box and attached to a nitrogen manifold by a needle. Deoxygenated 2:1 D₂O-acetonitrile (1 mL) was added to the vial via syringe. After mixing to dissolve all of the solids, a portion of this solution (0.4 to 0.5 mL) was transferred via syringe to an NMR tube that had been sealed under nitrogen with a septum. Samples were analyzed by ³¹P{¹H}, ¹H, or ¹³C{¹H} NMR spectroscopy immediately after preparation and then periodically over a period of several hours.

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Spectra of Complexation Studies

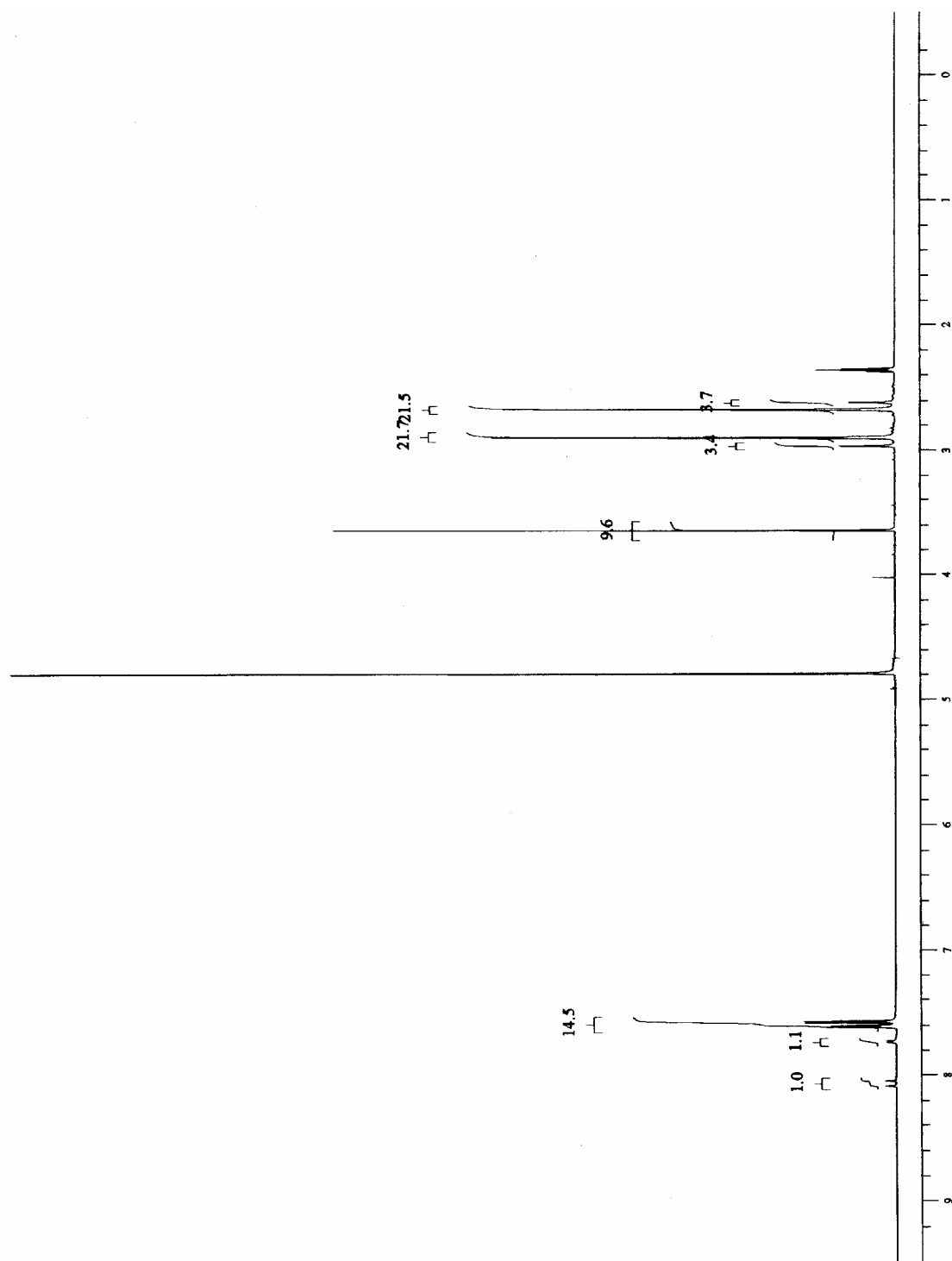


Figure S1. ^1H NMR spectrum of TXPTS $\cdot\text{Na}_3$ contaminated with approximately 15% oxide (360 MHz, 2:1 D_2O - CD_3CN).

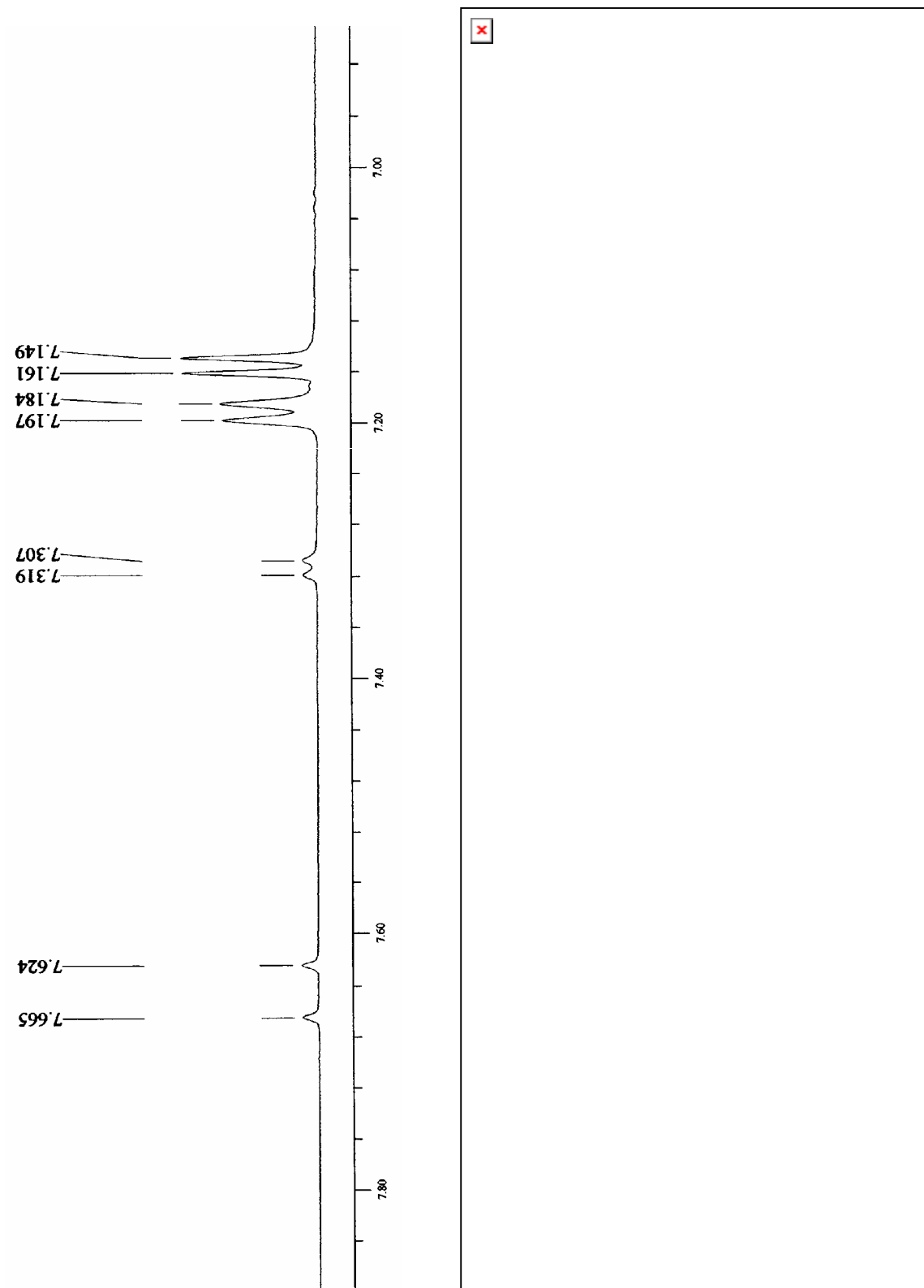


Figure S2. Expansions of ^1H NMR spectrum aliphatic and aromatic regions of TXPTS•Na₃ contaminated with approximately 15% oxide (360 MHz, 2:1 D₂O-CD₃CN).

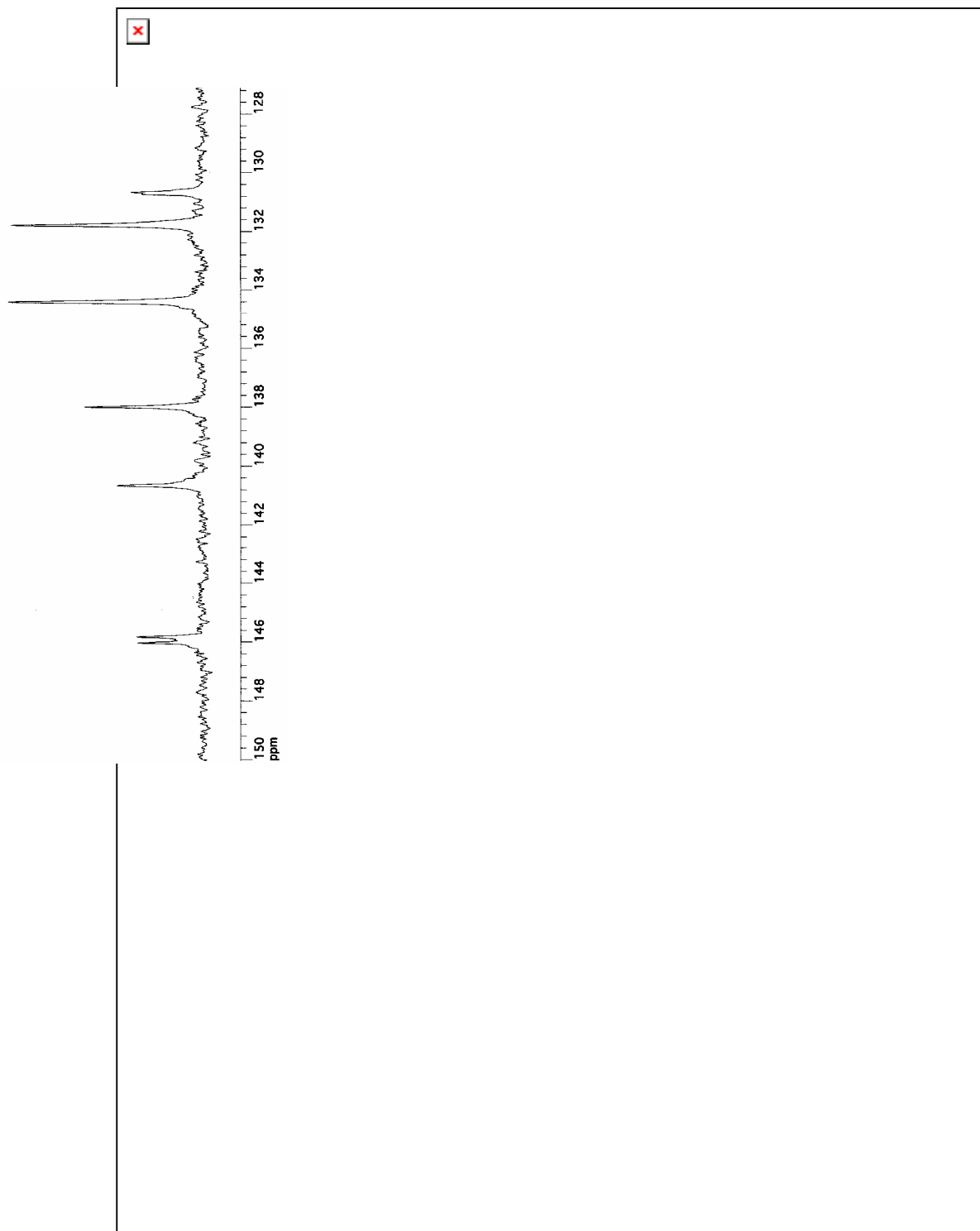


Figure S3. ^{13}C NMR spectrum of TXPTS $\cdot\text{Na}_3$ (125.8 MHz, 2:1 D_2O - CD_3CN).

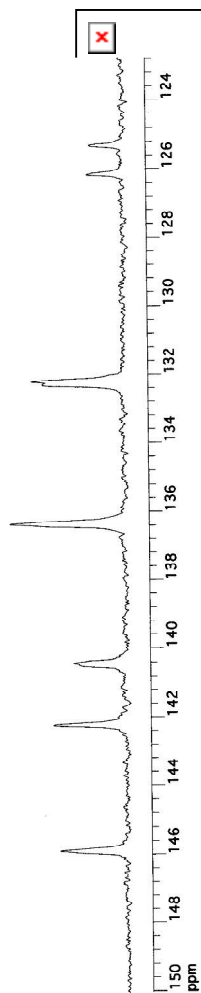


Figure S4. ^{13}C NMR spectrum of TXPTSO $\cdot\text{Na}_3$ (125.8 MHz, 2:1 D_2O - CD_3CN).

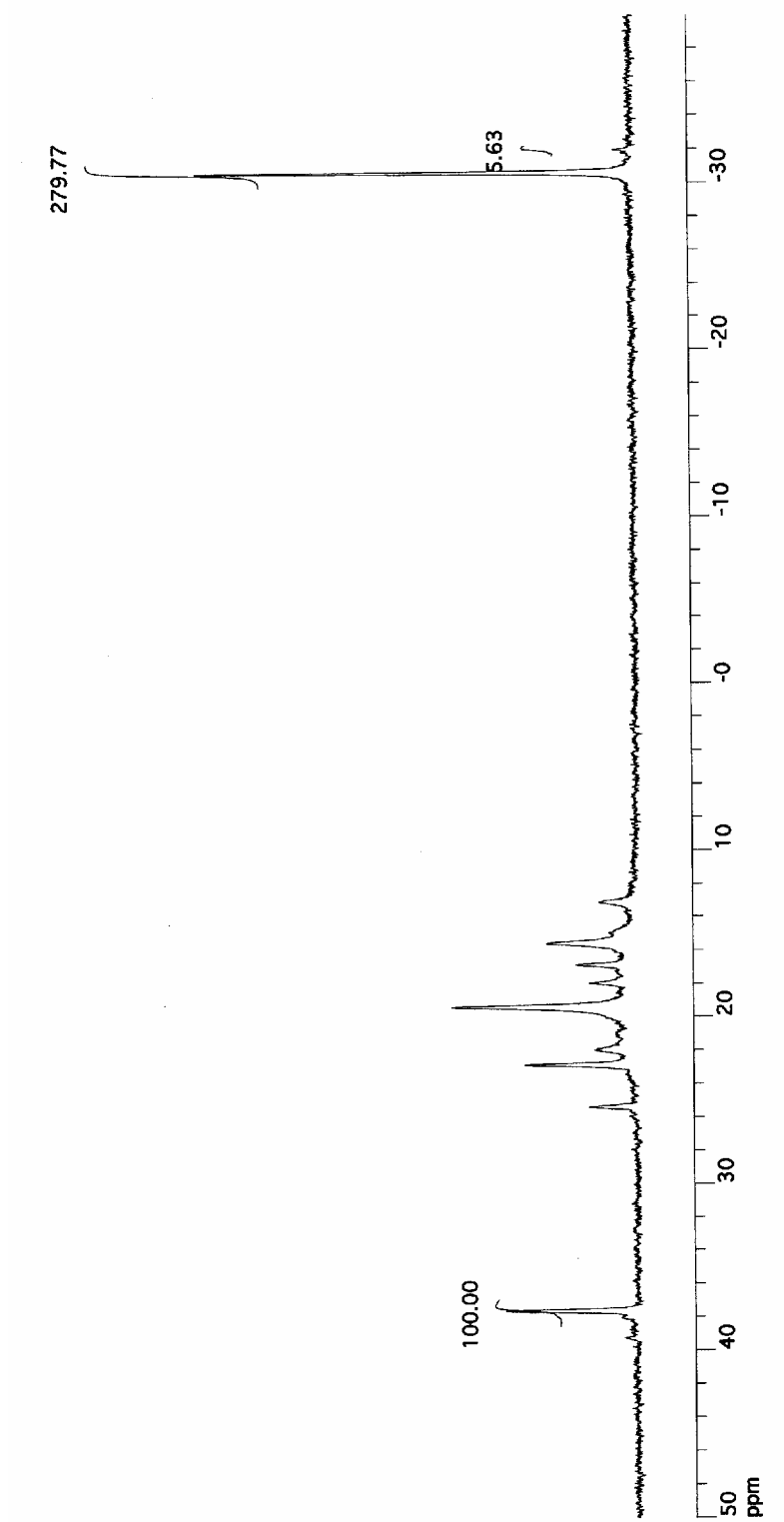


Figure S5. ^{31}P NMR spectrum of TXPTS + $\text{Pd}(\text{OAc})_2$ (2.5 : 1, 202.5 MHz, 2:1 D_2O - CD_3CN)

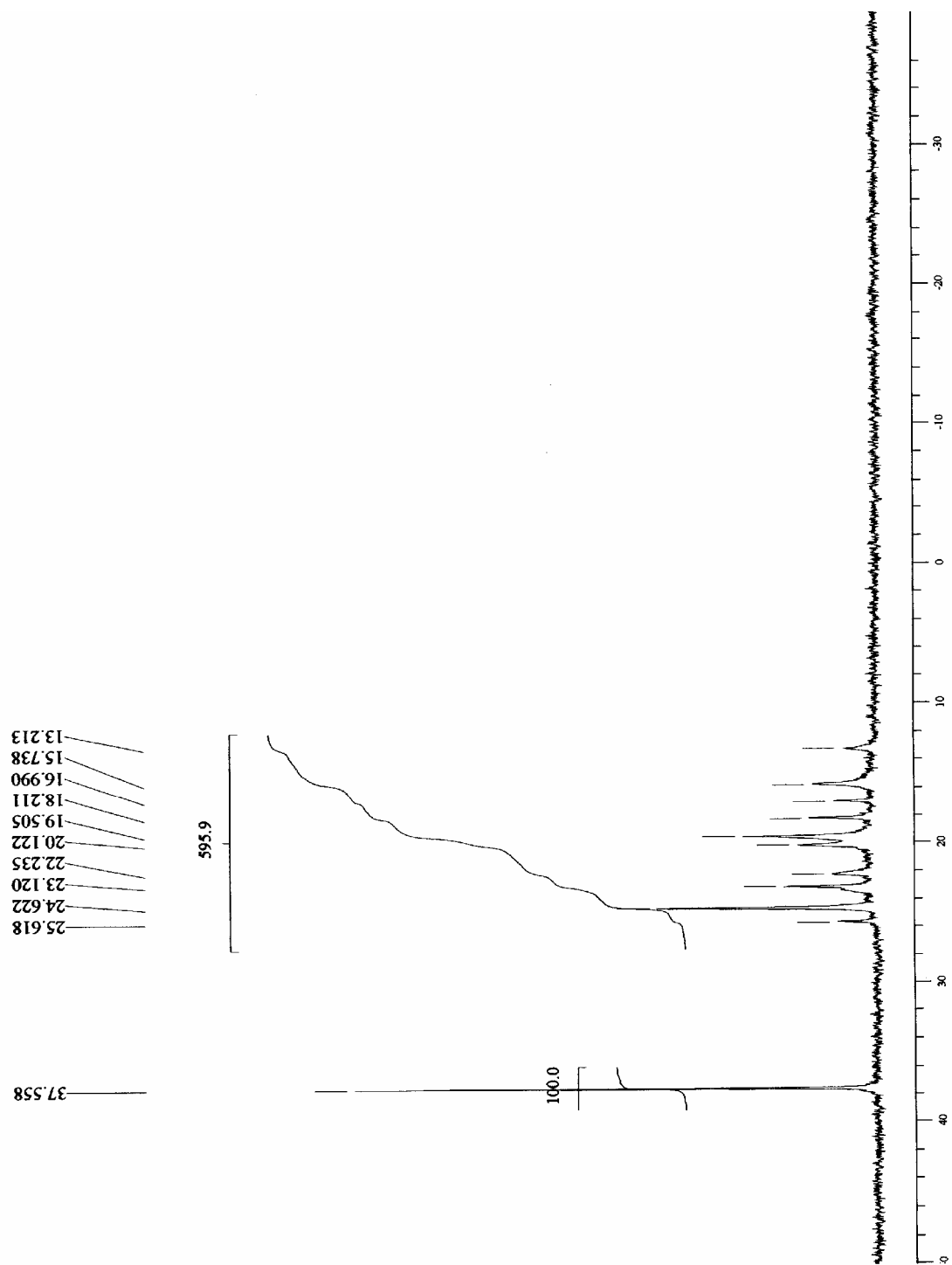


Figure S6. ^{31}P NMR spectrum of Na_2PdCl_4 (0.02 M) and TXPTS 0.05 M) immediately after mixing (202.5 MHz, 2:1 D_2O - CD_3CN).

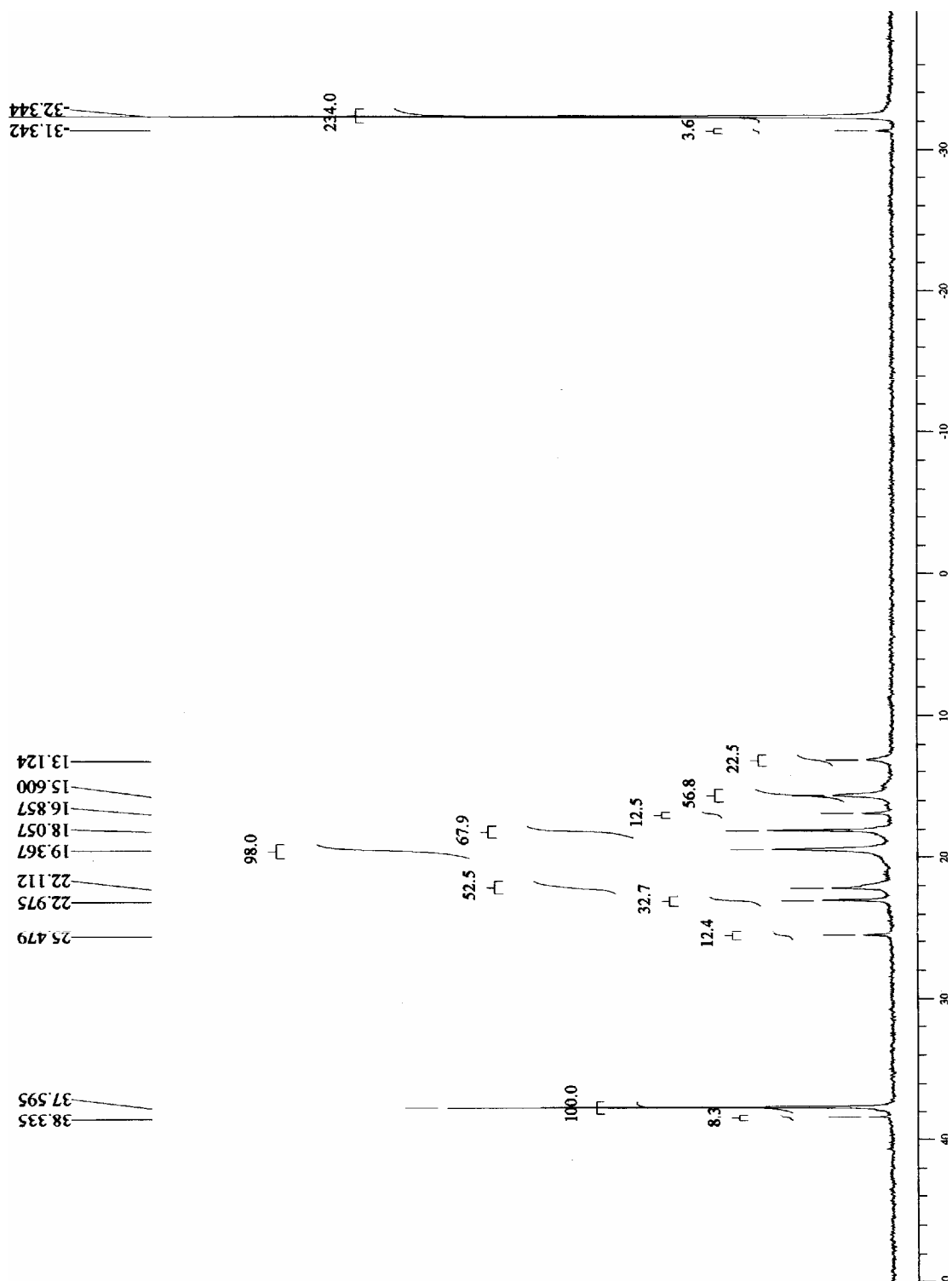


Figure S7. ^{31}P NMR spectrum of Na_2PdCl_4 (0.02 M) and TXPTS 0.10 M) immediately after mixing (202.5 MHz, 2:1 D_2O - CD_3CN).

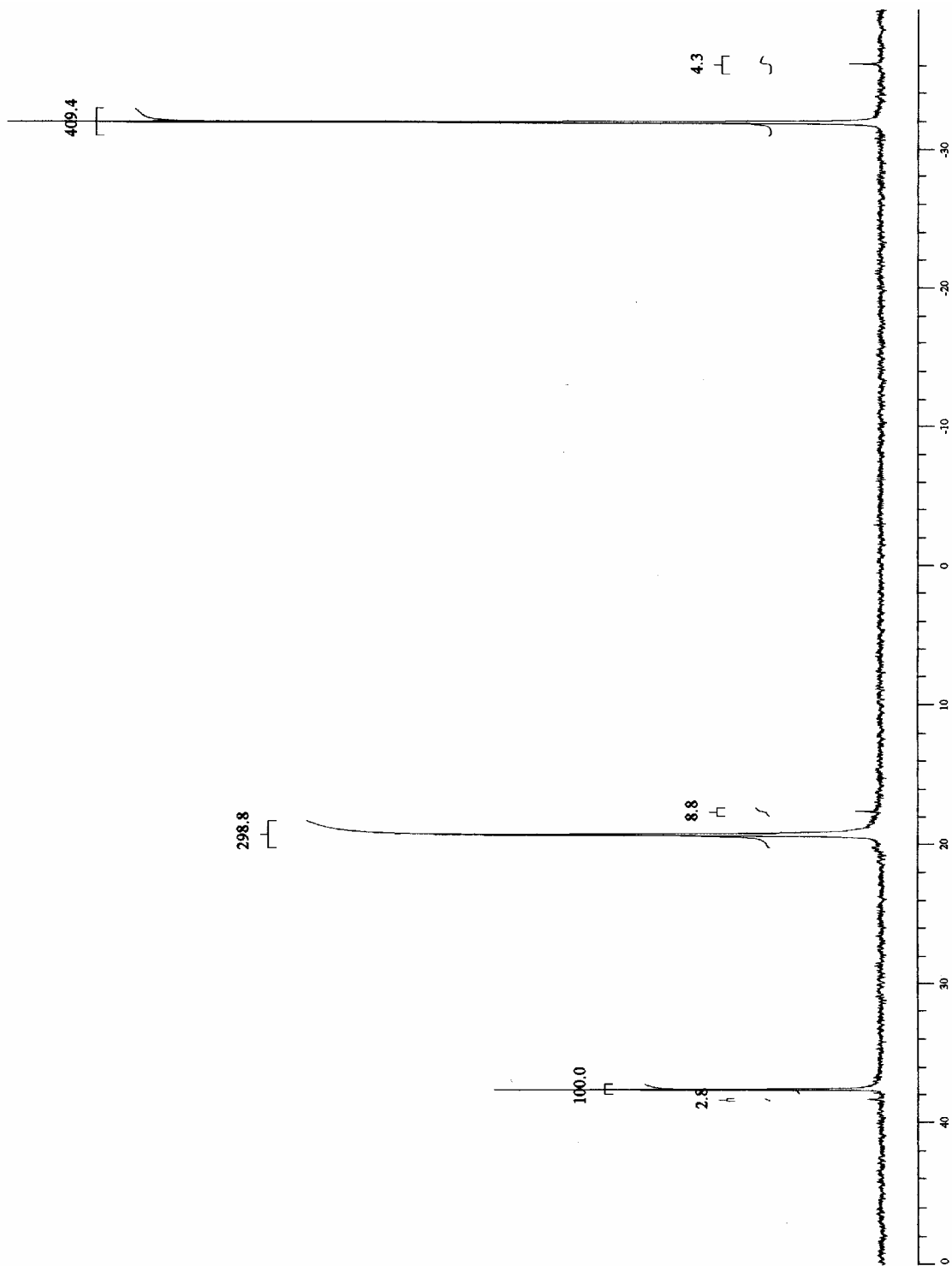


Figure S8. ^{31}P NMR spectrum of $\text{Pd}(\text{OAc})_2$ (0.02 M), Na_2CO_3 (6.5 eq) and TXPTS (2.7 eq) immediately after mixing (202.5 MHz, 2:1 D_2O - CD_3CN).

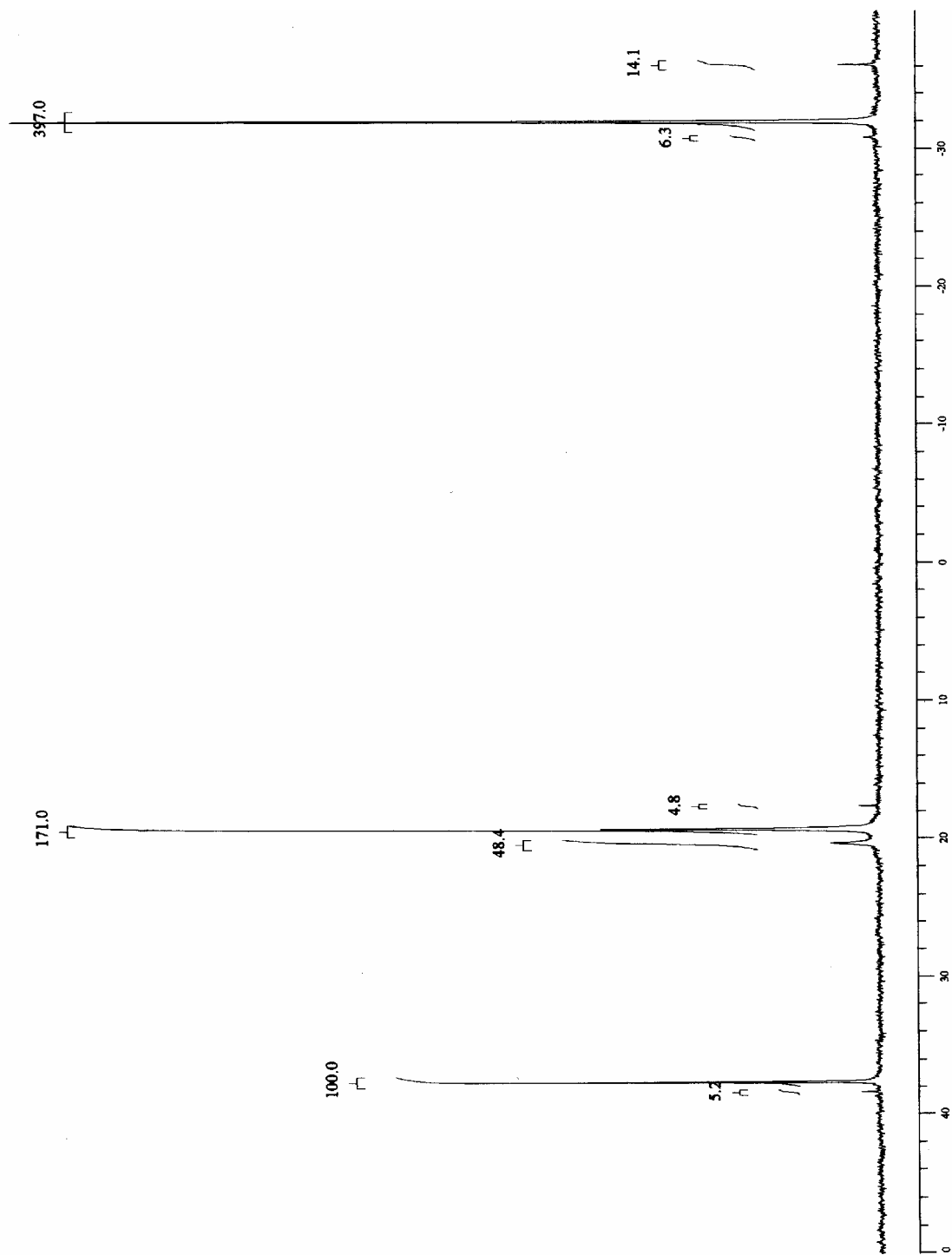


Figure S9. ^{31}P NMR spectrum of $\text{Pd}(\text{OAc})_2$ (0.02 M), Na_2CO_3 (6.5 eq) and TXPTS (2.7 eq) after 48 hours (202.5 MHz, 2:1 D_2O - CD_3CN).

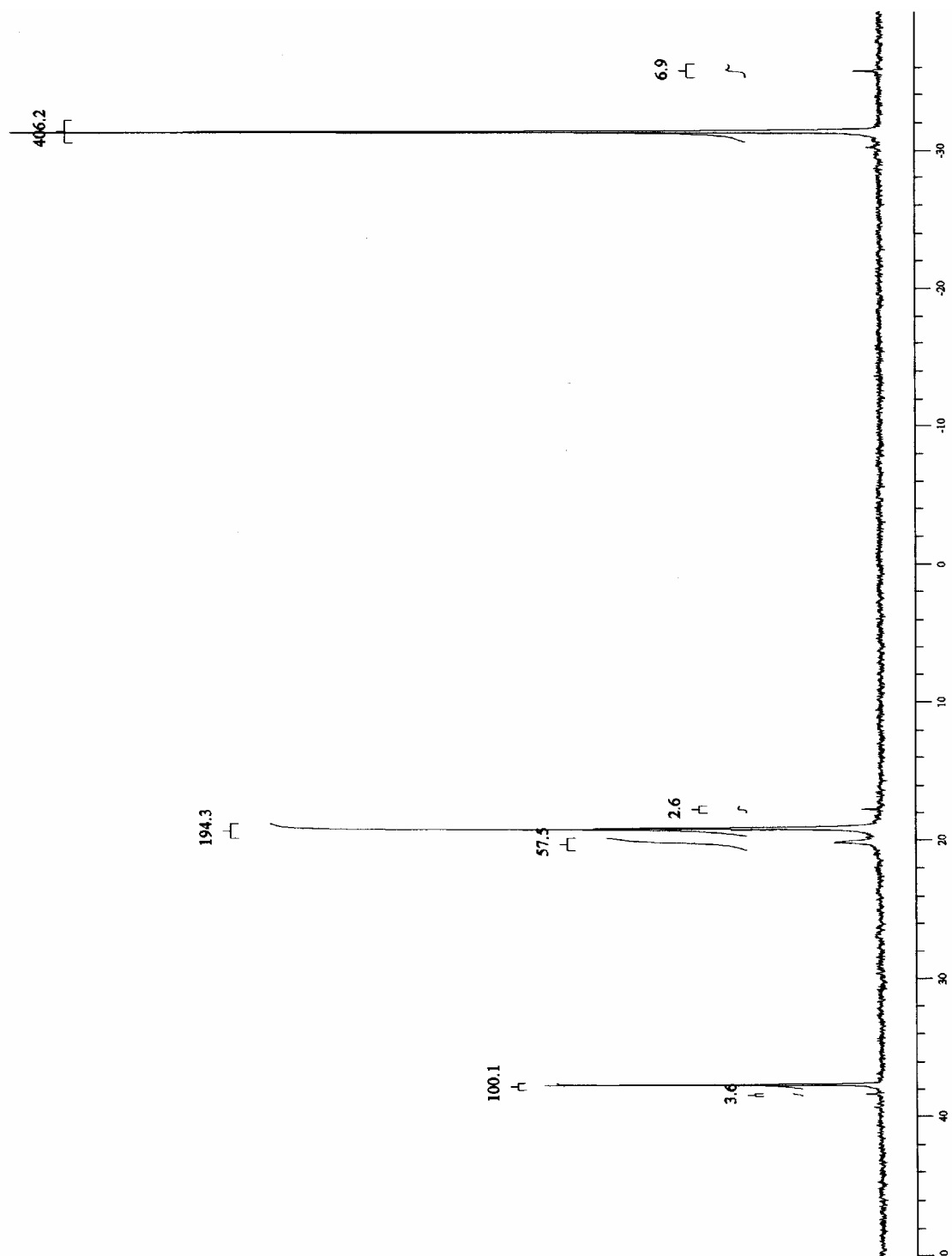


Figure S10. ^{31}P NMR spectrum of $\text{Pd}(\text{OAc})_2$ (0.02 M), Na_2CO_3 (6.5 eq) and TXPTS (2.7 eq) allowed to stand for 48 hours followed by addition of phenyl iodide (202.5 MHz, 2:1 D_2O - CD_3CN).

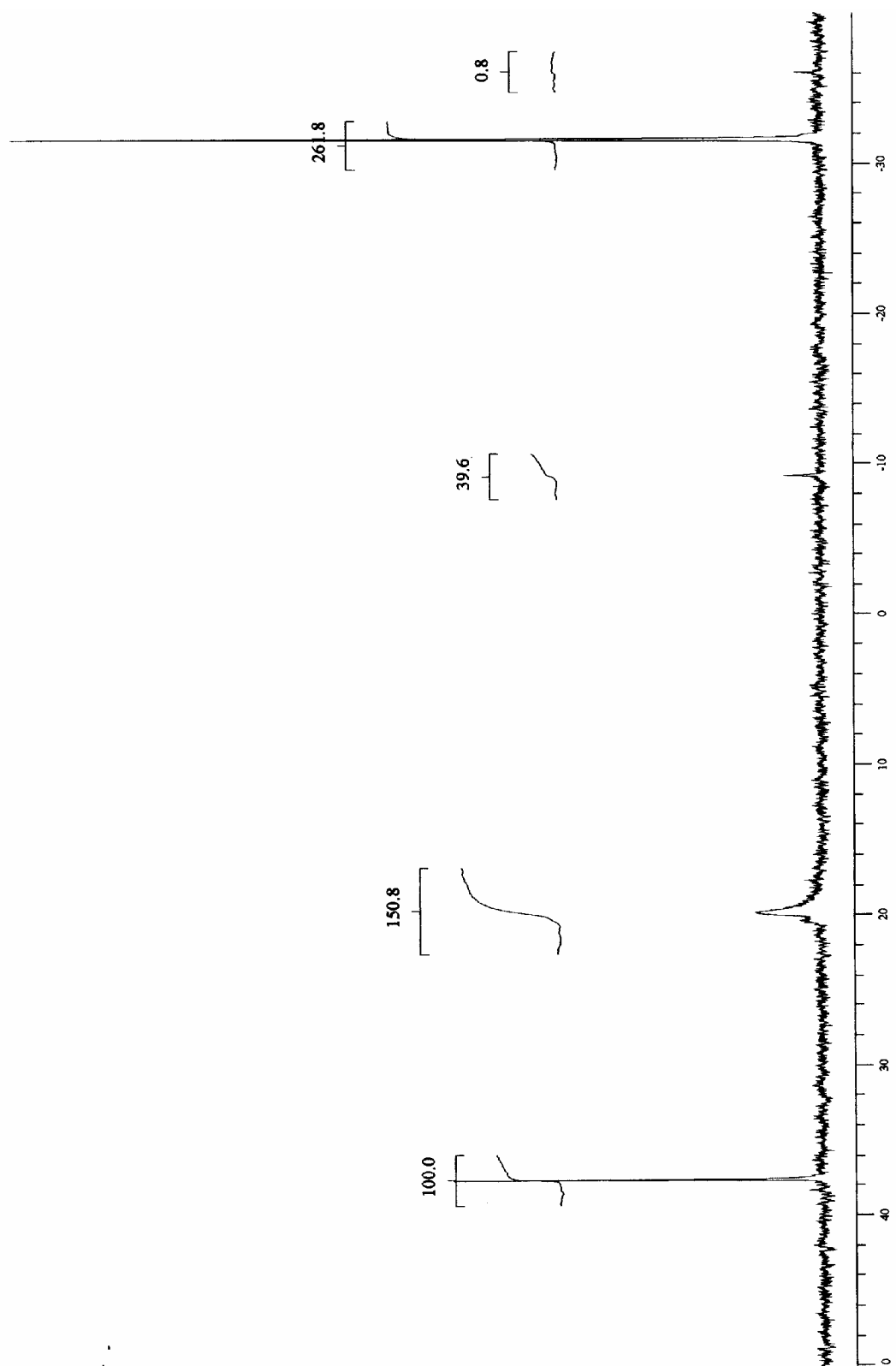


Figure S11. ^{31}P NMR spectrum of $\text{Pd}(\text{OAc})_2$ (0.01 M), Na_2CO_3 (26.6 eq) and TXPTS (2.5 eq) immediately after mixing (202.5 MHz, 2:1 D_2O - CD_3CN).

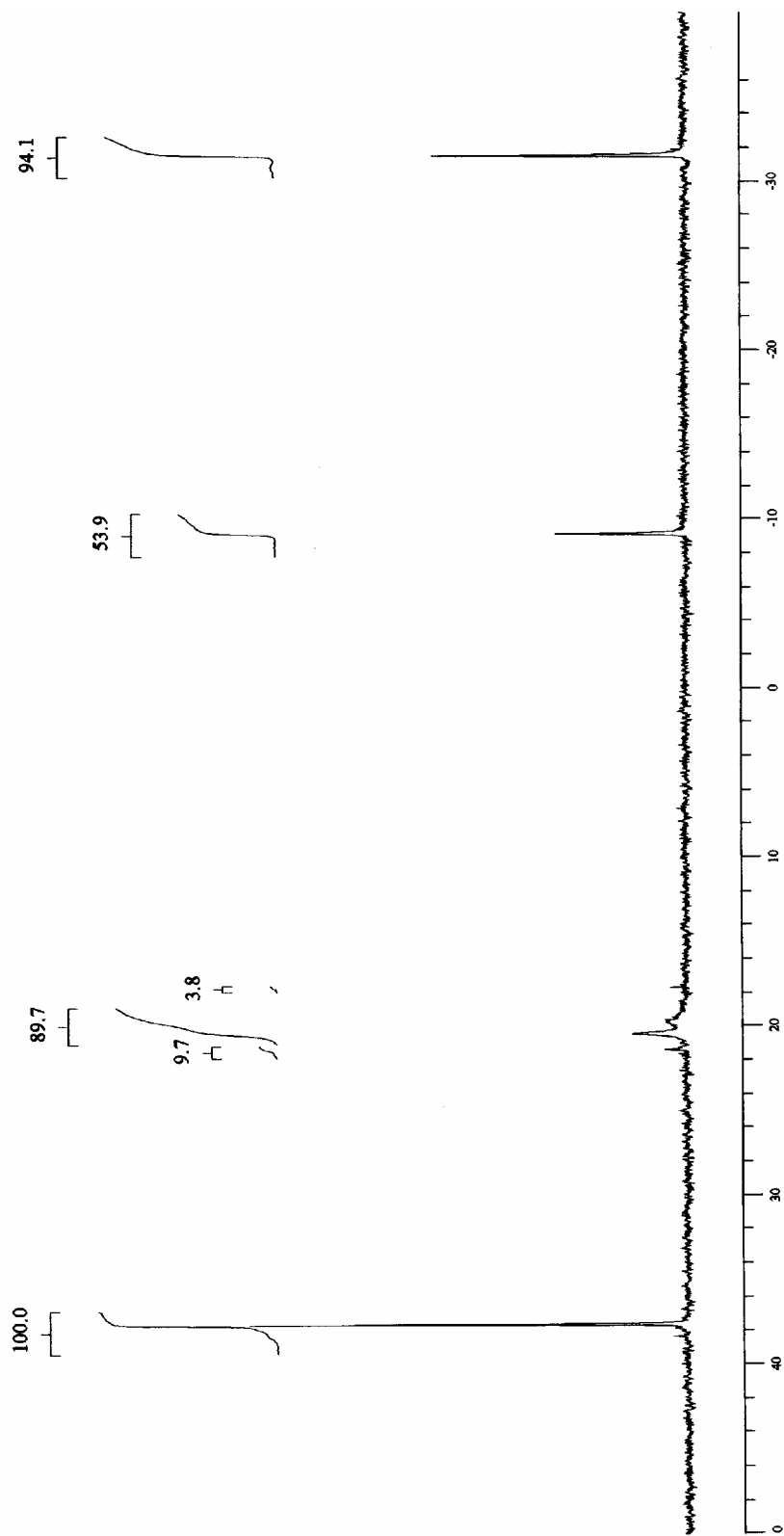


Figure S12. ^{31}P NMR spectrum of $\text{Pd}(\text{OAc})_2$ (0.01 M), Na_2CO_3 (26.6 eq) and TXPTS (2.5 eq) after 24 hours (202.5 MHz, 2:1 D_2O - CD_3CN).

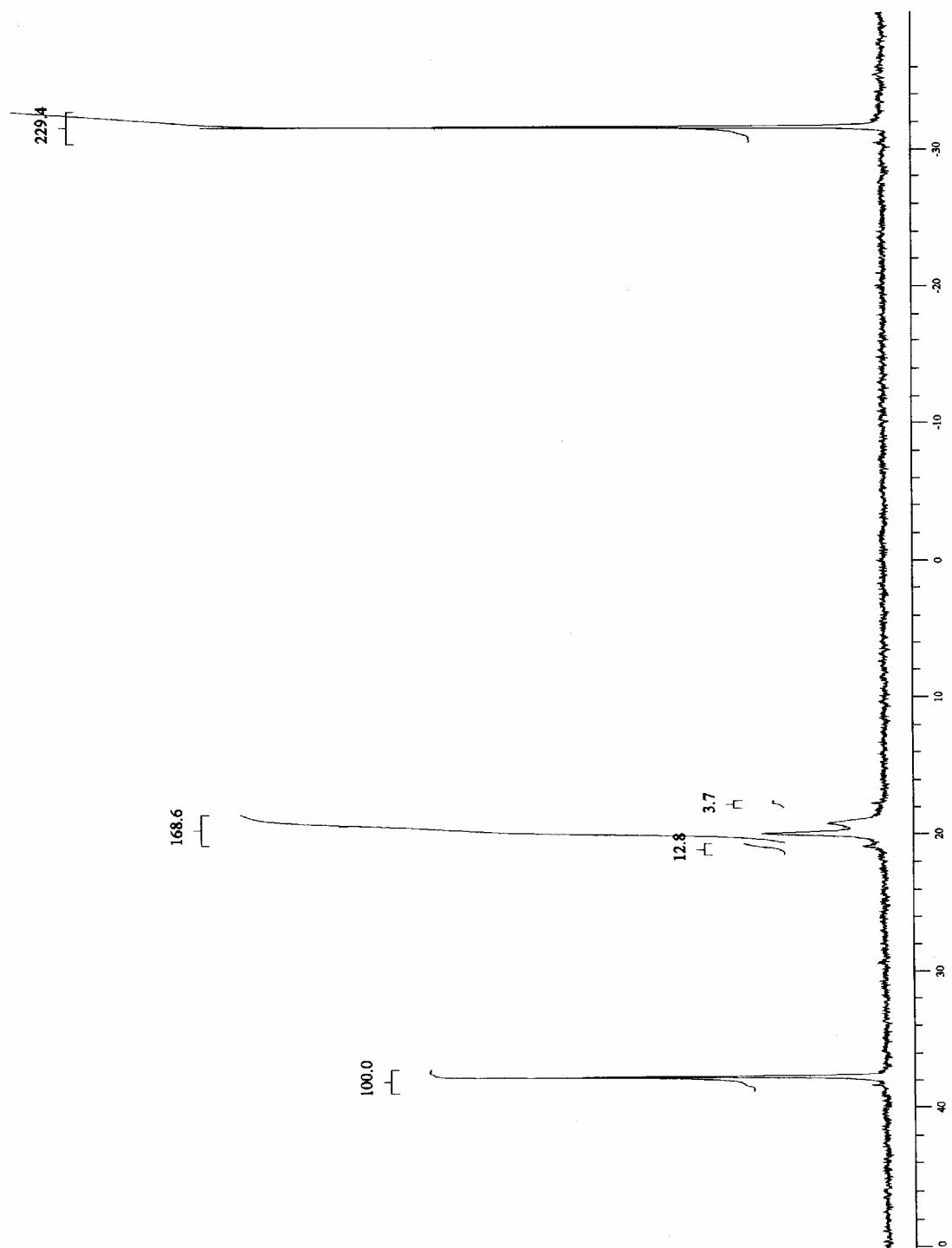


Figure S13. ^{31}P NMR spectrum after addition of phenyl iodide to a mixture of $\text{Pd}(\text{OAc})_2$ (0.01 M), Na_2CO_3 (26.6 eq) and TXPTS (2.5 eq) that had been standing for 24 hours (202.5 MHz, 2:1 D_2O - CD_3CN).

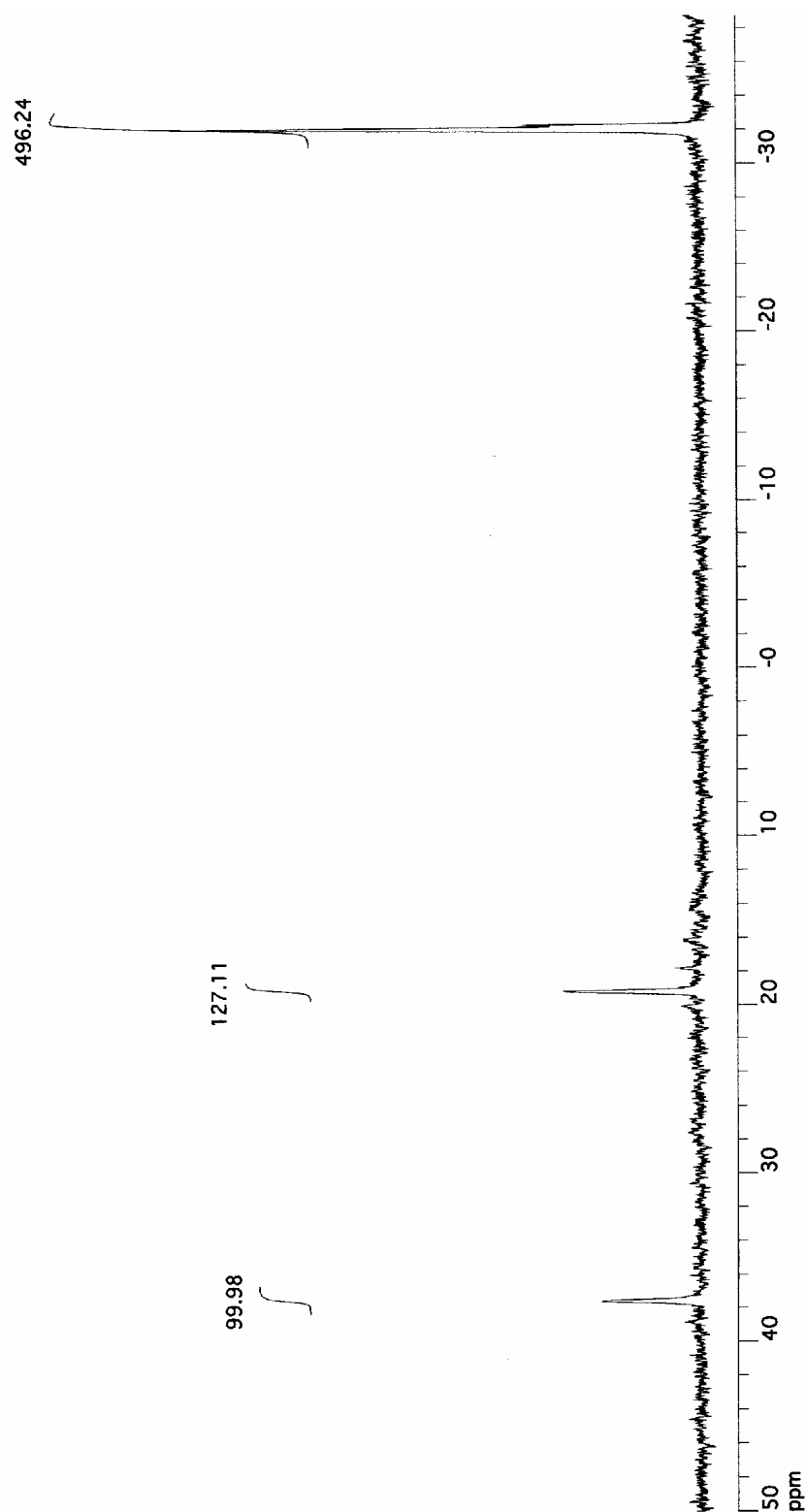


Figure S14. ^{31}P NMR spectrum of a mixture of $\text{Pd}(\text{OAc})_2$ (0.01 M), Na_2CO_3 (6.6 eq), TXPTS (2.4 eq) and $\text{PhB}(\text{OH})_2$ (16.4 eq) immediately after mixing (202.5 MHz, 2:1 D_2O - CD_3CN).

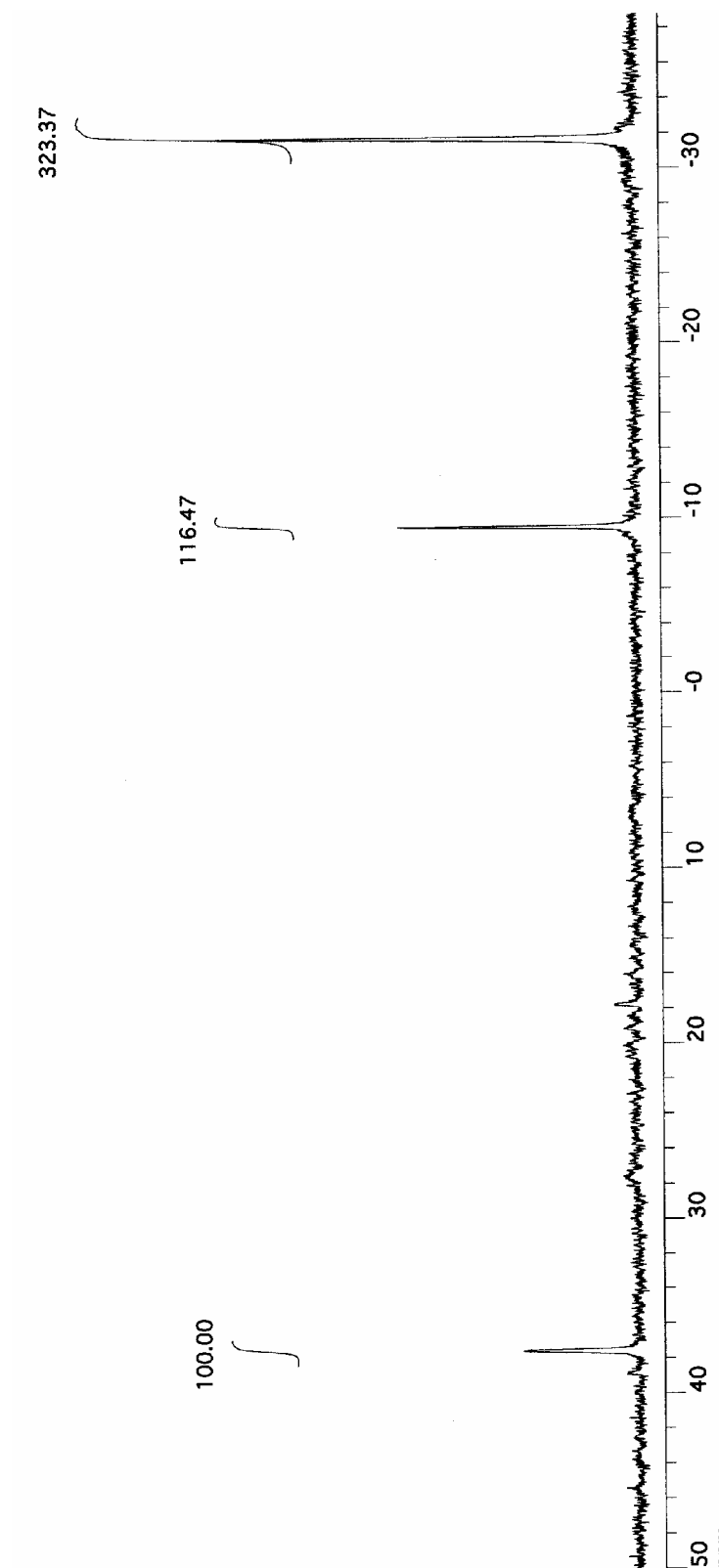


Figure S15. ^{31}P NMR spectrum of a mixture of $\text{Pd}(\text{OAc})_2$ (0.01 M), Na_2CO_3 (6.6 eq), TXPTS (2.4 eq) and $\text{PhB}(\text{OH})_2$ (16.4 eq) after 24 hours (202.5 MHz, 2:1 D_2O - CD_3CN).

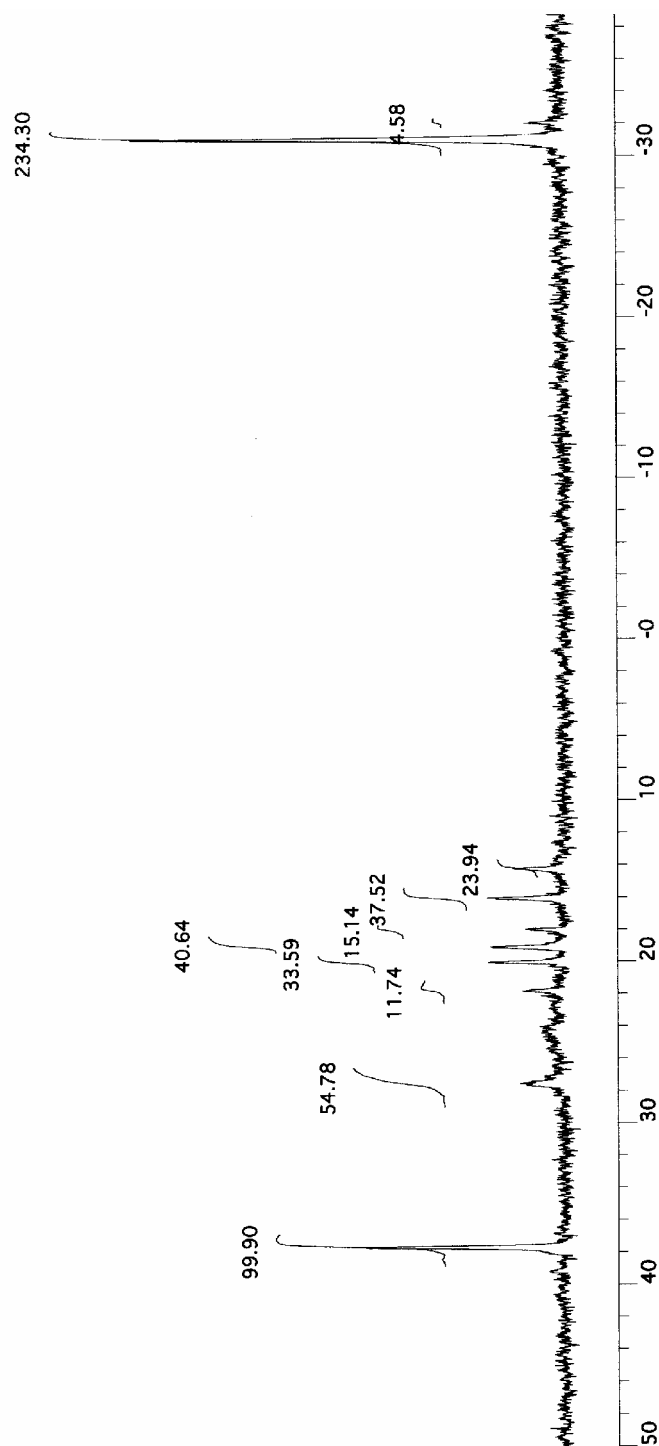


Figure S16. ^{31}P NMR spectrum after addition of phenyl iodide to a mixture of $\text{Pd}(\text{OAc})_2$ (0.01 M), Na_2CO_3 (6.6 eq), TXPTS (2.4 eq) and $\text{PhB}(\text{OH})_2$ (16.4 eq) that had been stirred for 24 hours (202.5 MHz, 2:1 D_2O - CD_3CN).

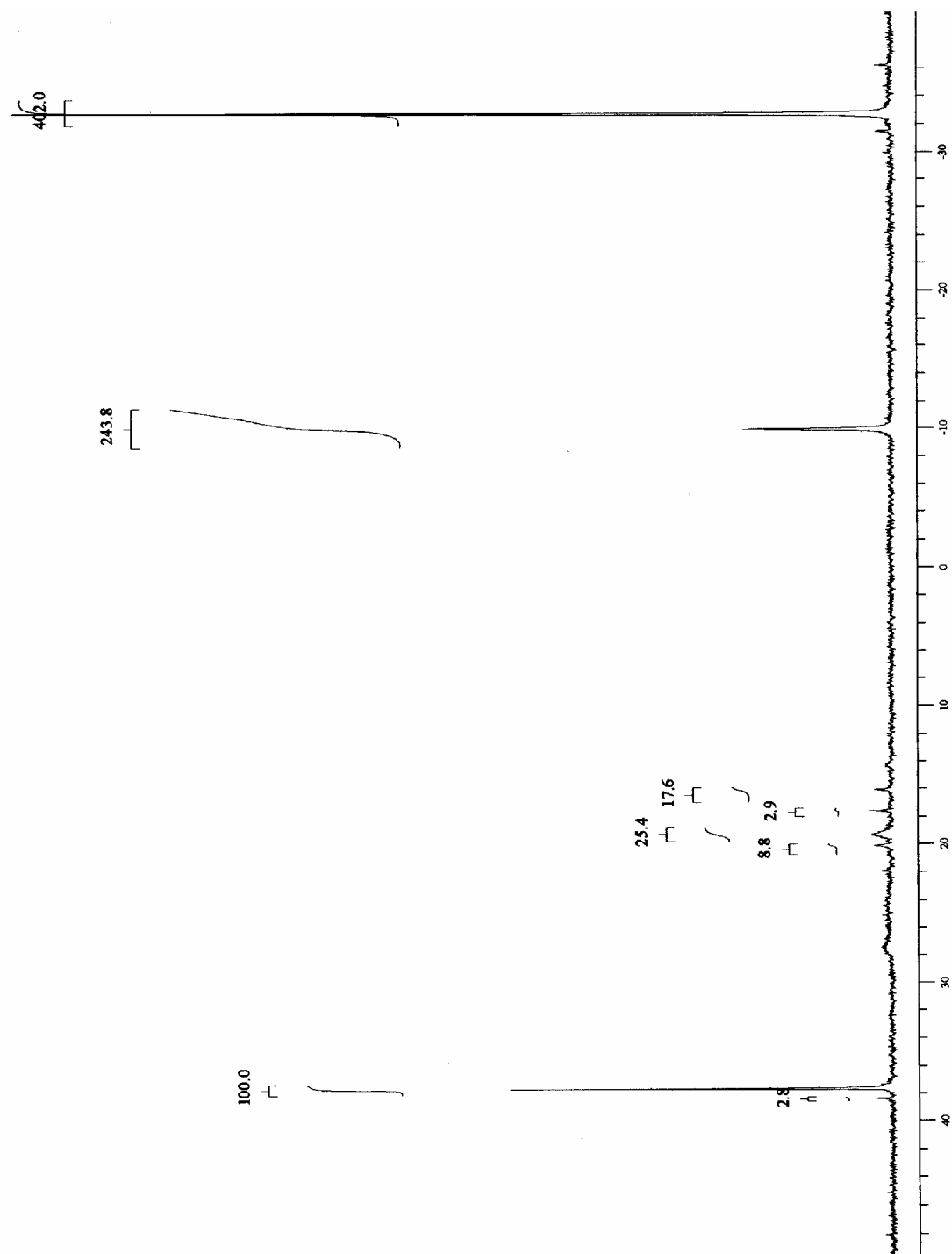


Figure S17. ^{31}P NMR spectrum of a mixture of $\text{Pd}(\text{OAc})_2$ (0.02 M), Na_2CO_3 (103.2 eq), TXPTS (2.8 eq) and $\text{PhB}(\text{OH})_2$ (3.9 eq) immediately after mixing (202.5 MHz, 2:1 D_2O - CD_3CN).

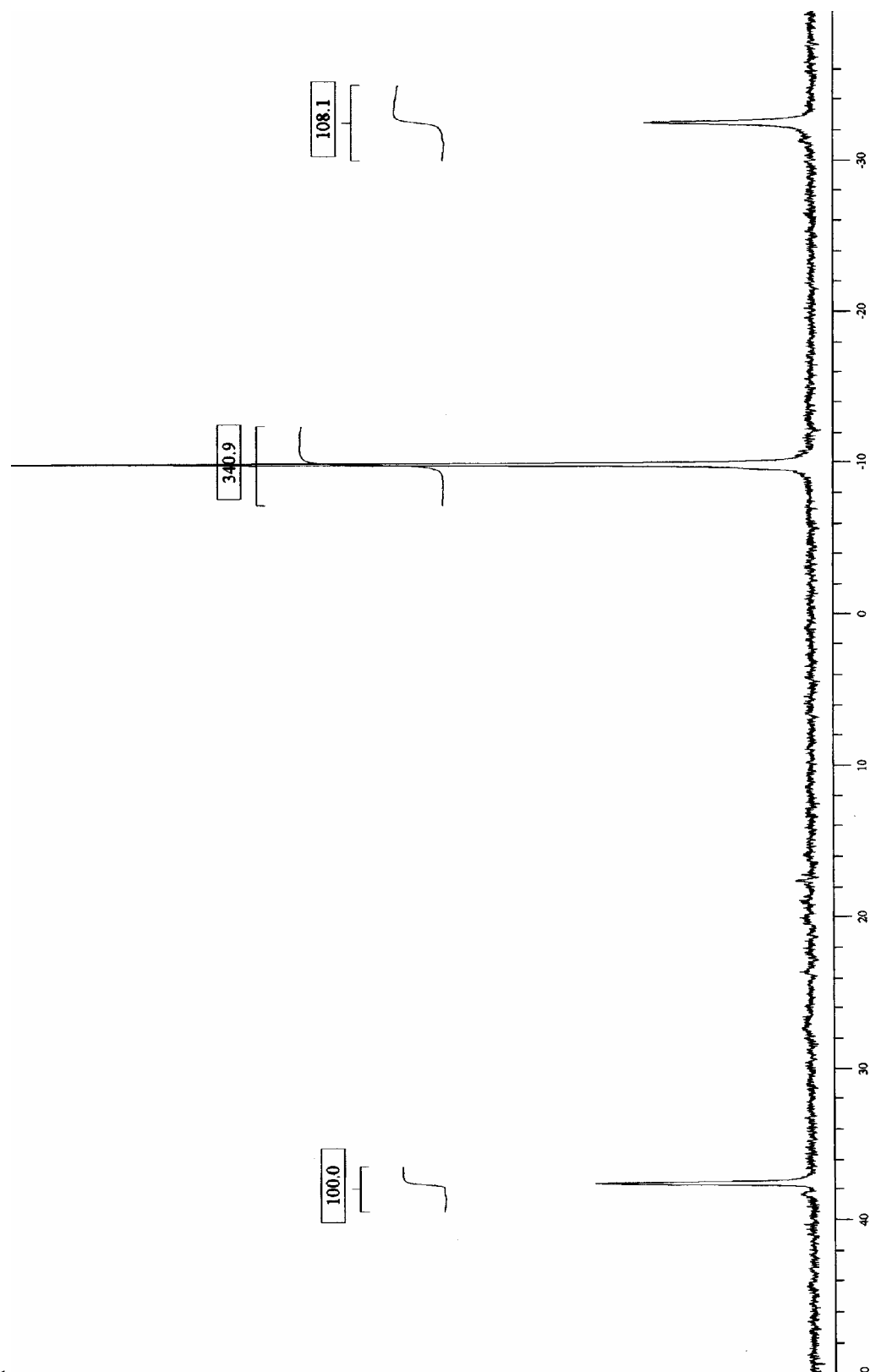


Figure S18. ^{31}P NMR spectrum of a mixture of $\text{Pd}(\text{OAc})_2$ (0.02 M), Na_2CO_3 (103.2 eq), TXPTS (2.8 eq) and $\text{PhB}(\text{OH})_2$ (3.9 eq) after 24 hours (202.5 MHz, 2:1 D_2O - CD_3CN).

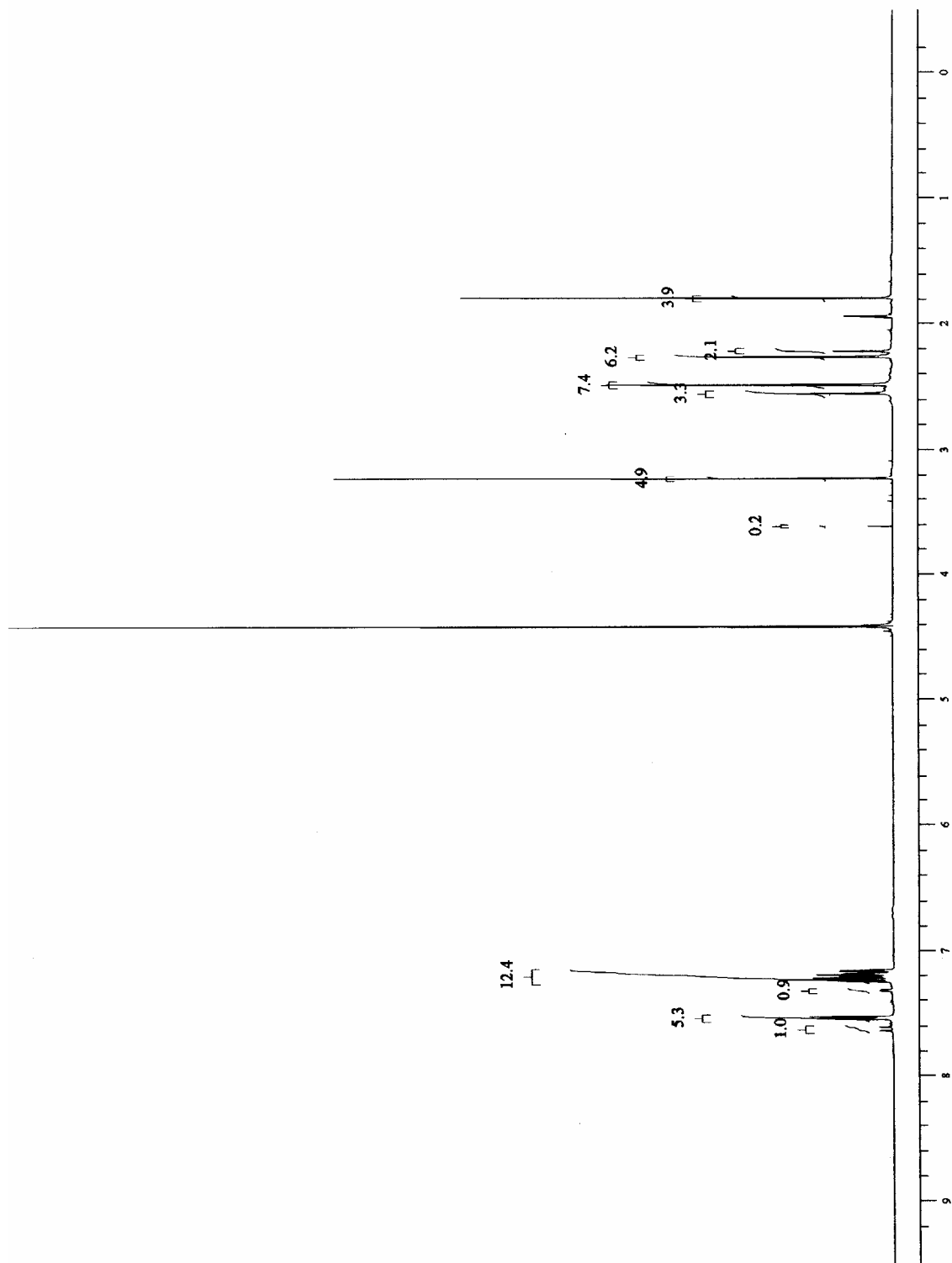


Figure S19. ^1H NMR spectrum of a mixture of $\text{Pd}(\text{OAc})_2$ (0.02 M), Na_2CO_3 (103.2 eq), TXPTS (2.8 eq) and $\text{PhB}(\text{OH})_2$ (3.9 eq) immediately after mixing (500 MHz, 2:1 D_2O - CD_3CN).

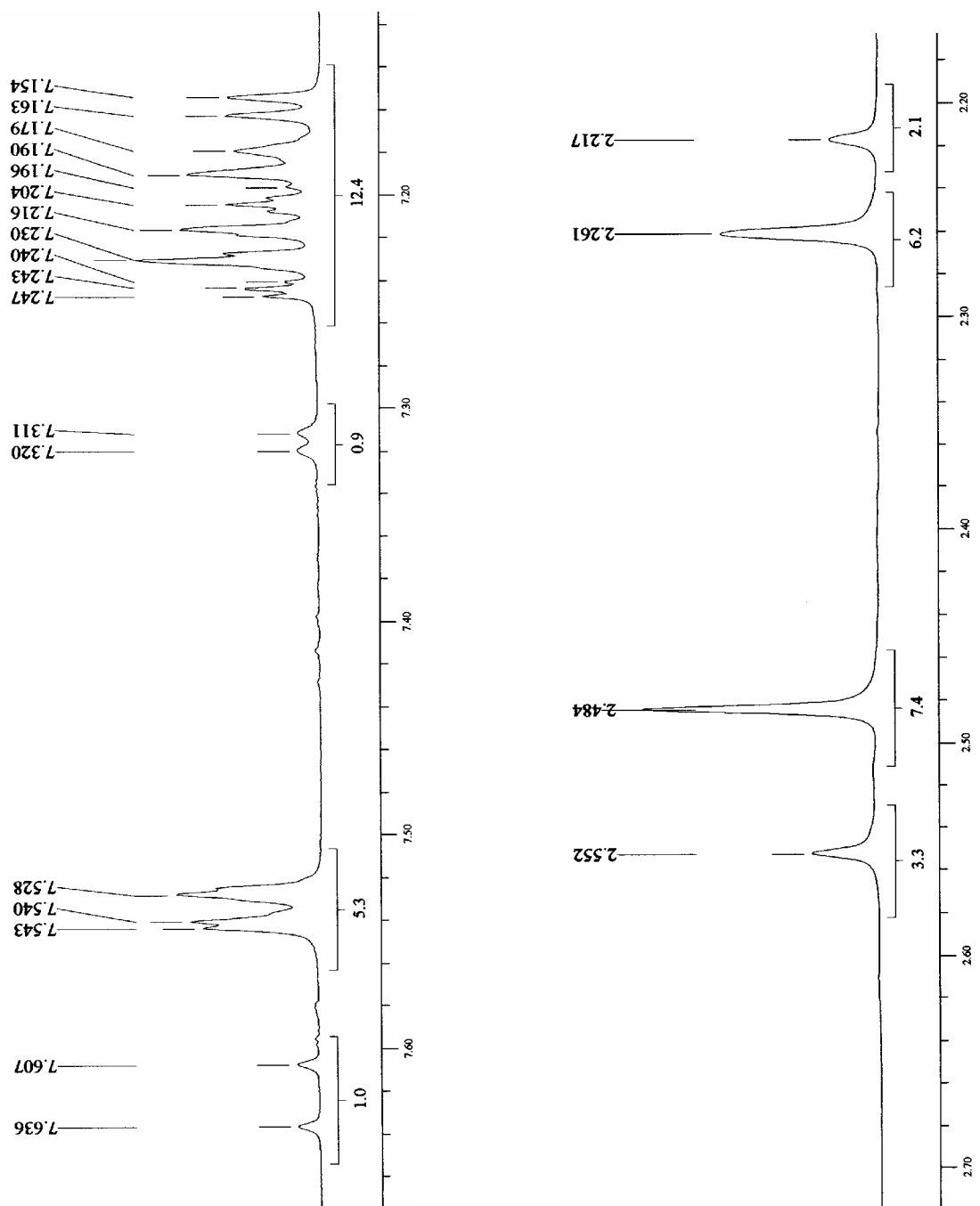


Figure S20. Expansions of the aromatic and aliphatic regions of the ^1H NMR spectrum of a mixture of $\text{Pd}(\text{OAc})_2$ (0.02 M), Na_2CO_3 (103.2 eq), TXPTS (2.8 eq) and $\text{PhB}(\text{OH})_2$ (3.9 eq) immediately after mixing (500 MHz, 2:1 D_2O - CD_3CN).

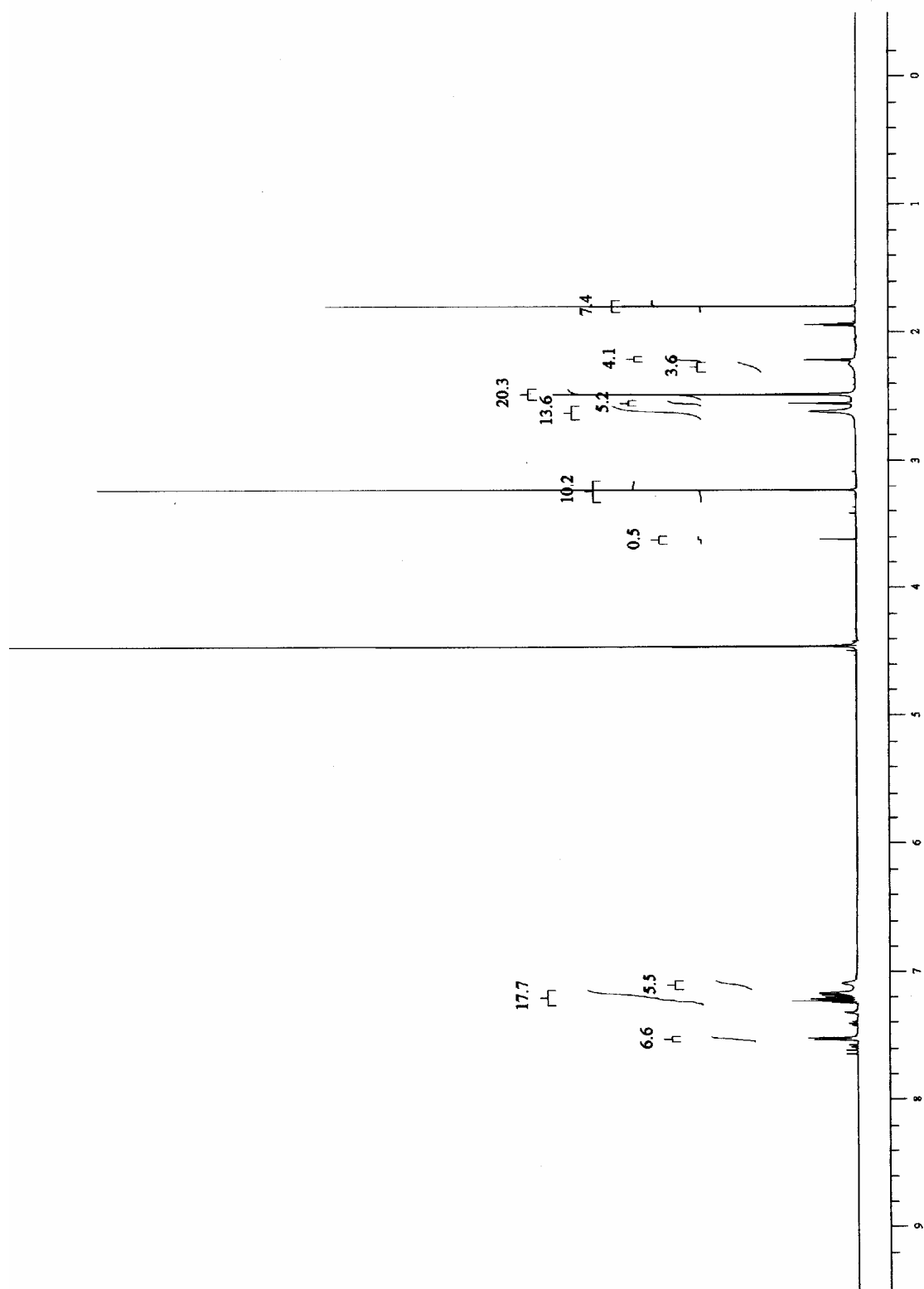


Figure S21. ^1H NMR spectrum of a mixture of $\text{Pd}(\text{OAc})_2$ (0.02 M), Na_2CO_3 (103.2 eq), TXPTS (2.8 eq) and $\text{PhB}(\text{OH})_2$ (3.9 eq) after 24 hours (500 MHz, 2:1 D_2O - CD_3CN).

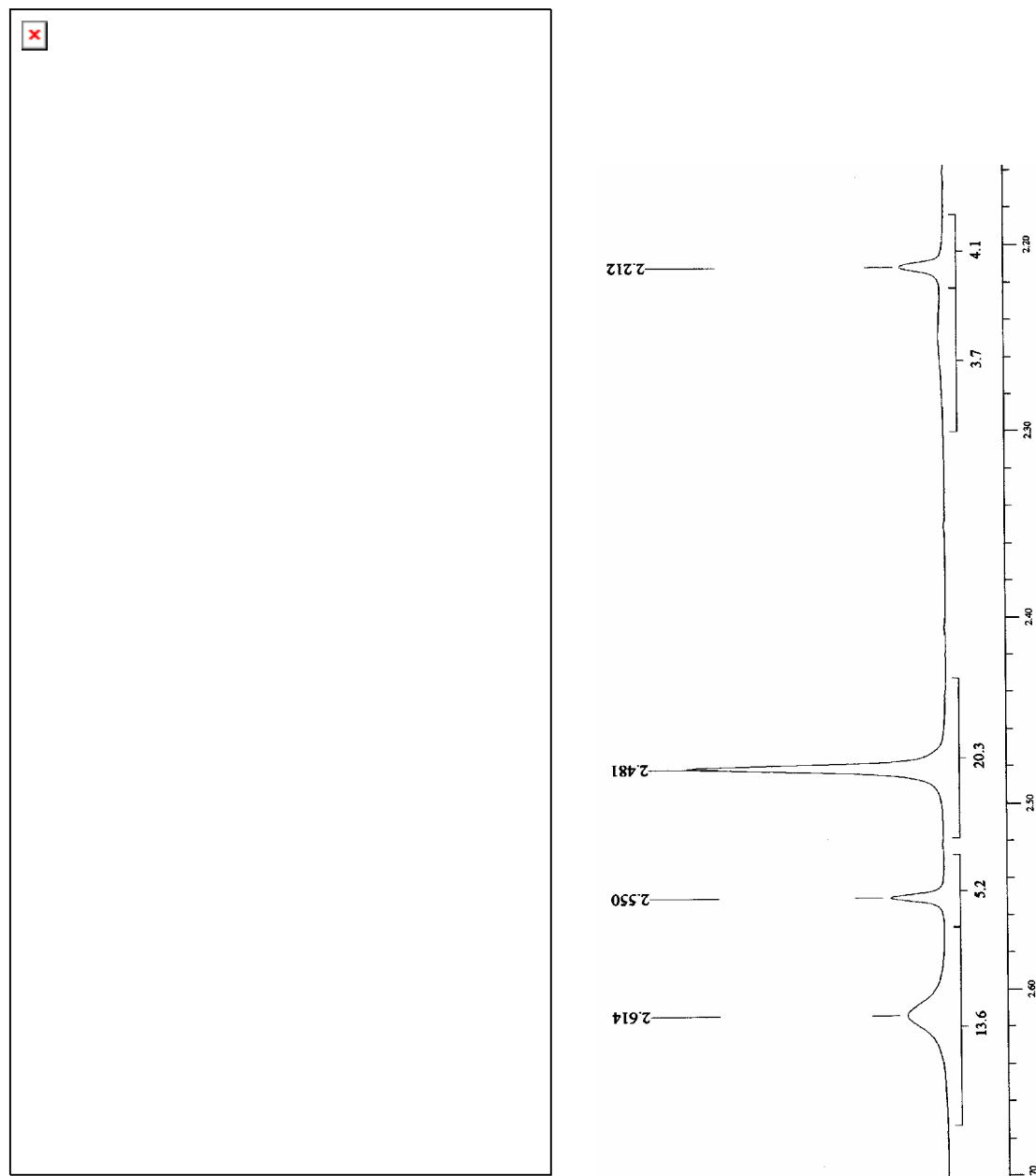


Figure S22. Expansions of the aromatic and aliphatic regions of the ^1H NMR spectrum of a mixture of $\text{Pd}(\text{OAc})_2$ (0.02 M), Na_2CO_3 (103.2 eq), TXPTS (2.8 eq) and $\text{PhB}(\text{OH})_2$ (3.9 eq) after 24 hours (500 MHz, 2:1 D_2O - CD_3CN).

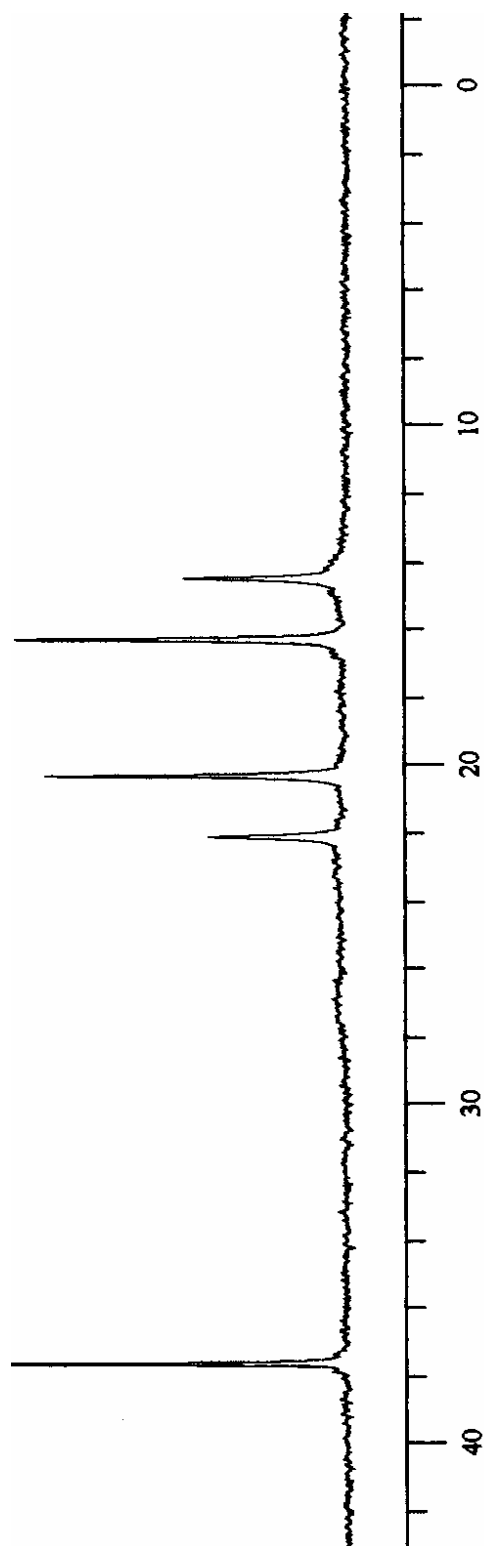


Figure S23. ^{31}P NMR spectrum of a mixture of $\text{Pd}(\text{OAc})_2$, TXPTS (2.5 eq) and $\text{PhB}(\text{OH})_2$ (4.0 eq) in 2:1 $\text{D}_2\text{O}/\text{CH}_3\text{CN}$ after 24 hours at room temperature.

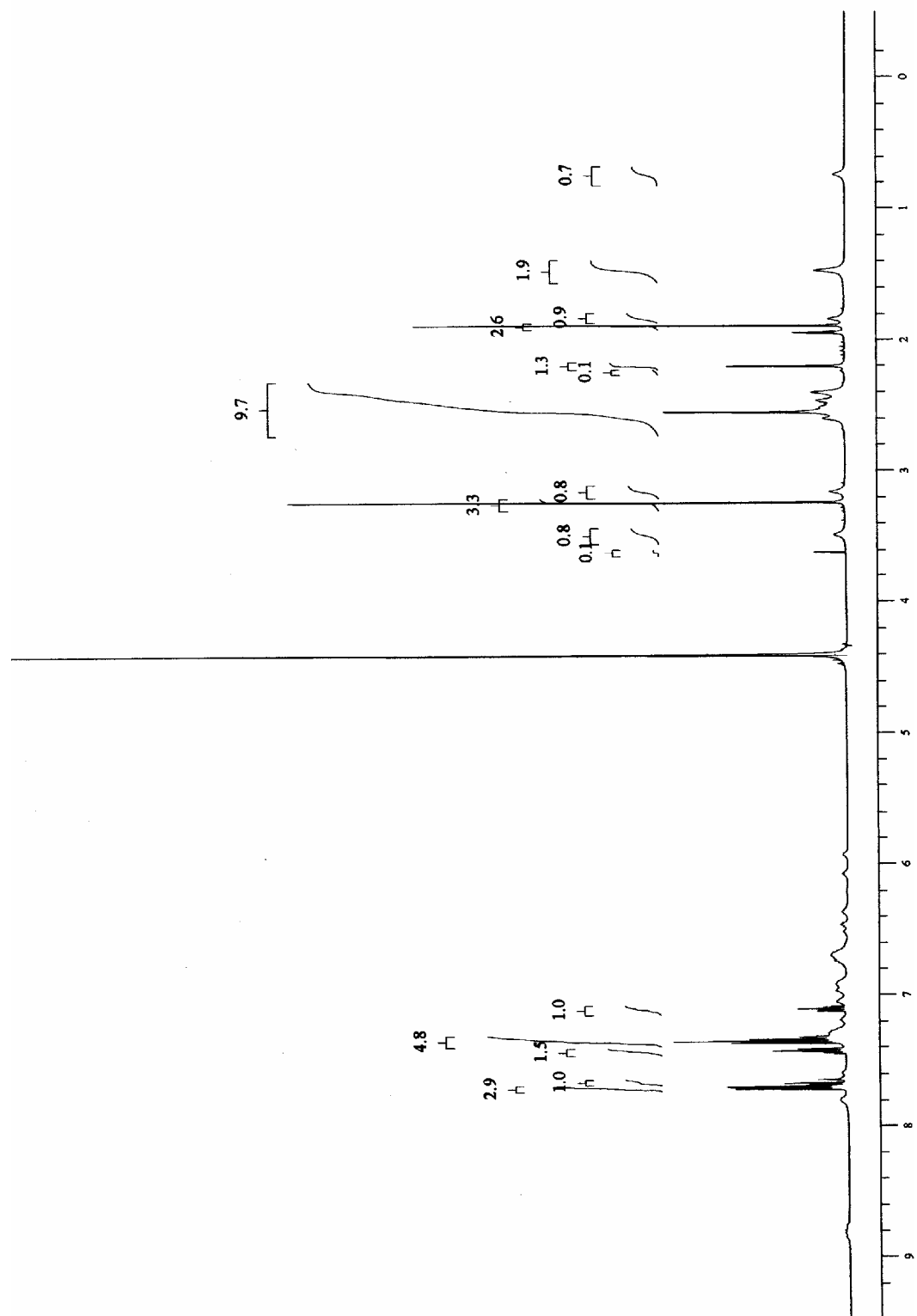


Figure S24. ^1H NMR spectrum of a mixture of $\text{Pd}(\text{OAc})_2$ (0.02 M), TXPTS (2.5 eq) and $\text{PhB}(\text{OH})_2$ (4.4 eq) after 48 hours (500 MHz, 2:1 D_2O - CH_3CN).

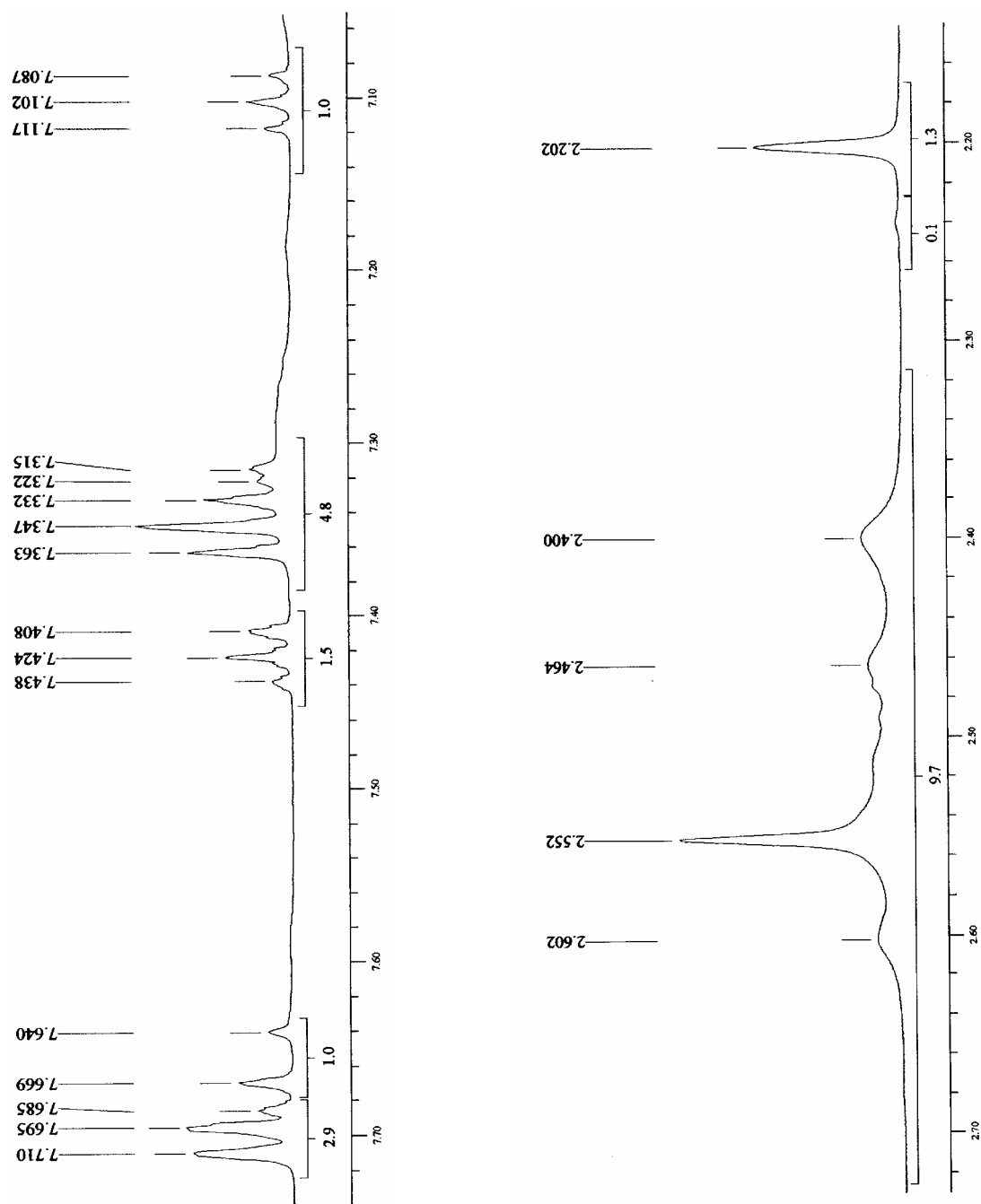


Figure S25. Expansions of the aromatic and alkyl regions of the ^1H NMR spectrum of a mixture of $\text{Pd}(\text{OAc})_2$ (0.02 M), TXPTS (2.5 eq) and $\text{PhB}(\text{OH})_2$ (4.4 eq) after 48 hours (500 MHz, 2:1 D_2O - CH_3CN).

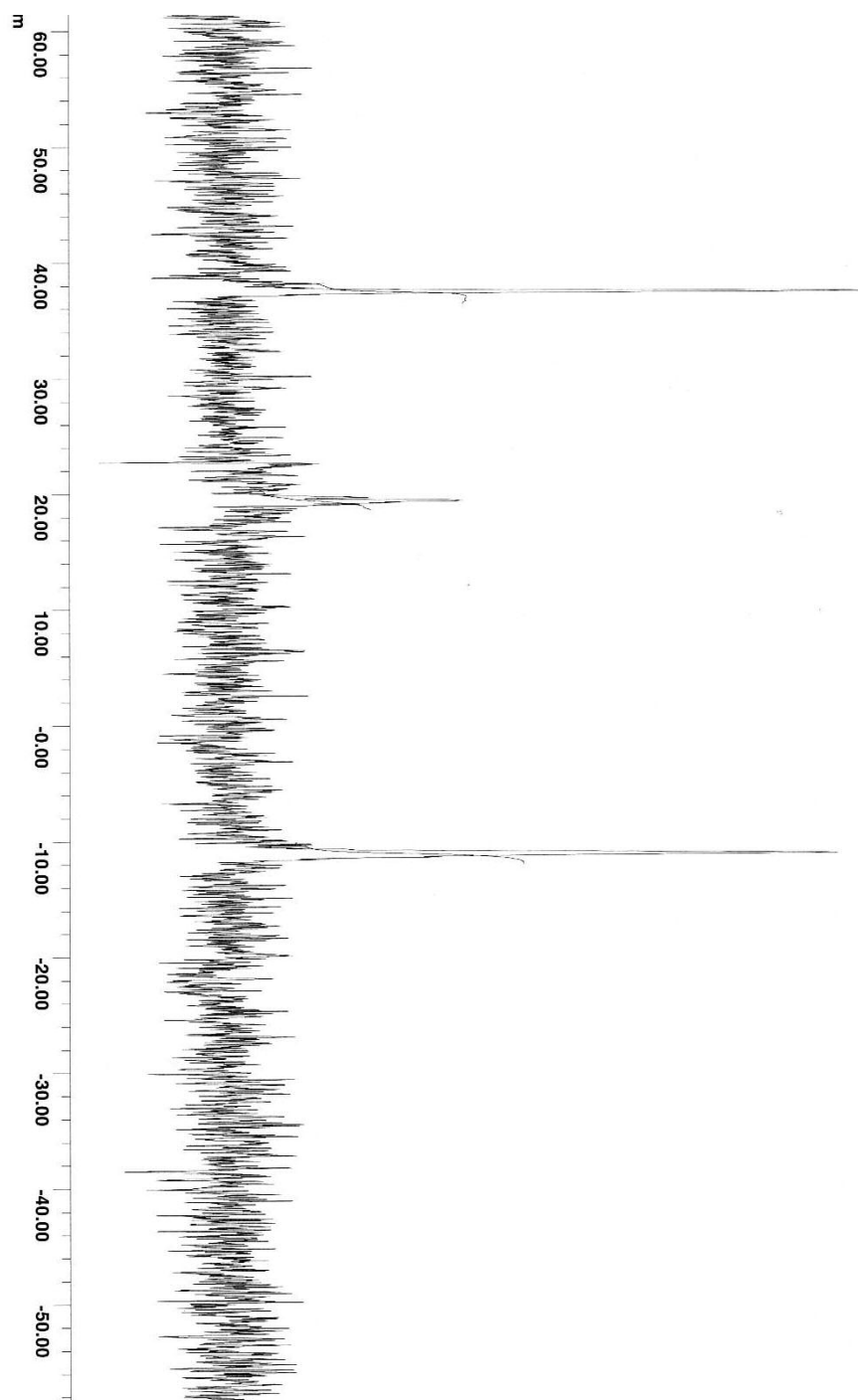


Figure S26. ^{31}P NMR spectrum of a mixture of TMAPTS•Na₃ (XX), Pd(OAc)₂ (XX) and Na₂CO₃ after 1 hour (202.5 MHz, 1:1 D₂O/CH₃CN).

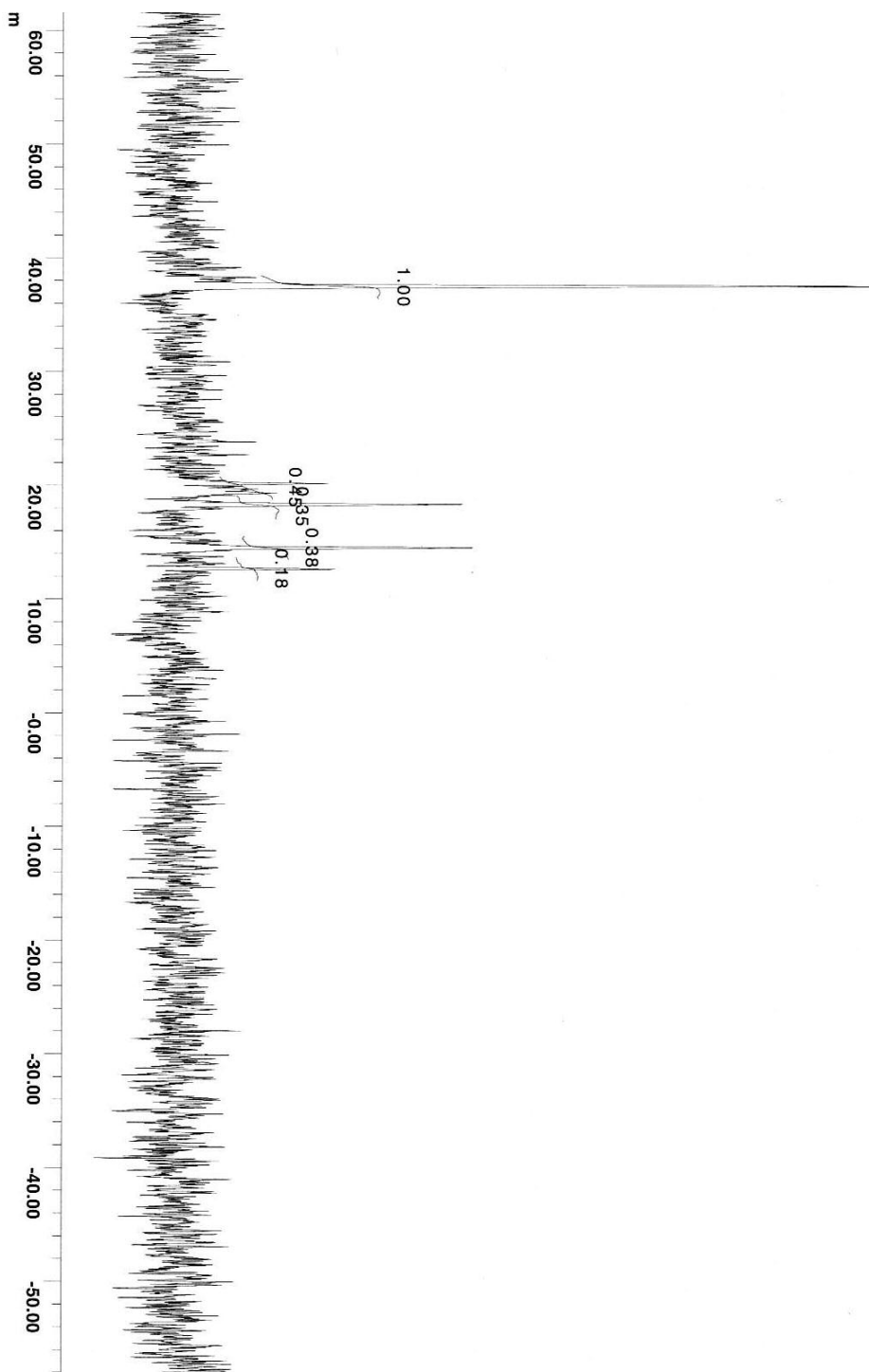


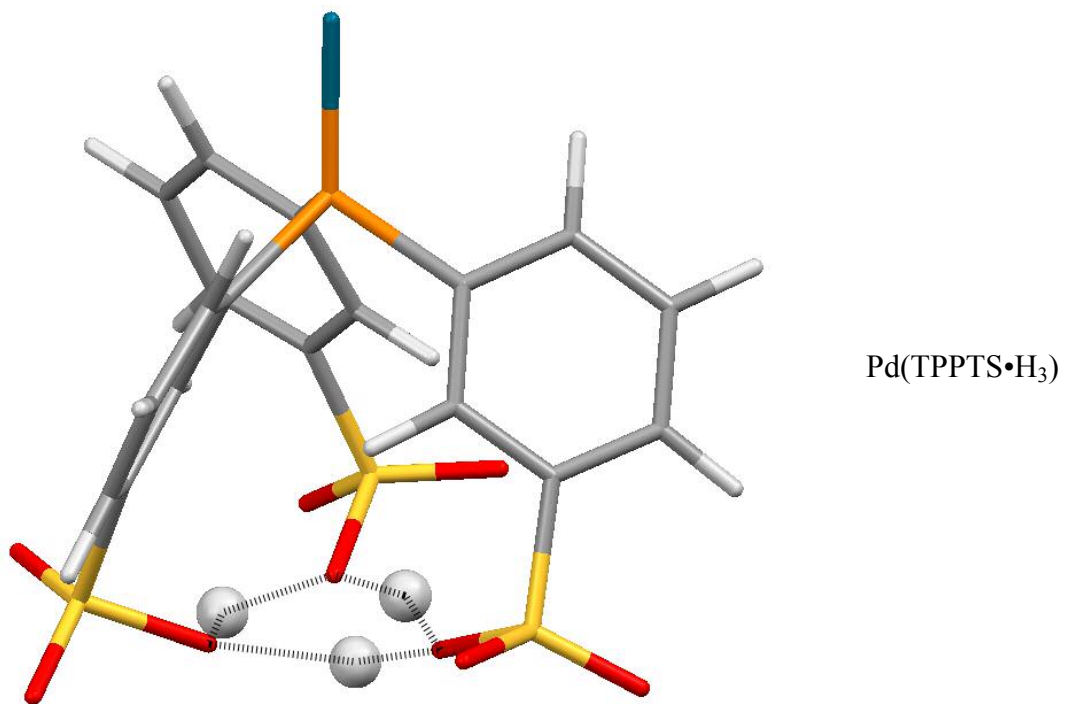
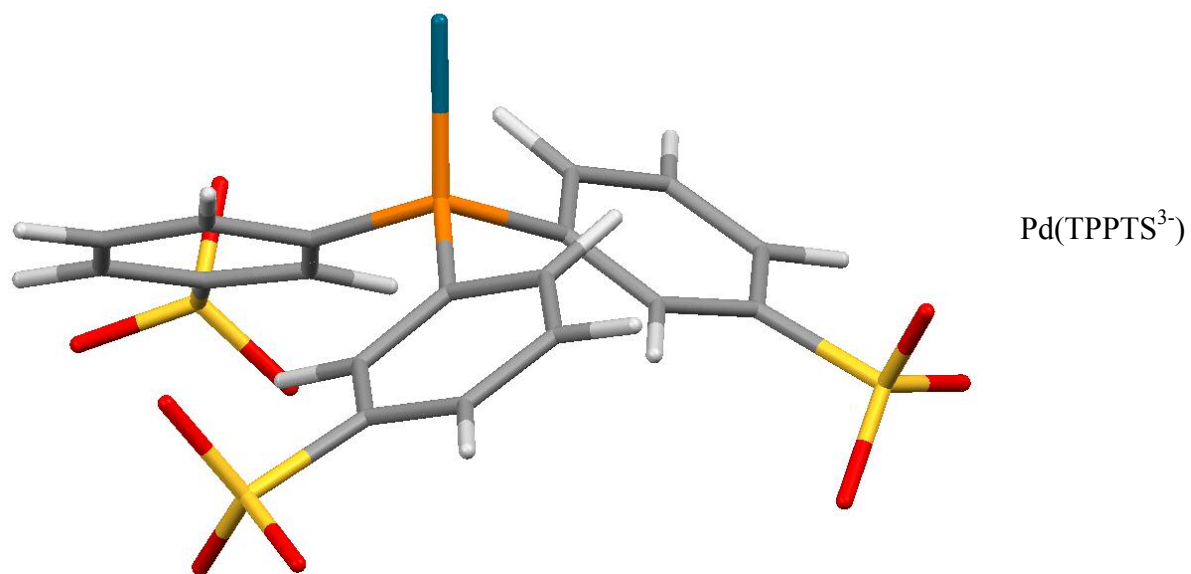
Figure S27. ^{31}P NMR spectrum of a mixture of TMAPTS•Na₃ (XX), Pd(OAc)₂ (XX), Na₂CO₃, and 4-ethyl-1-iodobenzene (XX) after 1 hour (202.5 MHz, 1:1 D₂O/CH₃CN).

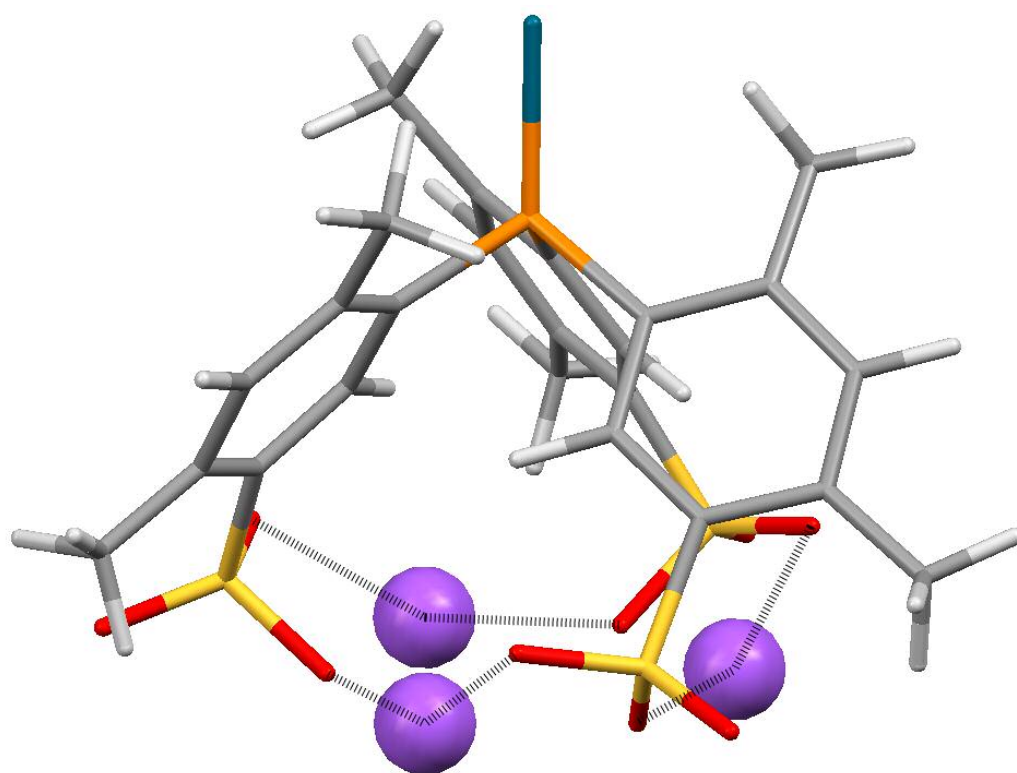
Computed Total Energies and Atomic Coordinates

Table S3. Pd, L, Pd(L), and Pd(L)₂ Total Electronic Energies in a.u.

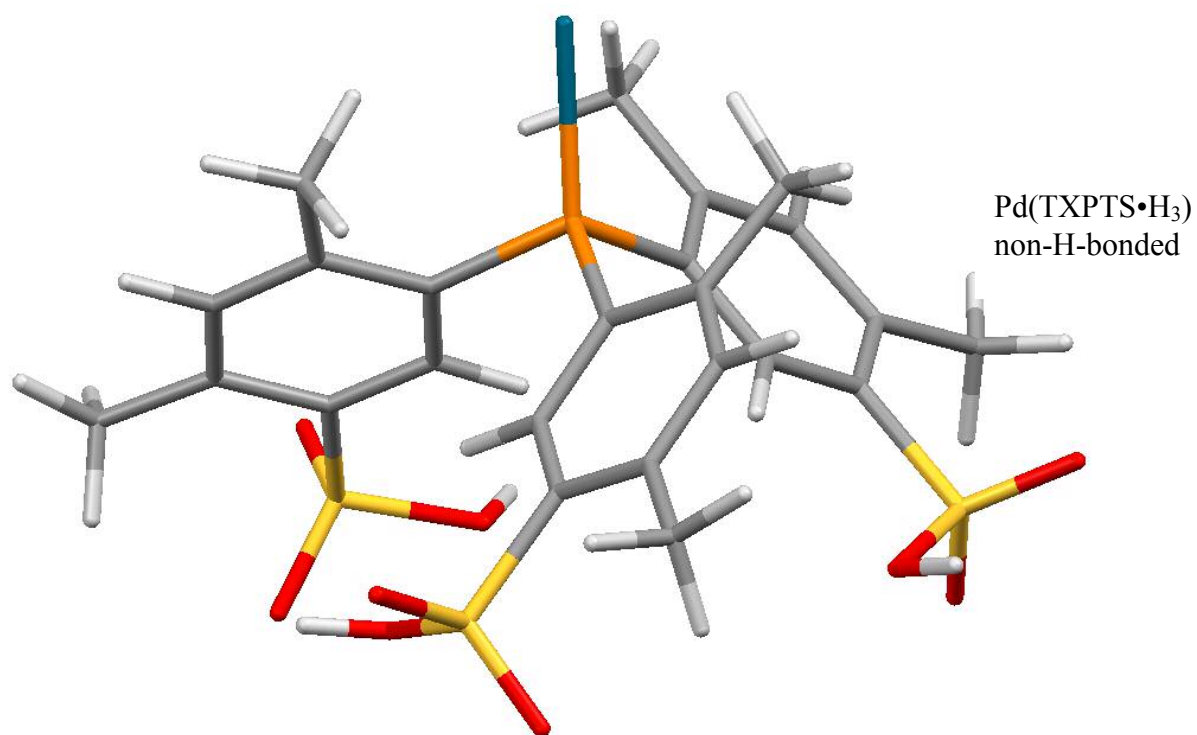
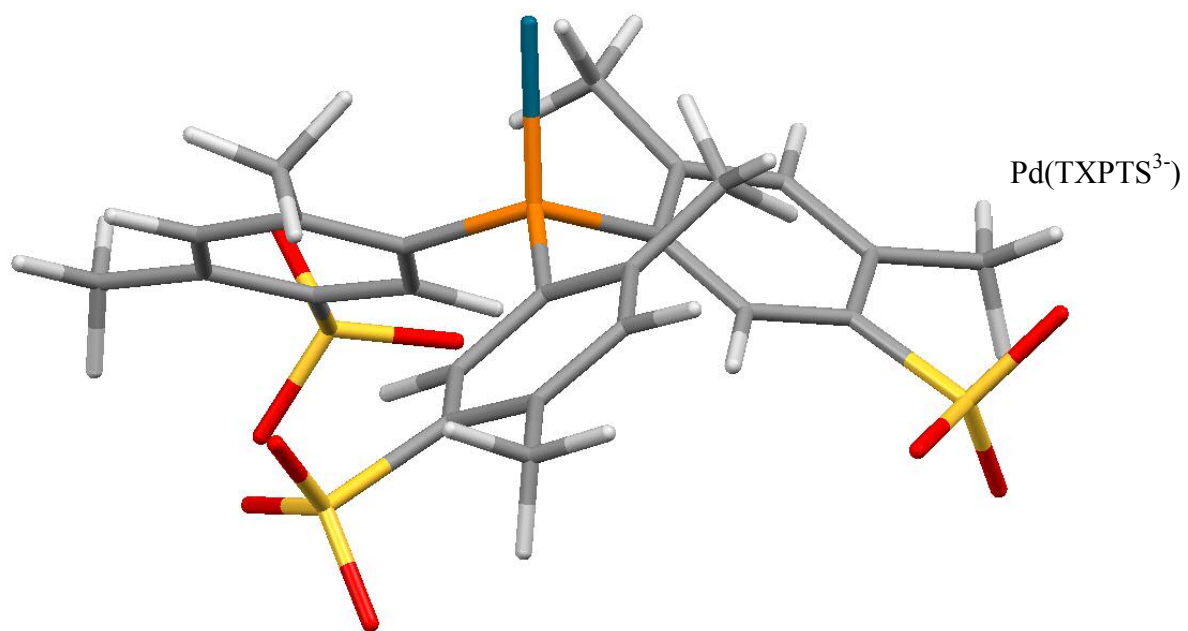
Species	E(B3LYP/AhlrichsVTZ+P; Stuttgart RSC 1997 for Pd)
Pd	-127.886371
PPh ₃	-1036.547116
Pd(PPh ₃)	-1164.492921
Pd(PPh ₃) ₂	-2201.089788
P(<i>o</i> -tol) ₃	-1154.531607
Pd(P(<i>o</i> -tol) ₃)	-1282.468989
Pd(P(<i>o</i> -tol) ₃) ₂	-2437.041041
TPPTS ³⁻	-2906.528628
TPPTS•H ₃	-2908.245887
TPPTS•Na ₃	-3393.695971
Pd(TPPTS ³⁻)	-3034.471745
Pd(TPPTS ³⁻) ₂	-5940.671933
Pd(TPPTS•Na ₃)	-3521.642414
Pd(TPPTS•H ₃)	-3036.190492
TXPTS ³⁻	-3142.490924
TXPTS•H ₃	-3144.243603
TXPTS•H ₃ no H-bond	-3144.214922
TXPTS•Na ₃	-3629.657093
Pd(TXPTS ³⁻)	-3270.435368
Pd(TXPTS ³⁻) ₂	-6412.600359
Pd(TXPTS•Na ₃)	-3757.601704
Pd(TXPTS•H ₃)	-3272.180833
Pd(TXPTS•H ₃ no H-bond)	-3272.168384
TMAPTS ³⁻	-3368.168285
TMAPTS•H ₃	-3369.902611
TMAPTS•H ₃ no H-bond	-3369.896888
TMAPTS•Na ₃	-3855.339931
Pd(TMAPTS ³⁻)	-3496.111549
Pd(TMAPTS ³⁻) ₂	-6863.960809
Pd(TMAPTS•Na ₃)	-3983.282002
Pd(TMAPTS•H ₃)	-3497.841632
Pd(TMAPTS•H ₃ no H-bond)	-3497.832799
P(Mes) ₃	-1390.477771
Pd(P(Mes) ₃)	-1518.406065
P(2,4- <i>t</i> -Bu ₂ C ₆ H ₃) ₃	-1980.331042
Pd(P(2,4- <i>t</i> -Bu ₂ C ₆ H ₃) ₃)	-2108.230672
TXP	-1272.522361
Pd(TXP)	-1400.460391
TMAP	-1498.221555
P(TMAP)	-1626.159809

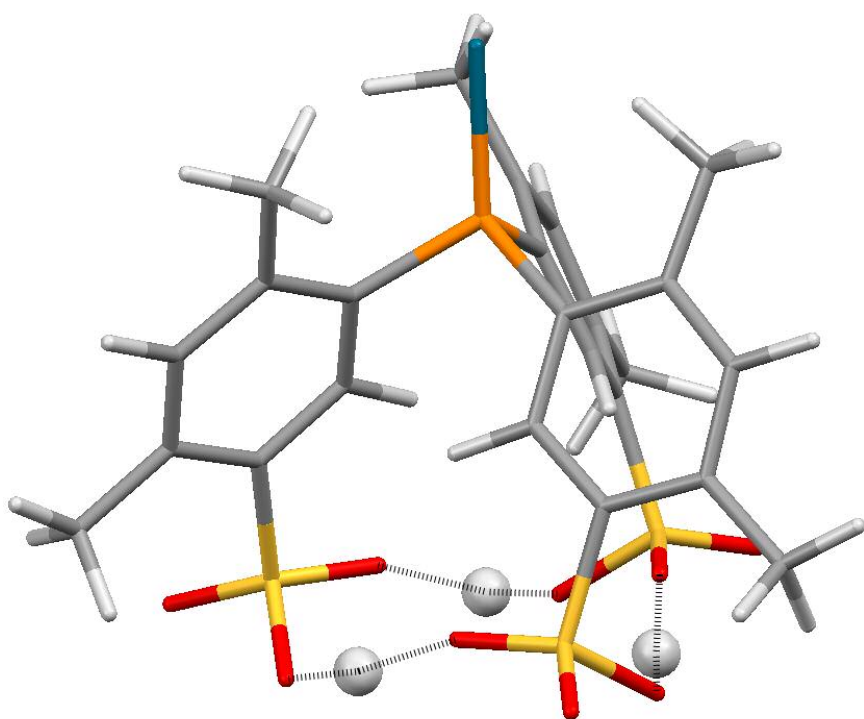
Cylindrical bond models of calculated structures for PdL complexes (L = sulfonated phosine). Carbon, grey; hydrogen, white; phosphorus, orange; sulfur, yellow; oxygen, red; palladium, blue; sodium, purple.



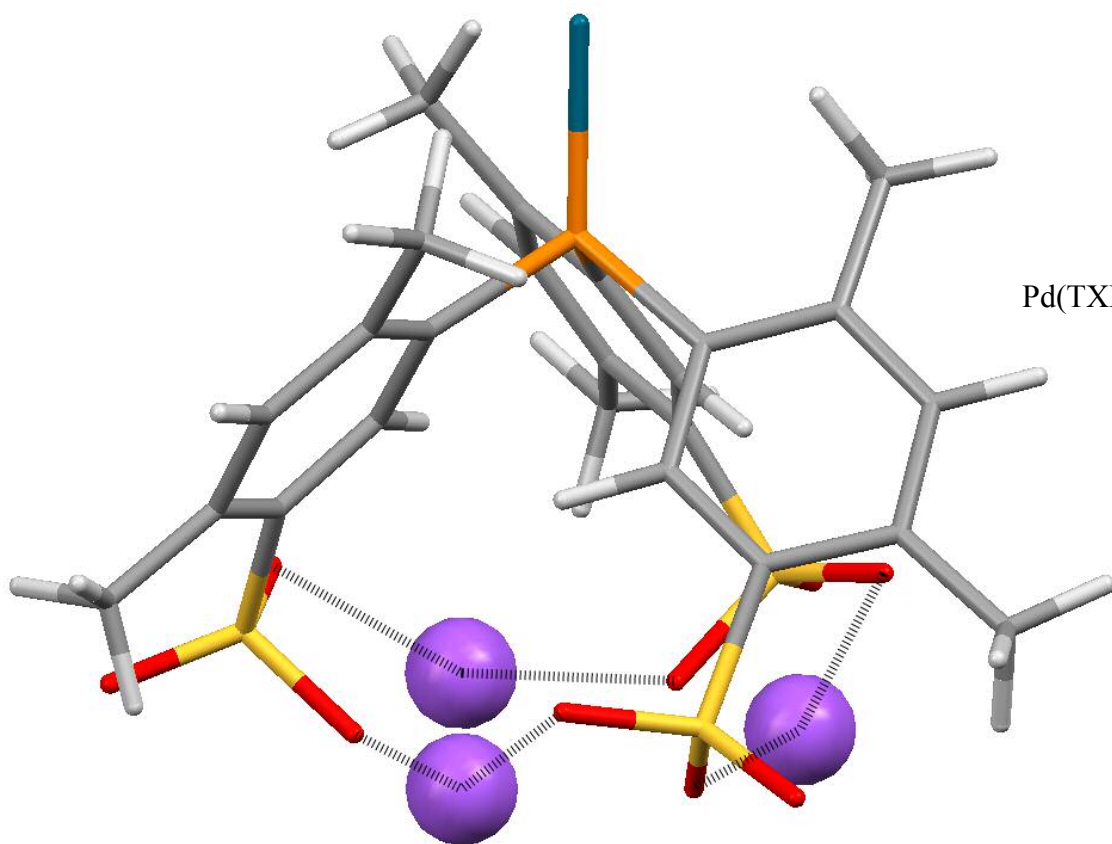


Pd(TPPTS·Na₃)

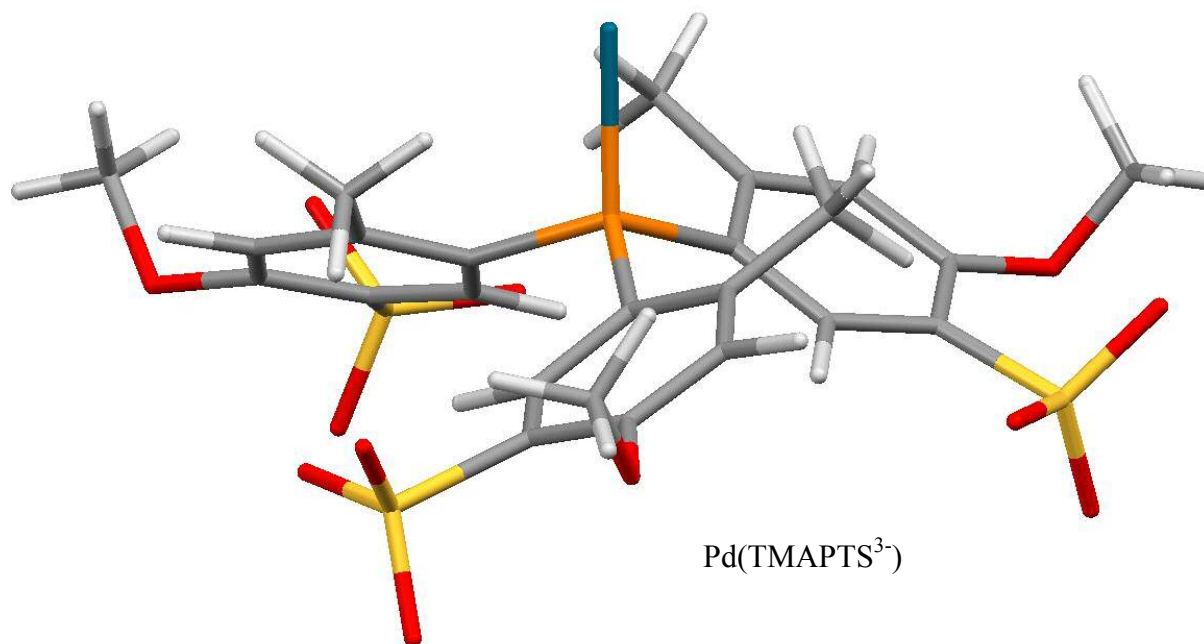




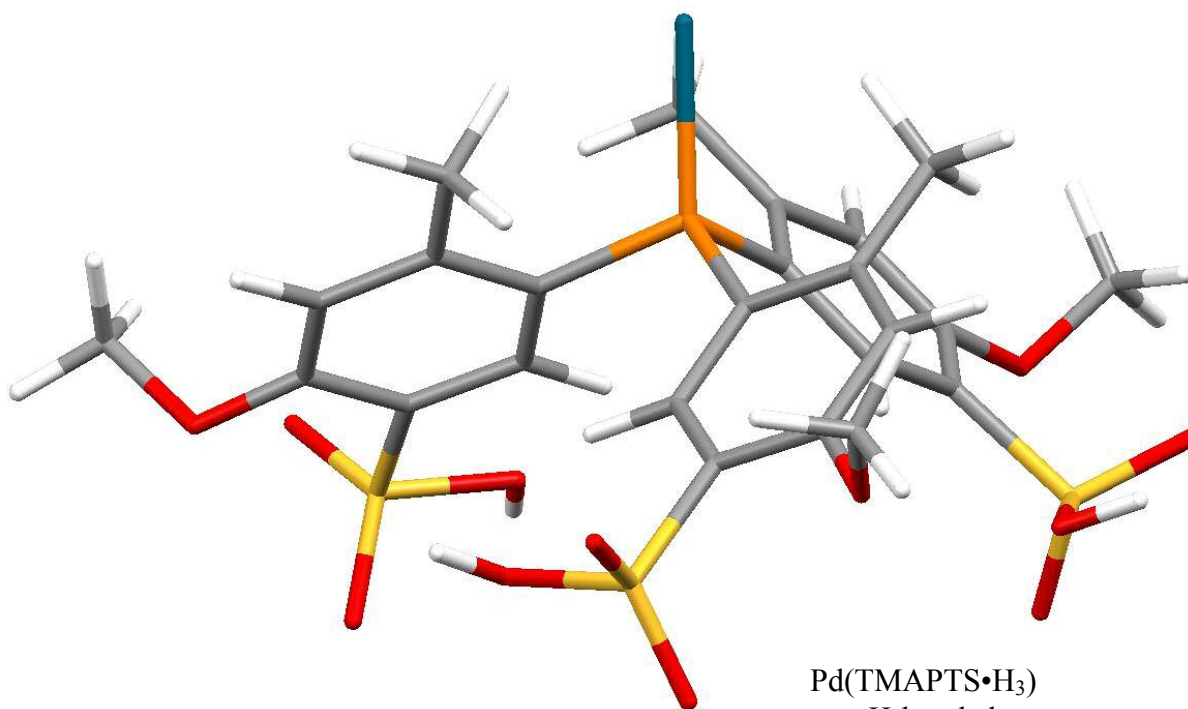
Pd(TXPTS•H₃)
H-bonded



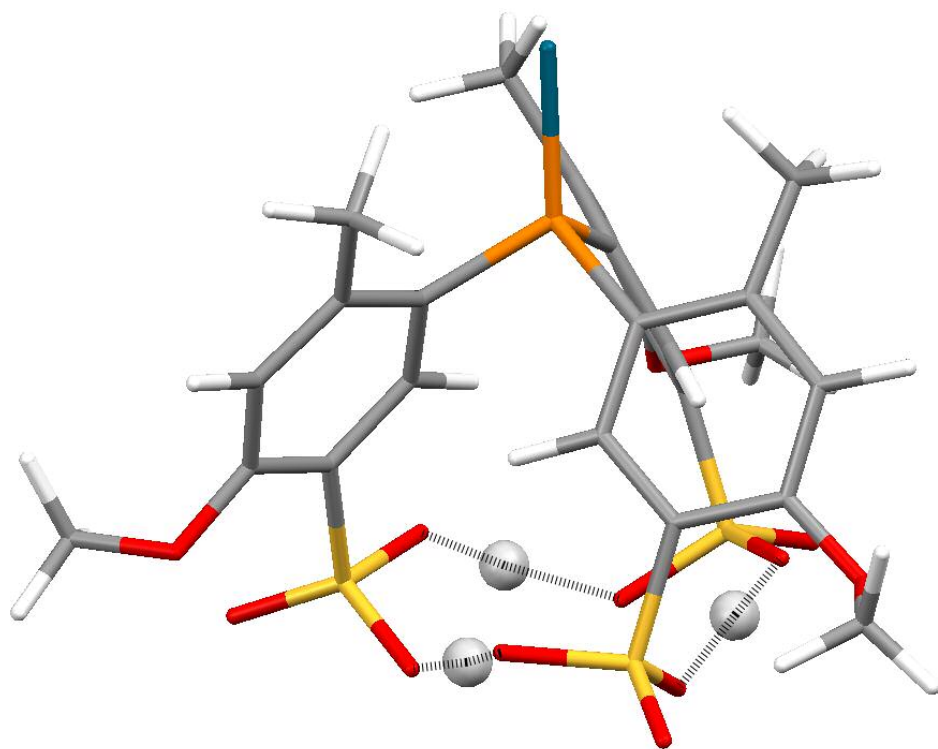
Pd(TXPTS•Na₃)



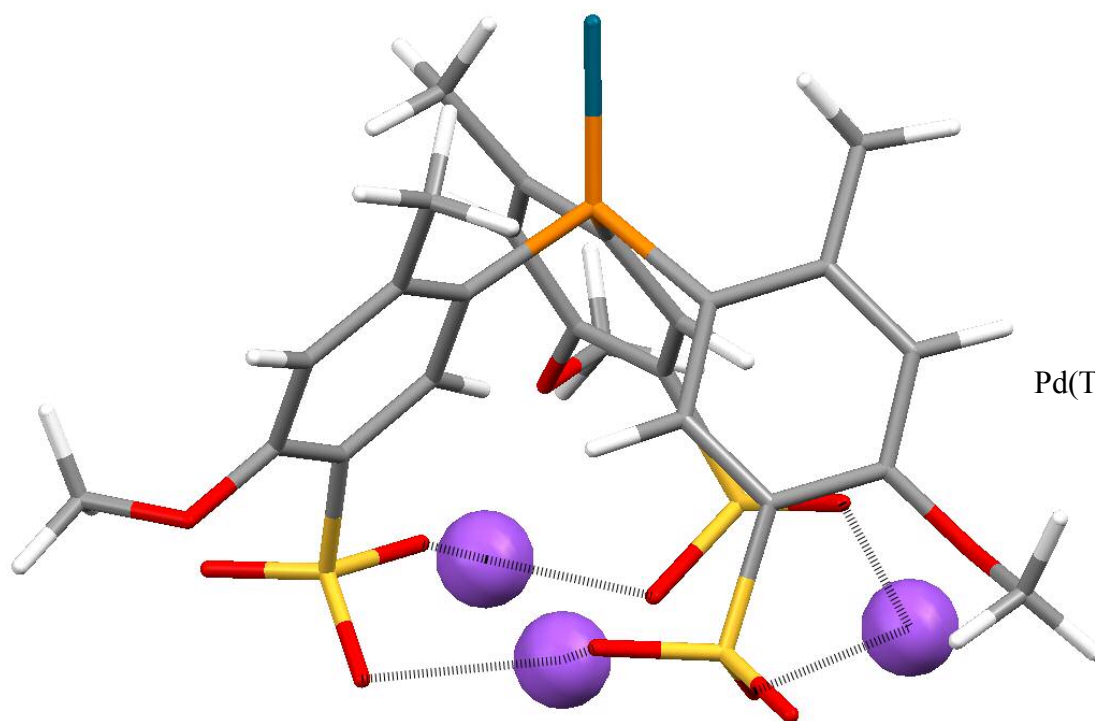
$\text{Pd}(\text{TMAPTS}^{3-})$



$\text{Pd}(\text{TMAPTS} \cdot \text{H}_3)$
non-H-bonded

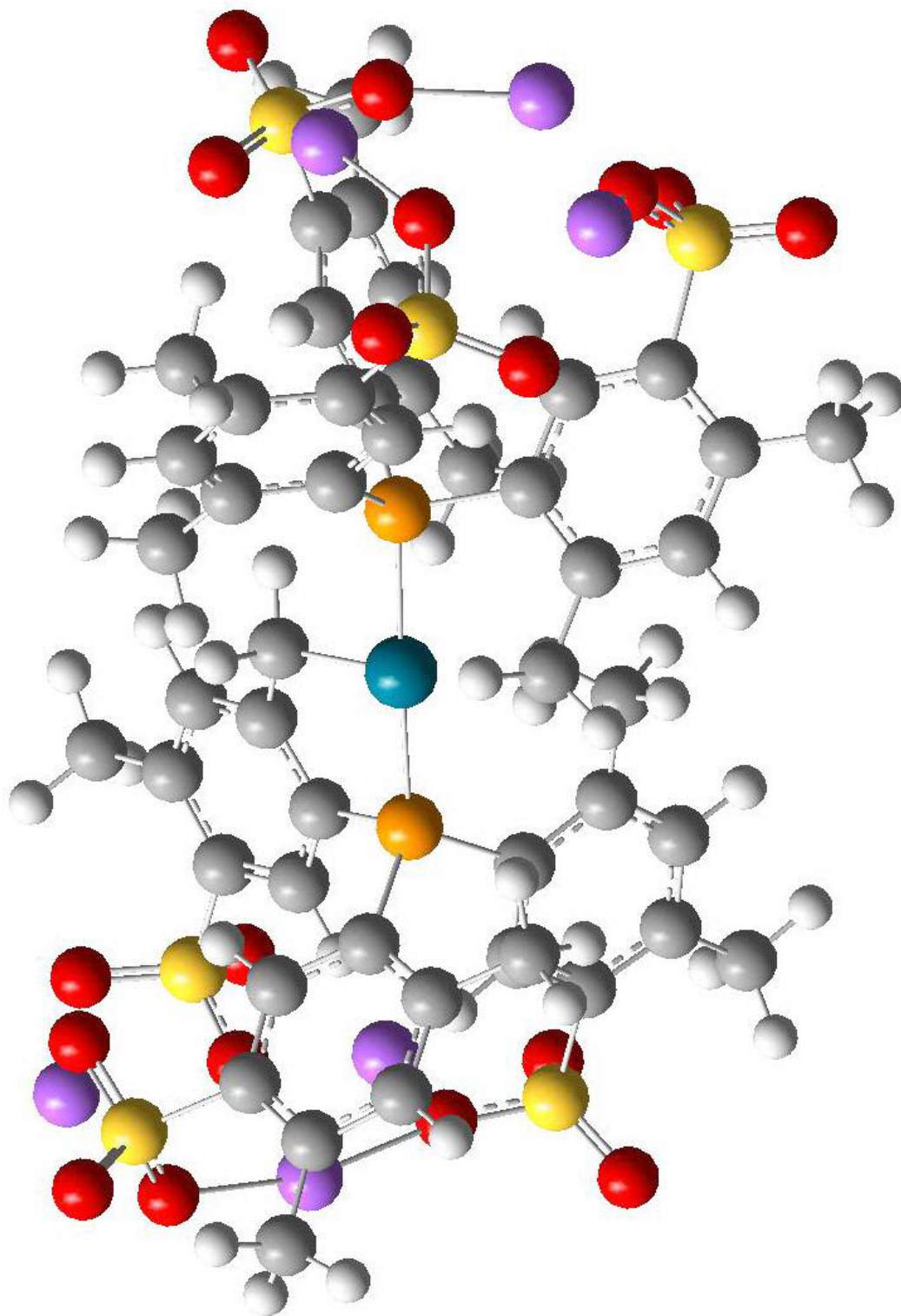


Pd(TMAPTS·H₃)
H-bonded



Pd(TMAPTS·Na₃)

Ball and stick model of calculated structure of $\text{Pd}(\kappa^2C,P\text{-TXPTS}\cdot\text{Na}_3)(\kappa P\text{-TXPTS}\cdot\text{Na}_3)$ (**16**).



Local DFT optimized geometries (coordinates) in x,y,z format in Å.

PPh₃

P	0.00133	0.0017	-1.28773
C	-1.67479	3.81821	0.73449
C	-0.69774	1.47038	-0.45307
C	-0.78096	3.89466	-0.33591
C	-0.30554	2.72826	-0.93259
C	-1.59484	1.40197	0.61941
C	-2.08303	2.57037	1.20626
H	-2.0591	4.73629	1.19813
H	-0.45923	4.87291	-0.71714
H	-2.78757	2.50363	2.04613
H	0.38636	2.79019	-1.78576
H	-1.91178	0.41994	1.00032
C	4.22297	-0.35247	0.58689
C	1.65426	-0.08465	-0.51153
C	3.79188	-1.2325	-0.40829
C	2.52065	-1.09114	-0.96148
C	2.09365	0.79433	0.48539
C	3.37304	0.66228	1.02767
H	5.22848	-0.4552	1.01574
H	4.45673	-2.03039	-0.76488
H	3.70718	1.35897	1.80819
H	2.18825	-1.77557	-1.75621
H	1.42302	1.59031	0.84154
C	-2.33958	-3.3646	0.86854
C	-0.86709	-1.34289	-0.40471
C	-2.9186	-2.61933	-0.16094
C	-2.18256	-1.62357	-0.80047
C	-0.29293	-2.09522	0.62675
C	-1.02516	-3.103	1.25632
H	-2.91436	-4.15685	1.36604
H	-3.95063	-2.82289	-0.47602
H	-0.56336	-3.68715	2.06363
H	-2.63513	-1.04733	-1.62117
H	0.73994	-1.88506	0.94126

Pd(PPh₃)

Pd	0.04361	0.07594	-2.54125
P	0.00821	0.01117	-0.41073
C	1.00627	3.99545	1.70527
C	0.34452	1.59109	0.43665
C	1.66143	3.62178	0.52933
C	1.32523	2.42938	-0.10706
C	-0.31275	1.96939	1.61217

C	0.01651	3.17107	2.24118
H	1.26356	4.94021	2.20207
H	2.43309	4.27282	0.09768
H	-0.50842	3.46668	3.15934
H	1.80742	2.13319	-1.0521
H	-1.09375	1.31979	2.03447
C	2.95533	-2.97297	1.52739
C	1.20815	-1.11996	0.36847
C	2.29358	-3.28508	0.33714
C	1.43154	-2.3588	-0.24464
C	1.87511	-0.80827	1.55816
C	2.74913	-1.73285	2.13219
H	3.64301	-3.69855	1.98146
H	2.46115	-4.2556	-0.14832
H	3.27574	-1.47957	3.06194
H	0.92543	-2.57431	-1.19903
H	1.71239	0.16952	2.03587
C	-4.04652	-1.16818	1.4643
C	-1.57046	-0.5106	0.3394
C	-3.98857	-0.37277	0.31719
C	-2.75636	-0.05361	-0.24798
C	-1.63145	-1.31024	1.48567
C	-2.8679	-1.64007	2.04271
H	-5.01792	-1.42852	1.90499
H	-4.91407	-0.00832	-0.14786
H	-2.90974	-2.27424	2.93826
H	-2.69177	0.54558	-1.16998
H	-0.70187	-1.68167	1.94203

Pd(PPh₃)₂

P	-0.00961	-2.32029	-0.07692
C	-4.21965	-3.83291	-1.3752
C	-1.63386	-3.02183	-0.54817
C	-3.07752	-4.28275	-2.0594
C	-1.80586	-3.88753	-1.64245
C	-2.77268	-2.54737	0.1412
C	-4.03045	-2.97902	-0.28948
H	-4.91691	-2.61477	0.25577
H	-0.93738	-4.27182	-2.20319
C	1.02124	-3.96955	4.15522
C	0.42179	-3.07486	1.53461
C	-0.11556	-4.4467	3.48059
C	-0.40162	-4.00931	2.18684
C	1.5625	-2.57558	2.20304
C	1.83058	-3.04905	3.49073
H	2.72517	-2.66353	4.00742

H	-1.30033	-4.41542	1.6928
C	3.19352	-3.71563	-3.15665
C	1.19796	-2.97527	-1.28718
C	3.1995	-4.25057	-1.85708
C	2.20941	-3.88906	-0.94279
C	1.18526	-2.41658	-2.5852
C	2.18022	-2.8151	-3.48261
H	2.16365	-2.38476	-4.49764
H	2.24833	-4.33886	0.06347
O	-1.92589	-5.62983	-4.01035
O	-4.01428	-6.56348	-2.98977
O	-4.14382	-4.55469	-4.44334
S	-3.29381	-5.3544	-3.50273
O	4.27204	-5.75081	0.02608
O	4.42083	-6.53313	-2.34882
O	5.78888	-4.60149	-1.59912
S	4.52956	-5.38705	-1.39023
O	-2.31103	-5.90171	3.38163
O	-0.35334	-6.7875	4.66868
O	-1.65329	-4.87144	5.56552
S	-1.21233	-5.60616	4.33571
C	1.35172	-4.41843	5.54033
C	-5.59257	-4.24287	-1.79542
C	4.23823	-4.08616	-4.15704
H	-5.66995	-5.3484	-1.7918
H	-5.76372	-3.94788	-2.85007
H	-6.35648	-3.7943	-1.13267
H	1.4423	-5.52265	5.56381
H	0.50645	-4.18641	6.21882
H	2.28376	-3.94031	5.89619
H	4.24941	-5.18562	-4.29594
H	5.24186	-3.83858	-3.75707
H	4.06053	-3.57089	-5.1198
C	-2.6679	-1.59853	1.2836
C	0.16568	-1.41671	-3.00738
C	2.4604	-1.55998	1.58694
H	-2.01781	-0.72291	1.00667
H	-2.1808	-2.06454	2.16359
H	-3.66057	-1.22333	1.59095
H	1.86121	-0.6893	1.19972
H	2.99789	-1.96455	0.70607
H	3.20643	-1.18595	2.31086
H	0.09918	-0.58066	-2.25637
H	-0.85048	-1.85778	-3.05086
H	0.40422	-0.98796	-3.99726
Pd	-0.02171	-0.00366	0.00262

P	-0.01842	2.31225	0.08143
C	-4.30537	3.82187	1.10327
C	-1.67084	3.01233	0.44538
C	-3.21009	4.2731	1.85943
C	-1.91395	3.87882	1.52558
C	-2.76214	2.53762	-0.31659
C	-4.0455	2.96834	0.03192
H	-4.89441	2.60374	-0.56998
H	-1.08387	4.26461	2.14093
C	1.2812	3.966	-4.07462
C	0.51482	3.06745	-1.4992
C	0.10166	4.43945	-3.47521
C	-0.26649	4.00076	-2.20283
C	1.69748	2.57113	-2.09279
C	2.04785	3.04681	-3.35971
H	2.97512	2.66421	-3.81741
H	-1.19592	4.40478	-1.76769
C	2.97438	3.72503	3.35902
C	1.10756	2.97186	1.36572
C	3.06561	4.25308	2.05981
C	2.13834	3.88546	1.08404
C	1.01085	2.41891	2.66275
C	1.94352	2.82392	3.6219
H	1.86062	2.39855	4.63581
H	2.24246	4.33096	0.08049
O	-2.18699	5.62339	3.87858
O	-4.20818	6.55271	2.72718
O	-4.42599	4.54431	4.17072
S	-3.51946	5.34513	3.28548
O	4.25824	5.7448	0.24336
O	4.24998	6.54016	2.61849
O	5.66593	4.60607	1.97093
S	4.42233	5.38894	1.67551
O	-2.10086	5.88572	-3.52161
O	-0.06396	6.78036	-4.67359
O	-1.29394	4.86067	-5.6577
S	-0.93968	5.59597	-4.40049
C	1.70013	4.41885	-5.43436
C	-5.70289	4.23011	1.43416
C	3.9495	4.10296	4.4247
H	-5.77975	5.33565	1.42964
H	-5.9427	3.9313	2.47424
H	-6.42173	3.78388	0.72133
H	1.787	5.52357	-5.45021
H	0.90243	4.18464	-6.16748
H	2.65578	3.9458	-5.72921

H	3.95095	5.20336	4.5563
H	4.97781	3.85311	4.09502
H	3.70747	3.59413	5.3768
C	-2.583	1.59057	-1.45138
C	-0.0316	1.4179	3.02174
C	2.55634	1.55705	-1.42099
H	-1.9486	0.71654	-1.13662
H	-2.04346	2.05997	-2.29839
H	-3.55326	1.21255	-1.82042
H	1.93724	0.68262	-1.07632
H	3.03258	1.96181	-0.50548
H	3.35043	1.18786	-2.09463
H	-0.04497	0.57851	2.27235
H	-1.0498	1.85533	2.99657
H	0.14254	0.99498	4.02742

P(*o*-tol)₃

P	0.000000	0.000000	0.911053
C	0.984769	4.113250	-0.965062
C	0.363697	1.601539	0.112635
C	1.662309	2.979076	-1.411518
C	1.349304	1.732103	-0.872737
C	-0.324238	2.747021	0.569844
C	0.000000	3.989006	0.014401
H	-0.537623	4.881428	0.367037
H	1.870891	0.831309	-1.230557
C	-4.054563	-1.203790	-0.965062
C	-1.568822	-0.485799	0.112635
C	-3.411110	-0.049936	-1.411518
C	-2.174697	0.302480	-0.872737
C	-2.216871	-1.654309	0.569844
C	-3.454581	-1.994503	0.014401
H	-3.958629	-2.906309	0.367037
H	-1.655381	1.204585	-1.230557
C	3.069794	-2.909460	-0.965062
C	1.205125	-1.115740	0.112635
C	1.748801	-2.929140	-1.411518
C	0.825393	-2.034583	-0.872737
C	2.541109	-1.092712	0.569844
C	3.454581	-1.994503	0.014401
H	4.496252	-1.975119	0.367037
H	-0.215511	-2.035894	-1.230557
C	-1.401141	2.635435	1.596696
C	2.982924	-0.104294	1.596696
C	-1.581783	-2.531141	1.596696
H	-1.084567	1.993809	2.442875

H	-2.307912	2.157218	1.174466
H	-1.691634	3.624329	1.992086
H	-1.184406	-1.936168	2.442875
H	-0.714249	-3.077319	1.174466
H	-2.292944	-3.277163	1.992086
H	2.268973	-0.057642	2.442875
H	3.022161	0.920102	1.174466
H	3.984578	-0.347167	1.992086
H	2.436383	3.062646	-2.185898
H	1.223985	5.101088	-1.380826
H	-3.870521	0.578646	-2.185898
H	-5.029665	-1.490542	-1.380826
H	1.434138	-3.641293	-2.185898
H	3.805679	-3.610547	-1.380826

Pd(P(*o*-tol)₃)

P	0.000000	0.000000	0.171881
C	1.495967	3.987429	-1.605281
C	0.543372	1.571965	-0.562804
C	2.023604	2.779982	-2.063060
C	1.546848	1.580566	-1.539821
C	0.000000	2.791016	-0.094513
C	0.496229	3.982668	-0.633741
H	0.080191	4.934638	-0.273068
H	1.954493	0.623412	-1.899197
C	-4.201198	-0.698169	-1.605281
C	-1.633047	-0.315408	-0.562804
C	-3.419337	0.362502	-2.063060
C	-2.142234	0.549327	-1.539821
C	-2.417091	-1.395508	-0.094513
C	-3.697206	-1.561588	-0.633741
H	-4.313617	-2.397872	-0.273068
H	-1.517137	1.380934	-1.899197
C	2.705231	-3.289259	-1.605281
C	1.089675	-1.256556	-0.562804
C	1.395733	-3.142484	-2.063060
C	0.595386	-2.129892	-1.539821
C	2.417091	-1.395508	-0.094513
C	3.200978	-2.421081	-0.633741
H	4.233426	-2.536766	-0.273068
H	-0.437355	-2.004346	-1.899197
C	-1.064797	2.821607	0.944026
C	2.975982	-0.488662	0.944026
C	-1.911185	-2.332945	0.944026
H	-0.777960	2.159850	1.807279
H	-2.018387	2.401749	0.566533

H	-1.253504	3.847035	1.306899
H	-1.481505	-1.753658	1.807279
H	-1.070782	-2.948848	0.566533
H	-2.704878	-3.009084	1.306899
H	2.259465	-0.406192	1.807279
H	3.089169	0.547100	0.566533
H	3.958382	-0.837951	1.306899
H	2.808120	2.769462	-2.831105
H	1.864775	4.940456	-2.007335
H	-3.802484	1.047173	-2.831105
H	-5.210948	-0.855285	-2.007335
H	0.994364	-3.816635	-2.831105
H	3.346173	-4.085171	-2.007335
PD	0.000000	0.000000	2.334896

Pd(P(*o*-tol)₃)₂

Pd	0.000000	0.000000	0.000000
P	0.000000	0.000000	2.260153
C	0.000000	1.660858	3.002399
C	-1.438345	-0.830429	3.002399
C	1.438345	-0.830429	3.002399
C	0.925915	1.996291	3.996753
C	-0.898156	2.635778	2.510949
C	-2.191796	-0.196280	3.996753
C	-1.833573	-2.095715	2.510949
C	1.265881	-1.800011	3.996753
C	2.731729	-0.540063	2.510949
C	0.978574	3.287459	4.517643
H	1.615997	1.223571	4.368633
C	-0.827045	3.925253	3.049010
C	-1.898988	2.314048	1.456004
C	-3.336309	-0.796260	4.517643
H	-1.867642	0.787709	4.368633
C	-2.985846	-2.678868	3.049010
C	-1.054530	-2.801596	1.456004
C	2.357736	-2.491199	4.517643
H	0.251645	-2.011280	4.368633
C	3.812891	-1.246384	3.049010
C	2.953518	0.487548	1.456004
C	0.096912	4.256569	4.039386
H	1.709390	3.534809	5.298833
H	-1.521731	4.689898	2.671690
H	-1.406219	1.790855	0.591866
H	-2.666476	1.603675	1.824380
H	-2.411835	3.220078	1.088367
C	-3.734753	-2.044356	4.039386

H	-3.915929	-0.287029	5.298833
H	-3.300705	-3.662807	2.671690
H	-0.847817	-2.113249	0.591866
H	-0.055586	-3.111074	1.824380
H	-1.582752	-3.698750	1.088367
C	3.637841	-2.212213	4.039386
H	2.206539	-3.247779	5.298833
H	4.822436	-1.027091	2.671690
H	2.254035	0.322393	0.591866
H	2.722062	1.507398	1.824380
H	3.994587	0.478671	1.088367
H	0.128366	5.279033	4.438930
H	-4.635960	-2.528348	4.438930
H	4.507594	-2.750685	4.438930
P	0.000000	0.000000	-2.260153
C	0.000000	-1.660858	-3.002399
C	1.438345	0.830429	-3.002399
C	-1.438345	0.830429	-3.002399
C	-0.925915	-1.996291	-3.996753
C	0.898156	-2.635778	-2.510949
C	2.191796	0.196280	-3.996753
C	1.833573	2.095715	-2.510949
C	-1.265881	1.800011	-3.996753
C	-2.731729	0.540063	-2.510949
C	-0.978574	-3.287459	-4.517643
H	-1.615997	-1.223571	-4.368633
C	0.827045	-3.925253	-3.049010
C	1.898988	-2.314048	-1.456004
C	3.336309	0.796260	-4.517643
H	1.867642	-0.787709	-4.368633
C	2.985846	2.678868	-3.049010
C	1.054530	2.801596	-1.456004
C	-2.357736	2.491199	-4.517643
H	-0.251645	2.011280	-4.368633
C	-3.812891	1.246384	-3.049010
C	-2.953518	-0.487548	-1.456004
C	-0.096912	-4.256569	-4.039386
H	-1.709390	-3.534809	-5.298833
H	1.521731	-4.689898	-2.671690
H	1.406219	-1.790855	-0.591866
H	2.666476	-1.603675	-1.824380
H	2.411835	-3.220078	-1.088367
C	3.734753	2.044356	-4.039386
H	3.915929	0.287029	-5.298833
H	3.300705	3.662807	-2.671690
H	0.847817	2.113249	-0.591866

H	0.055586	3.111074	-1.824380
H	1.582752	3.698750	-1.088367
C	-3.637841	2.212213	-4.039386
H	-2.206539	3.247779	-5.298833
H	-4.822436	1.027091	-2.671690
H	-2.254035	-0.322393	-0.591866
H	-2.722062	-1.507398	-1.824380
H	-3.994587	-0.478671	-1.088367
H	-0.128366	-5.279033	-4.438930
H	4.635960	2.528348	-4.438930
H	-4.507594	2.750685	-4.438930

TPPTS³⁻

P	0.01193866	-0.01079171	1.46493161
C	-0.35070041	4.46007729	0.35271901
C	-0.11459878	1.69583857	0.82914960
C	0.81637412	3.78220391	0.00899552
C	0.92451429	2.40221500	0.20472746
C	-1.27364361	2.39671803	1.21265137
C	-1.40269756	3.75604630	0.93969291
H	-2.33824253	4.27030993	1.20230401
H	1.83625257	1.89164698	-0.14129272
C	-3.67631149	-2.53376412	0.28498492
C	-1.40261114	-0.95779818	0.80473411
C	-3.67244744	-1.17661059	-0.02738275
C	-2.53215861	-0.39731202	0.18987547
C	-1.43012607	-2.32095647	1.15596414
C	-2.54181242	-3.10603809	0.86176234
H	-2.51925015	-4.17922449	1.09921765
H	-2.54461479	0.65566379	-0.13049147
C	4.03434753	-1.93268096	0.25263855
C	1.53768802	-0.74666530	0.78369868
C	2.85538077	-2.59112024	-0.08577985
C	1.61276627	-1.98989773	0.13963214
C	2.73439097	-0.10345425	1.15452313
C	3.96759987	-0.67571527	0.85648149
H	4.88833332	-0.13423596	1.11682796
H	0.70237803	-2.51583791	-0.18524043
O	3.08358955	4.90522718	0.60640210
O	2.82675076	3.94035220	-1.68426788
O	1.60392404	6.03682137	-1.05404842
S	2.21663594	4.75254107	-0.59941560
O	2.37275290	-5.11320591	0.34656349
O	2.19029212	-4.27572393	-2.00018811
O	4.43752098	-4.49582100	-0.91748887
S	2.97035980	-4.27689648	-0.73474312

O	-4.81261873	0.48791733	-1.71997321
O	-6.03331995	-1.60178757	-1.06529689
O	-5.75713873	0.25334305	0.58143026
S	-5.21056700	-0.43507165	-0.62514889
H	-0.39634189	5.53768063	0.13901907
H	-2.08712506	1.86820602	1.73166990
H	-4.58687115	-3.10622811	0.05648198
H	-0.56678474	-2.77385306	1.66596365
H	4.98174095	-2.44646764	0.03427650
H	2.69690204	0.85760504	1.68878484

TPPTS•H₃

P	0.000000	0.000000	3.124061
C	-0.204529	1.573205	2.191949
C	0.440108	1.802566	0.975399
C	-1.207800	2.464224	2.599039
C	0.000000	2.831259	0.151840
H	1.251270	1.146479	0.627653
C	-1.601408	3.523399	1.779477
C	-1.020549	3.700145	0.521796
S	0.725395	2.931313	-1.464901
H	-2.398730	4.200861	2.110029
O	2.173910	2.787320	-1.363512
O	0.191613	1.507236	-2.123819
O	0.070980	3.999482	-2.199146
H	0.933476	0.815428	-2.131320
C	-1.260171	-0.963730	2.191949
C	-1.781122	-0.520138	0.975399
C	-1.530180	-2.278098	2.599039
C	-2.451942	-1.415629	0.151840
H	-1.618515	0.510392	0.627653
C	-2.250650	-3.148560	1.779477
C	-2.694145	-2.733894	0.521796
S	-2.901289	-0.837446	-1.464901
H	-2.438687	-4.177791	2.110029
O	-3.500845	0.489001	-1.363512
O	-1.401111	-0.587676	-2.123819
O	-3.499143	-1.938270	-2.199146
H	-1.172920	0.400700	-2.131320
C	1.464700	-0.609476	2.191949
C	1.341014	-1.282428	0.975399
C	2.737981	-0.186126	2.599039
C	2.451942	-1.415629	0.151840
H	0.367245	-1.656872	0.627653
C	3.852057	-0.374840	1.779477
C	3.714694	-0.966251	0.521796

S	2.175894	-2.093867	-1.464901
H	4.837417	-0.023070	2.110029
O	1.326935	-3.276321	-1.363512
O	1.209498	-0.919560	-2.123819
O	3.428163	-2.061212	-2.199146
H	0.239444	-1.216128	-2.131320
H	2.853450	0.335949	3.559927
H	4.558408	-1.073359	-0.173353
H	-1.717665	2.303186	3.559927
H	-1.349648	4.484377	-0.173353
H	-1.135785	-2.639135	3.559927
H	-3.208761	-3.411018	-0.173353

TPPTS•Na₃

P	0.72376	-2.01038	2.41733
C	-1.21808	2.17912	2.95844
C	0.11354	-0.29271	2.68188
C	-0.55568	1.84228	1.77852
C	0.13072	0.64409	1.64581
C	-0.54068	0.03744	3.87256
C	-1.18174	1.27279	4.01665
H	-1.69597	1.51364	4.95585
H	0.62379	0.4119	0.68946
C	-1.94384	-3.27359	-1.1908
C	-0.38163	-2.47214	1.02167
C	-2.2162	-2.09059	-0.50811
C	-1.47069	-1.6989	0.6029
C	-0.10556	-3.66625	0.338
C	-0.87991	-4.06403	-0.75148
H	-0.64799	-5.00399	-1.26894
H	-1.76831	-0.78176	1.13155
C	4.48921	-0.49525	0.19413
C	2.237	-1.61012	1.459
C	3.26969	-0.59366	-0.47439
C	2.16933	-1.18922	0.12771
C	3.46106	-1.52689	2.13144
C	4.58479	-0.99754	1.49126
H	5.54032	-0.93737	2.02822
H	1.23259	-1.28355	-0.43937
O	0.46631	3.75921	0.22336
O	-0.70403	1.8819	-0.8321
O	-2.04915	3.50671	0.43313
S	-0.71403	2.86327	0.32752
O	3.61124	-0.58022	-3.12428
O	1.5345	0.41939	-2.11703
O	3.64384	1.5868	-1.82853

S	3.04594	0.23036	-2.04667
O	-2.74044	-0.06874	-2.07066
O	-4.4961	-1.83662	-1.79218
O	-3.94595	-0.16868	0.03427
S	-3.49703	-1.00187	-1.12498
H	-1.77956	3.12095	3.02249
H	-0.5751	-0.6966	4.69024
H	-2.57776	-3.56592	-2.03955
H	0.74129	-4.29173	0.65708
H	5.3402	0.00203	-0.29053
H	3.52909	-1.85722	3.17799
NA	-0.57707	0.08758	-2.18867
NA	-3.16984	1.81507	-0.72608
NA	1.70083	2.64555	-1.34408

Pd(TPPTS³⁻)

P	0.00646	-0.01148	0.99354
C	-0.41568	4.41568	-0.2322
C	-0.13756	1.69388	0.36596
C	0.73981	3.73196	-0.60002
C	0.86823	2.36341	-0.34308
C	-1.28525	2.39651	0.77064
C	-1.43564	3.73898	0.43964
H	-2.35909	4.26391	0.72215
H	1.76717	1.83846	-0.70125
C	-3.64962	-2.55276	-0.2134
C	-1.41657	-0.96792	0.37457
C	-3.64825	-1.19803	-0.53321
C	-2.52067	-0.40971	-0.28242
C	-1.43668	-2.32733	0.73082
C	-2.53257	-3.1189	0.40438
H	-2.51521	-4.1905	0.64835
H	-2.52717	0.6434	-0.60239
C	3.99218	-1.8774	-0.38636
C	1.52542	-0.74443	0.30162
C	2.80714	-2.53178	-0.70866
C	1.57045	-1.95257	-0.40494
C	2.7252	-0.10293	0.65533
C	3.94676	-0.65083	0.28069
H	4.87568	-0.11777	0.52804
H	0.64899	-2.46736	-0.71631
O	3.01617	4.90992	-0.16872
O	2.66771	3.81456	-2.38765
O	1.44766	5.93078	-1.81878
S	2.09911	4.68155	-1.32365
O	2.45004	-5.08263	-0.33951

O	2.00902	-4.15793	-2.61811
O	4.3594	-4.34249	-1.76957
S	2.91121	-4.18502	-1.43775
O	-4.73967	0.45548	-2.26385
O	-5.96139	-1.64917	-1.65857
O	-5.77002	0.2068	-0.00117
S	-5.17134	-0.47265	-1.18704
H	-0.47937	5.48144	-0.4957
H	-2.0555	1.88136	1.3638
H	-4.54877	-3.13189	-0.46939
H	-0.58684	-2.75638	1.28237
H	4.93301	-2.36983	-0.67243
H	2.68986	0.82441	1.24639
Pd	0.0624	-0.02943	3.14217

[Pd(TPPTS)₂]⁶⁻

P	-0.03412	-2.27907	0.09553
C	4.18233	-2.84877	-1.73347
C	1.62042	-2.65414	-0.61307
C	3.75667	-3.78904	-0.79536
C	2.46945	-3.71299	-0.24928
C	2.06972	-1.69765	-1.53666
C	3.33441	-1.80689	-2.1094
H	3.66298	-1.04922	-2.83602
H	2.1459	-4.48178	0.46965
C	-3.40097	-4.26258	-2.38086
C	-1.27605	-3.14959	-0.9378
C	-2.08996	-4.6445	-2.66359
C	-1.0218	-4.10954	-1.9304
C	-2.59552	-2.74139	-0.69029
C	-3.6531	-3.31478	-1.39022
H	-4.68334	-3.00389	-1.16567
H	0.00458	-4.45045	-2.13869
C	-0.0012	-4.27338	4.28136
C	-0.05324	-3.19915	1.6894
C	-1.08413	-4.52702	3.44121
C	-1.11356	-4.00004	2.14428
C	1.03232	-2.95095	2.54275
C	1.06072	-3.49379	3.82386
H	1.92181	-3.28909	4.476
H	-1.98795	-4.20189	1.50527
O	5.60711	-4.443	0.94261
O	4.19559	-6.27506	-0.00409
O	5.91316	-5.13689	-1.42864
S	4.9683	-5.03354	-0.27113
O	-3.6626	-5.0851	3.45126

O	-2.04095	-6.96204	3.77679
O	-2.3712	-5.29028	5.58761
S	-2.41707	-5.55799	4.1139
O	-0.7599	-6.71426	-3.6385
O	-3.19767	-6.48794	-4.15966
O	-1.55529	-4.94654	-5.21823
S	-1.86708	-5.80804	-4.04018
H	5.19204	-2.97032	-2.15189
H	1.41086	-0.84179	-1.76829
H	-4.20268	-4.74414	-2.95925
H	-2.77567	-1.94669	0.05111
H	-0.03983	-4.6763	5.30351
H	1.85785	-2.31095	2.19773
Pd	-0.31861	-0.0101	0.18678
P	-0.25977	2.27291	0.06839
C	-3.97365	4.03886	-2.0747
C	-1.70417	3.10546	-0.71226
C	-3.82128	4.29428	-0.7131
C	-2.68769	3.83862	-0.02877
C	-1.86711	2.85472	-2.08312
C	-2.98757	3.32836	-2.75882
H	-3.09446	3.12301	-3.83354
H	-2.59852	4.04307	1.04991
C	3.41676	3.22527	-2.58095
C	1.16372	2.79326	-0.97139
C	2.32325	4.0871	-2.66423
C	1.20302	3.8914	-1.84711
C	2.25853	1.91702	-0.91558
C	3.38622	2.14376	-1.70057
H	4.23585	1.44824	-1.63528
H	0.36079	4.59776	-1.9119
C	0.02283	4.12377	4.29851
C	-0.07849	3.11511	1.68857
C	0.94969	4.55205	3.34922
C	0.89885	4.06053	2.03722
C	-0.99539	2.6778	2.65695
C	-0.95563	3.19402	3.94842
H	-1.68208	2.84205	4.69467
H	1.64872	4.39362	1.30261
O	-5.18431	4.73493	1.5017
O	-4.75845	6.66478	-0.03196
O	-6.36875	4.89139	-0.69969
S	-5.14683	5.23012	0.09884
O	3.46857	5.33612	3.26542
O	1.69079	7.08274	3.47959
O	2.19598	5.5884	5.40453

S	2.19508	5.74884	3.91366
O	1.70459	6.57027	-3.33327
O	3.86712	5.60147	-4.14409
O	1.71216	4.81234	-5.10963
S	2.40071	5.39479	-3.91965
H	-4.89768	4.38301	-2.56087
H	-1.10812	2.26617	-2.61964
H	4.28189	3.44017	-3.22496
H	2.18831	1.02983	-0.26167
H	0.12887	4.51699	5.31988
H	-1.71927	1.89175	2.39034

Pd(TPPTS•H₃)

P	-2.302698	0.000432	0.000701
C	-1.412603	1.596853	-0.148005
C	-0.193859	1.798144	0.500442
C	-1.822731	2.514268	-1.124346
C	0.631677	2.836811	0.086876
H	0.153188	1.116734	1.290813
C	-1.001139	3.581028	-1.488686
C	0.260058	3.735159	-0.907087
S	2.250238	2.912802	0.810137
H	-1.331627	4.283949	-2.263712
O	2.152118	2.728759	2.254329
O	2.903078	1.501375	0.235936
O	2.986036	3.996438	0.183602
H	2.914260	0.792102	0.960969
C	-1.411590	-0.924461	-1.307622
C	-0.190893	-0.464481	-1.801421
C	-1.823944	-2.226612	-1.619351
C	0.634349	-1.340844	-2.495758
H	0.157331	0.558872	-1.600498
C	-1.002115	-3.074834	-2.361696
C	0.260698	-2.649253	-2.781957
S	2.253187	-0.751574	-2.921173
H	-1.333964	-4.096161	-2.587009
O	2.154961	0.594398	-3.476132
O	2.908757	-0.550649	-1.411769
O	2.987627	-1.832763	-3.553364
H	2.914964	0.430707	-1.155569
C	-1.406362	-0.667380	1.454188
C	-0.186861	-1.327388	1.300985
C	-1.815949	-0.284877	2.738294
C	0.638997	-1.492257	2.406454
H	0.160154	-1.666272	0.314077
C	-0.992513	-0.503386	3.842794

C	0.268655	-1.083154	3.682692
S	2.255859	-2.160019	2.108518
H	-1.322275	-0.186618	4.840237
O	2.155168	-3.307523	1.212730
O	2.918662	-0.950483	1.189169
O	2.986806	-2.178251	3.362918
H	2.927947	-1.216541	0.210203
H	-2.787225	0.219052	2.856836
H	0.965788	-1.215459	4.521257
H	-2.792393	2.361016	-1.621918
H	0.956744	4.526661	-1.214954
H	-2.795282	-2.580001	-1.241311
H	0.957083	-3.310830	-3.314877
PD	-4.416994	-0.004206	0.004241

Pd(TPPTS•Na₃)

Pd	4.47416	-1.09669	0.40861
P	2.42565	-0.38561	0.14822
C	1.29934	-0.50422	1.59559
C	1.37906	-1.19126	-1.12509
C	2.16854	1.37119	-0.2952
C	0.01435	0.03768	1.52901
C	1.64779	-1.2827	2.70138
C	0.17609	-1.84276	-0.83165
C	1.79667	-1.11157	-2.46166
C	0.974	1.78243	-0.89202
C	3.06587	2.33776	0.16756
C	-0.91415	-0.25671	2.51692
H	-0.29503	0.6459	0.66597
C	0.71984	-1.52984	3.71767
H	2.65974	-1.71708	2.74009
C	-0.60907	-2.3461	-1.86736
H	-0.16938	-1.98358	0.2026
C	1.01626	-1.6466	-3.4851
H	2.7513	-0.61809	-2.69906
C	0.63655	3.12898	-0.91876
H	0.27367	1.04672	-1.31139
C	2.75242	3.69491	0.06397
H	4.00977	2.00781	0.62936
C	-0.58167	-1.03901	3.62228
S	-2.59631	0.2626	2.24532
H	1.00497	-2.14808	4.5785
C	-0.20241	-2.26621	-3.19701
S	-2.21591	-3.03504	-1.48074
H	1.36129	-1.57827	-4.525

C	1.51974	4.09967	-0.44804
S	-1.02788	3.58467	-1.39066
H	3.46356	4.44854	0.42635
H	-1.34664	-1.28178	4.3722
O	-2.77891	1.63397	2.78627
O	-2.74957	0.29268	0.7339
O	-3.44747	-0.81227	2.81718
H	-0.83361	-2.70673	-3.9814
O	-3.13622	-1.81414	-1.48844
O	-2.53088	-4.01912	-2.51618
O	-2.14359	-3.51108	-0.06373
H	1.22485	5.15768	-0.45746
O	-1.02691	4.16279	-2.73359
O	-1.78915	2.26899	-1.26405
O	-1.49269	4.46498	-0.27104
Na	-2.45399	0.24898	-1.50342
Na	-3.59091	-2.0175	0.8182
Na	-2.61427	2.86076	0.86701

TXPTS³⁻

P	0.01711	0.01387	1.29621
C	-0.25935	4.48853	0.09864
C	-0.23586	1.69429	0.62562
C	0.82411	3.68969	-0.29883
C	0.80133	2.31488	-0.09115
C	-1.31239	2.49123	1.07814
C	-1.31069	3.85426	0.75932
H	-2.17588	4.46009	1.0769
H	1.64669	1.72772	-0.48064
C	-3.76787	-2.45569	0.24397
C	-1.339	-1.04179	0.67639
C	-3.63544	-1.11467	-0.14847
C	-2.42533	-0.44855	0.01125
C	-1.4725	-2.37483	1.12827
C	-2.66615	-3.05314	0.85497
H	-2.74486	-4.10725	1.16981
H	-2.35662	0.58025	-0.3732
C	4.00059	-2.02692	0.07493
C	1.58201	-0.62967	0.60773
C	2.75802	-2.57968	-0.27214
C	1.58411	-1.86398	-0.06394
C	2.82069	-0.08104	1.01215
C	3.99252	-0.77582	0.69045
H	4.95704	-0.31891	0.96867
H	0.64411	-2.31554	-0.41533

O	3.2948	3.33793	-1.07384
O	1.92436	5.07861	-2.2581
O	2.68991	5.46866	0.07895
S	2.31761	4.45618	-0.95979
O	1.19985	-4.57249	-0.92802
O	3.36111	-4.30445	-2.18037
O	3.37705	-5.06807	0.18952
S	2.65926	-4.28138	-0.86335
O	-4.60313	1.20948	-0.84879
O	-5.47142	-0.83225	-2.02714
O	-6.0921	-0.40037	0.3452
S	-5.07489	-0.19886	-0.73514
C	-5.04605	-3.19895	0.0423
C	-0.26966	5.95977	-0.15095
C	5.27359	-2.76332	-0.17783
H	-0.0986	6.16331	-1.22635
H	0.58928	6.43094	0.36746
H	-1.22394	6.41258	0.17716
H	-5.36092	-3.13112	-1.01763
H	-5.85796	-2.70407	0.61168
H	-4.94259	-4.258	0.34393
H	5.33712	-3.05634	-1.24423
H	5.26589	-3.72105	0.37995
H	6.15048	-2.15086	0.10367
C	-2.45204	1.94521	1.87613
C	2.93504	1.20519	1.76444
C	-0.39752	-3.09366	1.87738
H	-2.15821	1.04003	2.44332
H	-3.30343	1.65768	1.22018
H	-2.8248	2.70399	2.59036
H	0.26435	-2.39029	2.42004
H	0.24719	-3.6854	1.19038
H	-0.83834	-3.79826	2.60818
H	2.0223	1.41505	2.35644
H	3.08278	2.06544	1.07497
H	3.80291	1.17768	2.45058

TXPTS•H₃

P	-0.09450400	0.00918600	2.85332500
C	0.30584700	1.56385400	1.94617600
C	0.94028100	1.52043300	0.70545000
C	-0.22342700	2.79199200	2.38820200
C	0.98041500	2.63562900	-0.11760100
H	1.35261800	0.58002700	0.31635800
C	-0.09090700	3.91899000	1.56535700
C	-0.98083800	2.88896700	3.66991600

C	0.48062300	3.88216900	0.28968000
S	1.56986600	2.36625100	-1.76814900
H	-0.49983600	4.87758100	1.91941100
H	-2.00145200	2.47367400	3.55294200
H	-0.49691900	2.30531400	4.47449200
H	-1.08717100	3.93584100	4.00249100
C	0.52354100	5.08435700	-0.58715900
O	2.56440800	3.35049200	-2.15854800
O	1.90386300	0.92426900	-1.83388100
O	0.28981400	2.64158100	-2.67264100
H	1.56057500	5.31578900	-0.89382800
H	-0.03431100	4.90503100	-1.52683300
H	0.08994200	5.96312100	-0.08193500
C	-1.60236200	-0.44681000	1.89508100
C	-1.80126800	0.05779300	0.61080900
C	-2.45537700	-1.46896100	2.35419200
C	-2.76108100	-0.47999800	-0.23238000
H	-1.14967100	0.84412700	0.20803300
C	-3.46817800	-1.93388500	1.50330800
C	-2.25251900	-2.10422800	3.68886800
C	-3.64248800	-1.48726900	0.18967100
S	-2.72361600	0.08376200	-1.91314700
H	-4.13786900	-2.72630800	1.87089000
H	-1.40325000	-2.81500800	3.65872600
H	-2.00473800	-1.35580700	4.46375300
H	-3.14410000	-2.66957500	4.01024400
C	-4.67668700	-2.07040500	-0.70816100
O	-4.04118600	0.47309100	-2.38494100
O	-1.60654200	1.05519100	-1.97275200
O	-2.31797800	-1.21543300	-2.73728800
H	-5.35581700	-1.28784900	-1.09479500
H	-4.20707900	-2.52805700	-1.60063900
H	-5.26939300	-2.84089700	-0.18799700
C	1.09927200	-1.09478600	1.98507000
C	0.81692600	-1.58506500	0.71072700
C	2.39756800	-1.27372900	2.50135400
C	1.80601900	-2.15983100	-0.07255300
H	-0.17888300	-1.45630900	0.26627700
C	3.35096000	-1.93392300	1.71346800
C	2.78607200	-0.70962500	3.82659600
C	3.10797000	-2.37031500	0.40734100
S	1.37012500	-2.48891200	-1.75973400
H	4.36172600	-2.07779700	2.12483900
H	2.95387700	0.38297700	3.75227000
H	1.98907400	-0.85187800	4.57930700
H	3.71947600	-1.16135200	4.20415300

C	4.17622300	-2.98840400	-0.42500500
O	1.73972300	-3.83385900	-2.16568900
O	-0.03769300	-2.04682100	-1.89341400
O	2.30283000	-1.50058200	-2.58714000
H	3.87801600	-3.99475900	-0.77334800
H	4.35321200	-2.39375700	-1.34226300
H	5.12358100	-3.06457400	0.13367200
H	-1.36849700	-1.53720600	-2.50496500
H	-0.46685900	1.96891400	-2.49006900
H	2.10187300	-0.51179200	-2.38466100

TXPTS•H₃ no H-bond

P	-0.01045100	-0.00877200	2.09588800
C	-1.29518500	-1.02453000	1.29773400
C	-2.15723800	-0.49186500	0.33643400
C	-1.48985300	-2.34878600	1.74282500
C	-3.20304300	-1.25966900	-0.16268300
H	-2.00657400	0.52875100	-0.04529700
C	-2.54745500	-3.08971800	1.20737300
C	-0.57189500	-2.96186700	2.74419300
C	-3.43289400	-2.58049900	0.25568100
S	-4.31920400	-0.58044900	-1.35939500
H	-2.70019100	-4.12144400	1.55972400
H	0.41181800	-3.19750200	2.29034700
H	-0.36311900	-2.26202400	3.57765400
H	-0.98392600	-3.89622200	3.16176000
C	-4.55889200	-3.40211300	-0.27265900
O	-5.61422900	-0.28756900	-0.73474000
O	-3.61110900	0.86702800	-1.64534300
O	-4.24661400	-1.37146600	-2.57947900
H	-5.53064400	-2.89395200	-0.12220700
H	-4.45690200	-3.55857300	-1.36299500
H	-4.59928500	-4.38509000	0.22535600
H	-4.28205200	1.55893100	-1.42680800
C	1.52031900	-0.61235300	1.31267100
C	1.50110800	-1.60801800	0.33312000
C	2.75876800	-0.12791200	1.78307300
C	2.69513700	-2.12237800	-0.15931000
H	0.54633300	-1.97768800	-0.06968300
C	3.93558800	-0.66658900	1.25499300
C	2.81851700	0.95812600	2.80217900
C	3.94851300	-1.67091700	0.28529600
S	2.68248100	-3.40390500	-1.38263700
H	4.90134500	-0.29041600	1.62599300
H	2.52695200	1.93337500	2.36279100
H	2.10499100	0.77064700	3.62891900

H	3.83087400	1.06827000	3.22662300
C	5.22992500	-2.22721100	-0.23523200
O	3.07597700	-4.68192900	-0.77860200
O	1.07892000	-3.51585200	-1.68900100
O	3.34111700	-2.91800800	-2.58658700
H	5.27494300	-3.32463700	-0.09788200
H	5.32781700	-2.04701500	-1.32232800
H	6.09471600	-1.77602900	0.27894300
H	0.81438700	-4.44519100	-1.48167700
C	-0.24051600	1.61611500	1.30333900
C	0.64812500	2.09171600	0.33629100
C	-1.28464400	2.45076600	1.75354000
C	0.50824800	3.38153000	-0.16295800
H	1.45145800	1.44696000	-0.04999600
C	-1.39512900	3.73740100	1.21817700
C	-2.27448900	1.96549700	2.75673800
C	-0.51460700	4.24540000	0.26133000
S	1.65032400	4.00567200	-1.36519400
H	-2.20859600	4.38853300	1.57327800
H	-2.97420900	1.23426000	2.30383500
H	-1.77344400	1.43238500	3.58903300
H	-2.87405300	2.79168400	3.17515200
C	-0.66130200	5.63146900	-0.26737900
O	2.56083300	4.97337300	-0.74269200
O	2.53944900	2.66412300	-1.66123000
O	0.92319100	4.34764200	-2.57930700
H	0.26582400	6.21759500	-0.11844900
H	-0.84914400	5.62141100	-1.35744500
H	-1.49069100	6.15972000	0.23163200
H	3.47761700	2.89345500	-1.45171900

TXPTS•Na₃

P	0.00511	-0.0548	2.94277
C	-0.27214	1.52878	2.05517
C	0.50507	1.89808	0.95921
C	-1.3948	2.31274	2.38747
C	0.15426	2.98264	0.16274
H	1.3977	1.3179	0.68277
C	-1.69438	3.42582	1.59623
C	-2.29313	1.92369	3.5113
C	-0.96084	3.78509	0.45932
S	1.10918	3.18094	-1.33418
H	-2.57371	4.0317	1.85719
H	-2.9684	1.10246	3.1999
H	-1.71348	1.54533	4.37369
H	-2.921	2.76849	3.83835

C	-1.36983	4.96759	-0.35412
O	1.1163	4.59476	-1.72475
O	2.43683	2.5364	-1.0758
O	0.37083	2.27262	-2.33421
H	-0.57591	5.73502	-0.35755
H	-1.51349	4.71691	-1.42122
H	-2.30447	5.39988	0.03831
NA	2.14181	0.74788	-2.36754
C	-1.21537	-1.06546	2.01607
C	-1.91107	-0.55074	0.92495
C	-1.34562	-2.43597	2.31771
C	-2.67692	-1.37147	0.1043
H	-1.84598	0.51758	0.67459
C	-2.16332	-3.22666	1.50488
C	-0.57217	-3.04921	3.43435
C	-2.83212	-2.74188	0.3737
S	-3.29383	-0.59567	-1.38309
H	-2.26138	-4.29506	1.74456
H	0.48606	-3.19112	3.1389
H	-0.56572	-2.39275	4.32437
H	-0.97831	-4.03483	3.71419
C	-3.65929	-3.66472	-0.45779
O	-4.48477	-1.31309	-1.85074
O	-3.44927	0.86066	-1.06664
O	-2.09496	-0.70563	-2.34169
H	-4.71114	-3.33092	-0.48804
H	-3.34355	-3.67717	-1.51704
H	-3.60513	-4.69097	-0.06004
NA	-1.69024	1.59324	-2.2285
C	1.50447	-0.58444	2.02811
C	1.42113	-1.39672	0.90003
C	2.75384	-0.0342	2.37687
C	2.52863	-1.62627	0.09135
H	0.46327	-1.85269	0.61294
C	3.8609	-0.3248	1.5742
C	2.88189	0.89934	3.53164
C	3.79162	-1.0985	0.40869
S	2.18784	-2.48902	-1.43612
H	4.83387	0.1057	1.8509
H	2.51451	1.90714	3.25491
H	2.26731	0.56405	4.38764
H	3.93042	1.00148	3.85557
C	5.01889	-1.3252	-0.40918
O	3.41462	-3.1343	-1.91597
O	1.00676	-3.37125	-1.1678
O	1.68509	-1.36615	-2.36104

H	5.24645	-2.40226	-0.49105
H	4.89485	-0.98789	-1.45433
H	5.87694	-0.79491	0.03448
NA	-0.49949	-2.17189	-2.29082

Pd(TXPTS³⁻)

P	0.00969	0.00927	0.89123
C	-0.24112	4.46165	-0.36554
C	-0.20212	1.70142	0.26317
C	0.801	3.63761	-0.82203
C	0.79601	2.27541	-0.54191
C	-1.24192	2.51905	0.76449
C	-1.24224	3.86998	0.40403
H	-2.06827	4.50254	0.76894
H	1.61608	1.66729	-0.9582
C	-3.78789	-2.41933	-0.18248
C	-1.38575	-1.01137	0.33094
C	-3.62194	-1.09823	-0.6304
C	-2.42596	-0.42407	-0.40858
C	-1.54613	-2.32666	0.82635
C	-2.73375	-2.99916	0.52253
H	-2.84744	-4.03565	0.88063
H	-2.33403	0.59593	-0.81696
C	3.94001	-2.05946	-0.42797
C	1.5555	-0.68281	0.23192
C	2.68845	-2.56985	-0.81113
C	1.52258	-1.87131	-0.51669
C	2.80204	-0.1693	0.66041
C	3.95758	-0.86167	0.28582
H	4.9316	-0.44673	0.59339
H	0.57057	-2.29742	-0.87402
O	3.13503	3.23992	-1.9381
O	1.6412	5.00887	-2.90638
O	2.73242	5.37573	-0.70001
S	2.20921	4.37263	-1.68096
O	1.13672	-4.44331	-1.77832
O	3.37382	-4.07949	-2.85593
O	3.23744	-5.10305	-0.59164
S	2.58922	-4.19566	-1.59099
O	-4.50893	1.13799	-1.66161
O	-5.34439	-1.02571	-2.62023
O	-6.08312	-0.30244	-0.35648
S	-5.00986	-0.23541	-1.39856
C	-5.05666	-3.16276	-0.42862
C	-0.25954	5.92096	-0.67028
C	5.20026	-2.78829	-0.7495

H	-0.18711	6.07728	-1.76472
H	0.65365	6.39535	-0.2579
H	-1.16988	6.40177	-0.26679
H	-5.28672	-3.16466	-1.51239
H	-5.90119	-2.61559	0.0367
H	-4.99552	-4.19667	-0.0413
H	5.25661	-2.97857	-1.83947
H	5.17038	-3.79681	-0.28994
H	6.08707	-2.22431	-0.40567
C	-2.29053	2.00831	1.68933
C	2.91966	1.03536	1.52716
C	-0.53129	-2.98854	1.69104
H	-1.8128	1.38226	2.49307
H	-3.02213	1.35226	1.17675
H	-2.84672	2.8431	2.15369
H	-0.19227	-2.27235	2.49047
H	0.37823	-3.27942	1.12845
H	-0.94754	-3.898	2.16164
H	2.17181	0.97185	2.36537
H	2.69595	1.9729	0.97998
H	3.93855	1.12009	1.9474
Pd	0.0806	0.03118	3.07252

[Pd(TXPTS)₂]⁶⁻

P	-0.00961	-2.32029	-0.07692
C	-4.21965	-3.83291	-1.3752
C	-1.63386	-3.02183	-0.54817
C	-3.07752	-4.28275	-2.0594
C	-1.80586	-3.88753	-1.64245
C	-2.77268	-2.54737	0.1412
C	-4.03045	-2.97902	-0.28948
H	-4.91691	-2.61477	0.25577
H	-0.93738	-4.27182	-2.20319
C	1.02124	-3.96955	4.15522
C	0.42179	-3.07486	1.53461
C	-0.11556	-4.4467	3.48059
C	-0.40162	-4.00931	2.18684
C	1.5625	-2.57558	2.20304
C	1.83058	-3.04905	3.49073
H	2.72517	-2.66353	4.00742
H	-1.30033	-4.41542	1.6928
C	3.19352	-3.71563	-3.15665
C	1.19796	-2.97527	-1.28718
C	3.1995	-4.25057	-1.85708
C	2.20941	-3.88906	-0.94279
C	1.18526	-2.41658	-2.5852

C	2.18022	-2.8151	-3.48261
H	2.16365	-2.38476	-4.49764
H	2.24833	-4.33886	0.06347
O	-1.92589	-5.62983	-4.01035
O	-4.01428	-6.56348	-2.98977
O	-4.14382	-4.55469	-4.44334
S	-3.29381	-5.3544	-3.50273
O	4.27204	-5.75081	0.02608
O	4.42083	-6.53313	-2.34882
O	5.78888	-4.60149	-1.59912
S	4.52956	-5.38705	-1.39023
O	-2.31103	-5.90171	3.38163
O	-0.35334	-6.7875	4.66868
O	-1.65329	-4.87144	5.56552
S	-1.21233	-5.60616	4.33571
C	1.35172	-4.41843	5.54033
C	-5.59257	-4.24287	-1.79542
C	4.23823	-4.08616	-4.15704
H	-5.66995	-5.3484	-1.7918
H	-5.76372	-3.94788	-2.85007
H	-6.35648	-3.7943	-1.13267
H	1.4423	-5.52265	5.56381
H	0.50645	-4.18641	6.21882
H	2.28376	-3.94031	5.89619
H	4.24941	-5.18562	-4.29594
H	5.24186	-3.83858	-3.75707
H	4.06053	-3.57089	-5.1198
C	-2.6679	-1.59853	1.2836
C	0.16568	-1.41671	-3.00738
C	2.4604	-1.55998	1.58694
H	-2.01781	-0.72291	1.00667
H	-2.1808	-2.06454	2.16359
H	-3.66057	-1.22333	1.59095
H	1.86121	-0.6893	1.19972
H	2.99789	-1.96455	0.70607
H	3.20643	-1.18595	2.31086
H	0.09918	-0.58066	-2.25637
H	-0.85048	-1.85778	-3.05086
H	0.40422	-0.98796	-3.99726
Pd	-0.02171	-0.00366	0.00262
P	-0.01842	2.31225	0.08143
C	-4.30537	3.82187	1.10327
C	-1.67084	3.01233	0.44538
C	-3.21009	4.2731	1.85943
C	-1.91395	3.87882	1.52558
C	-2.76214	2.53762	-0.31659

C	-4.0455	2.96834	0.03192
H	-4.89441	2.60374	-0.56998
H	-1.08387	4.26461	2.14093
C	1.2812	3.966	-4.07462
C	0.51482	3.06745	-1.4992
C	0.10166	4.43945	-3.47521
C	-0.26649	4.00076	-2.20283
C	1.69748	2.57113	-2.09279
C	2.04785	3.04681	-3.35971
H	2.97512	2.66421	-3.81741
H	-1.19592	4.40478	-1.76769
C	2.97438	3.72503	3.35902
C	1.10756	2.97186	1.36572
C	3.06561	4.25308	2.05981
C	2.13834	3.88546	1.08404
C	1.01085	2.41891	2.66275
C	1.94352	2.82392	3.6219
H	1.86062	2.39855	4.63581
H	2.24246	4.33096	0.08049
O	-2.18699	5.62339	3.87858
O	-4.20818	6.55271	2.72718
O	-4.42599	4.54431	4.17072
S	-3.51946	5.34513	3.28548
O	4.25824	5.7448	0.24336
O	4.24998	6.54016	2.61849
O	5.66593	4.60607	1.97093
S	4.42233	5.38894	1.67551
O	-2.10086	5.88572	-3.52161
O	-0.06396	6.78036	-4.67359
O	-1.29394	4.86067	-5.6577
S	-0.93968	5.59597	-4.40049
C	1.70013	4.41885	-5.43436
C	-5.70289	4.23011	1.43416
C	3.9495	4.10296	4.4247
H	-5.77975	5.33565	1.42964
H	-5.9427	3.9313	2.47424
H	-6.42173	3.78388	0.72133
H	1.787	5.52357	-5.45021
H	0.90243	4.18464	-6.16748
H	2.65578	3.9458	-5.72921
H	3.95095	5.20336	4.5563
H	4.97781	3.85311	4.09502
H	3.70747	3.59413	5.3768
C	-2.583	1.59057	-1.45138
C	-0.0316	1.4179	3.02174
C	2.55634	1.55705	-1.42099

H	-1.9486	0.71654	-1.13662
H	-2.04346	2.05997	-2.29839
H	-3.55326	1.21255	-1.82042
H	1.93724	0.68262	-1.07632
H	3.03258	1.96181	-0.50548
H	3.35043	1.18786	-2.09463
H	-0.04497	0.57851	2.27235
H	-1.0498	1.85533	2.99657
H	0.14254	0.99498	4.02742

Pd(TXPTS•Na₃)

PD	4.4689	-0.00888	0.12153
P	2.26174	-0.00227	0.06012
C	1.36379	-0.3512	1.61308
C	1.44087	-1.19251	-1.05748
C	1.43529	1.54402	-0.44954
C	0.24893	0.41253	1.95757
C	1.68077	-1.48589	2.39057
C	0.31858	-1.8938	-0.61923
C	1.83106	-1.30814	-2.40936
C	0.33814	1.49272	-1.30765
C	1.78897	2.78113	0.13093
C	-0.58722	0.03947	3.00363
H	-0.01058	1.31535	1.38429
C	0.85093	-1.79956	3.47179
C	2.82275	-2.3754	2.0442
C	-0.45481	-2.64714	-1.49498
H	0.0061	-1.84257	0.4342
C	1.06671	-2.12364	-3.24986
C	2.98512	-0.54475	-2.95699
C	-0.44424	2.6149	-1.55442
H	0.05355	0.54566	-1.78905
C	1.01652	3.90307	-0.18511
C	2.91146	2.89619	1.10156
C	-0.3047	-1.08172	3.80261
S	-2.09675	0.98386	3.15532
H	1.09902	-2.68463	4.07724
H	2.58359	-2.99898	1.15977
H	3.72012	-1.77763	1.7551
H	3.08317	-3.05241	2.87591
C	-0.09423	-2.79467	-2.84541
S	-1.98841	-3.2651	-0.81454
H	1.37531	-2.21744	-4.30226
H	2.72989	0.52719	-3.07395
H	3.85094	-0.57095	-2.25229
H	3.30045	-0.92786	-3.94265

C	-0.11947	3.86619	-1.0035
S	-1.9416	2.30687	-2.48046
H	1.29604	4.86822	0.26424
H	2.63686	2.45222	2.07901
H	3.8013	2.31898	0.75241
H	3.19889	3.94747	1.27438
C	-1.15401	-1.51676	4.95046
O	-2.56463	0.92918	4.54153
O	-1.80778	2.33561	2.58483
O	-3.04236	0.28697	2.16343
C	-0.86405	-3.61278	-3.8284
O	-2.43618	-4.41744	-1.59888
O	-1.74668	-3.48162	0.64532
O	-2.92423	-2.05048	-0.92162
C	-0.90229	5.11334	-1.24697
O	-2.39807	3.55688	-3.09101
O	-1.64375	1.16417	-3.39805
O	-2.90366	1.76106	-1.4131
H	-1.18376	-0.74067	5.73653
H	-2.21326	-1.65938	4.66572
H	-0.77326	-2.45893	5.37965
Na	-2.93025	-1.74348	1.3976
H	-0.91077	-4.6705	-3.51305
H	-1.92228	-3.30075	-3.90463
H	-0.40499	-3.54787	-4.82936
Na	-2.81997	-0.39089	-2.31186
H	-0.9191	5.36928	-2.3215
H	-1.96767	5.0044	-0.97172
H	-0.47503	5.95508	-0.67617
Na	-3.00725	2.12447	0.71756

Pd(TXPTS•H₃ no H-bond)

P	0.007907	-0.012022	1.609797
C	-0.495424	-1.614618	0.818994
C	-1.458058	-1.618081	-0.201831
C	0.022364	-2.856245	1.267675
C	-1.923753	-2.812872	-0.751188
H	-1.844511	-0.682101	-0.585349
C	-0.474083	-4.034347	0.690873
C	1.095280	-2.965558	2.323469
C	-1.450983	-4.064198	-0.311905
S	-3.182262	-2.780784	-2.041255
H	-0.082021	-4.985059	1.046425
H	2.046702	-2.550229	1.972723
H	0.820192	-2.396598	3.223366
H	1.265877	-4.008675	2.602379

C	-1.940781	-5.386078	-0.857419
O	-4.489891	-3.136756	-1.482504
O	-3.248631	-1.169977	-2.378714
O	-2.672769	-3.461185	-3.221844
H	-3.026921	-5.480323	-0.754883
H	-1.708504	-5.485233	-1.921745
H	-1.475115	-6.215231	-0.319669
H	-4.168097	-0.878206	-2.221463
C	1.649086	0.372122	0.829620
C	2.137615	-0.437672	-0.207356
C	2.462222	1.433105	1.302158
C	3.406359	-0.229892	-0.748737
H	1.523652	-1.233659	-0.609784
C	3.731261	1.607713	0.731008
C	2.016790	2.393195	2.377851
C	4.249709	0.798742	-0.287457
S	4.014445	-1.306928	-2.060169
H	4.355536	2.416722	1.105072
H	1.187520	3.022153	2.034623
H	1.651603	1.851105	3.262059
H	2.835884	3.051370	2.679205
C	5.639122	1.049434	-0.827164
O	4.993460	-2.256203	-1.522482
O	2.663273	-2.184186	-2.403564
O	4.330149	-0.502007	-3.230253
H	6.266253	0.156125	-0.740288
H	5.608450	1.319279	-1.886857
H	6.121615	1.859136	-0.274894
H	2.884090	-3.125151	-2.258376
C	-1.141680	1.234268	0.850289
C	-0.687103	2.059539	-0.189877
C	-2.460628	1.420516	1.336975
C	-1.496708	3.063317	-0.721825
H	0.302823	1.913759	-0.604040
C	-3.240526	2.443178	0.777119
C	-3.069551	0.557491	2.415182
C	-2.801237	3.293279	-0.244873
S	-0.868950	4.124690	-2.036540
H	-4.247582	2.590011	1.162089
H	-3.212467	-0.472719	2.069907
H	-2.411553	0.502844	3.294504
H	-4.042977	0.946604	2.725135
C	-3.708497	4.381385	-0.771881
O	-0.498126	5.435561	-1.495360
O	0.543341	3.363885	-2.409615
O	-1.747268	4.023647	-3.191964

H	-3.234409	5.365561	-0.697490
H	-3.947848	4.219025	-1.826920
H	-4.640348	4.408517	-0.202331
H	1.264301	4.011623	-2.283371
Pd	0.022270	-0.042621	3.851362

Pd(TXPTS•H₃)

P	-2.152613	0.000000	0.000000
C	-1.300976	1.623003	-0.014611
C	-0.035781	1.707714	0.566886
C	-1.772408	2.714813	-0.773841
C	0.785014	2.800797	0.343475
H	0.372271	0.874856	1.154401
C	-0.947578	3.843192	-0.896797
C	-3.081769	2.682494	-1.480867
C	0.350249	3.919886	-0.384419
S	2.456992	2.647467	0.912666
H	-1.322723	4.700621	-1.476050
H	-3.003902	2.117208	-2.429964
H	-3.848579	2.133848	-0.875151
H	-3.442621	3.698111	-1.719985
C	1.223012	5.101028	-0.625757
O	2.885026	3.816297	1.661325
O	2.532585	1.306823	1.539411
O	3.312888	2.638088	-0.428840
H	1.568663	5.541337	0.328019
H	2.140997	4.805056	-1.169974
H	0.698360	5.872489	-1.213188
C	-1.300976	-0.824155	-1.398257
C	-0.035781	-0.362920	-1.762366
C	-1.772408	-2.027573	-1.964176
C	0.785014	-1.102941	-2.597299
H	0.372271	0.562312	-1.334848
C	-0.947578	-2.698244	-2.879903
C	-3.081769	-2.623715	-1.582674
C	0.350249	-2.292859	-3.202511
S	2.456992	-0.533342	-2.749106
H	-1.322723	-3.628607	-3.332833
H	-3.003902	-3.163014	-0.618574
H	-3.848579	-1.824828	-1.410391
H	-3.442621	-3.338606	-2.342666
C	1.223012	-3.092435	-4.104741
O	2.885026	-0.469399	-4.135673
O	2.532585	0.679758	-1.901448
O	3.312888	-1.690430	-2.070231
H	1.568663	-2.486595	-4.962949

H	2.140997	-3.415756	-3.576314
H	0.698360	-3.986896	-4.479131
C	-1.300976	-0.798848	1.412868
C	-0.035781	-1.344794	1.195480
C	-1.772408	-0.687239	2.738018
C	0.785014	-1.697856	2.253824
H	0.372271	-1.437169	0.180448
C	-0.947578	-1.144947	3.776700
C	-3.081769	-0.058779	3.063541
C	0.350249	-1.627027	3.586930
S	2.456992	-2.114125	1.836441
H	-1.322723	-1.072014	4.808883
H	-3.003902	1.045806	3.048538
H	-3.848579	-0.309021	2.285543
H	-3.442621	-0.359505	4.062651
C	1.223012	-2.008592	4.730498
O	2.885026	-3.346898	2.474348
O	2.532585	-1.986581	0.362036
O	3.312888	-0.947657	2.499070
H	1.568663	-3.054742	4.634928
H	2.140997	-1.389301	4.746288
H	0.698360	-1.885593	5.692319
H	3.107207	-1.786154	-1.066733
H	3.107207	1.816895	-1.013488
H	3.107207	-0.030741	2.080221
PD	-4.303112	0.000000	0.000000

TMAPTS³⁻

P	0.00580994	0.00823697	1.16092241
C	-0.59547991	4.43206120	0.00555089
C	-0.37678027	1.66704822	0.49558866
C	0.56355387	3.75348139	-0.38503575
C	0.62244409	2.37407470	-0.19189097
C	-1.52100086	2.37040234	0.94424099
C	-1.61618102	3.73186159	0.64494735
H	-2.52188396	4.28766727	0.93422723
H	1.52254093	1.85789967	-0.55830157
C	-3.53958106	-2.73125935	0.06958768
C	-1.24897611	-1.15519381	0.51939350
C	-3.53839350	-1.39001298	-0.32702833
C	-2.37139010	-0.64741707	-0.15389363
C	-1.27764165	-2.49606729	0.97353822
C	-2.41271114	-3.26147008	0.69424903
H	-2.43579936	-4.32264566	0.98792863
H	-2.38100457	0.38865736	-0.52414858
C	4.13246918	-1.69525349	0.00358639

C	1.63001072	-0.49927559	0.49447444
C	2.96392918	-2.36557722	-0.37243196
C	1.74026239	-1.72595668	-0.17958212
C	2.81293774	0.14594910	0.92952538
C	4.03857040	-0.45439267	0.63001460
H	4.97385406	0.05643754	0.90781808
H	0.84173024	-2.25275540	-0.53468388
O	3.10013032	3.55760598	-0.89335626
O	1.77593398	5.13601685	-2.31772447
O	2.25229788	5.68810225	0.07172950
S	2.05027843	4.61622047	-0.95549196
O	1.52537835	-4.47204590	-0.84555244
O	3.54063082	-4.12576199	-2.29211521
O	3.80369306	-4.78973770	0.10186567
S	2.96583223	-4.09054565	-0.92481339
O	-4.64457893	0.90144980	-0.83268178
O	-5.36822891	-1.04237068	-2.23672104
O	-6.05225563	-0.89291871	0.16137847
S	-5.03699064	-0.53739893	-0.88158107
C	-2.63062692	1.72748566	1.71006501
C	2.81434822	1.43716717	1.68057072
C	-0.15366161	-3.13070679	1.72515380
H	-2.28241014	0.83199519	2.26117849
H	-3.45071983	1.40122700	1.02907395
H	-3.06536031	2.44116068	2.43562007
H	0.45349091	-2.37782669	2.26508331
H	0.53003949	-3.67846179	1.03573883
H	-0.54222620	-3.86233735	2.45895910
H	1.86652517	1.59119892	2.23260355
H	2.94138408	2.30198455	0.98870695
H	3.65186214	1.46407115	2.40352225
O	5.38020515	-2.22129488	-0.22898091
O	-4.62168169	-3.55163670	-0.13959765
O	-0.76461542	5.77613020	-0.22385959
C	-0.42482015	6.57909632	0.88886112
C	-5.47189522	-3.65092754	0.98543870
C	5.91431141	-2.90563679	0.88670373
H	0.66636217	6.49472046	1.08278251
H	-1.01433837	6.28566122	1.78764176
H	-0.67797220	7.62096167	0.61622345
H	-5.94120502	-2.66220140	1.17952669
H	-4.91115475	-4.00959969	1.87895250
H	-6.25173426	-4.39219761	0.72796828
H	5.29909229	-3.80823874	1.09226489
H	5.95853186	-2.24045134	1.77943194
H	6.94239664	-3.20684052	0.61061275

TMAPTS•H₃

P	-0.002613	0.008733	2.955862
C	-3.748841	-0.409492	0.265670
C	-1.591724	0.061641	2.023358
C	-2.711663	0.466810	-0.089792
C	-1.675645	0.723869	0.797886
C	-2.633213	-0.807909	2.406962
C	-3.708450	-0.996292	1.532190
H	-4.519816	-1.691605	1.791750
H	-0.878290	1.401896	0.467162
C	2.234240	-3.023637	0.267784
C	0.745080	-1.397960	2.028193
C	0.952191	-2.573021	-0.083335
C	0.210047	-1.808316	0.806446
C	2.022469	-1.857916	2.408404
C	2.724928	-2.692082	1.532308
H	3.735977	-3.040674	1.787876
H	-0.779944	-1.463796	0.481351
C	1.520595	3.445394	0.250915
C	0.842449	1.352273	2.018299
C	1.754311	2.106459	-0.099422
C	1.453916	1.086190	0.792419
C	0.620934	2.691750	2.398301
C	0.998254	3.711663	1.517983
H	0.810247	4.764182	1.775104
H	1.637336	0.054663	0.465950
O	-1.443220	2.139304	-1.642257
O	-1.925332	-0.118627	-2.526618
O	-3.775406	1.576096	-2.270523
S	-2.533527	1.013981	-1.769023
O	2.569112	0.160004	-1.634074
O	0.858350	1.696451	-2.535502
O	3.249738	2.457565	-2.280523
S	2.141522	1.666245	-1.774836
O	-1.138187	-2.319836	-1.623610
O	1.051616	-1.621520	-2.531192
O	0.507635	-4.068117	-2.247250
S	0.379394	-2.706316	-1.758122
C	-2.547127	-1.599214	3.668810
C	-0.096282	3.024884	3.663375
C	2.665723	-1.382858	3.667787
H	-2.169650	-0.988034	4.508916
H	-1.837871	-2.442254	3.549236
H	-3.524496	-2.026773	3.949296
H	1.951388	-1.371771	4.511153

H	3.029404	-0.342671	3.549591
H	3.533286	-2.006276	3.942758
H	0.201692	2.353836	4.489527
H	-1.189699	2.899851	3.534079
H	0.081836	4.069755	3.969204
O	1.703572	4.452329	-0.633788
O	3.021543	-3.678666	-0.616204
O	-4.716041	-0.758725	-0.613400
C	-5.850019	0.105532	-0.634071
C	2.857840	-5.095149	-0.635300
C	3.020523	4.998541	-0.658803
H	-5.561673	1.116724	-0.979907
H	-6.318993	0.153991	0.369109
H	-6.559348	-0.335264	-1.351886
H	1.840930	-5.363726	-0.980431
H	3.056047	-5.522267	0.368132
H	3.598984	-5.480280	-1.353024
H	3.750834	4.236817	-0.992967
H	3.296169	5.392754	0.339851
H	2.997284	5.823612	-1.387760
H	1.895676	-0.546615	-2.050244
H	-0.494808	1.906546	-2.057270
H	-1.411770	-1.383196	-2.041442

TMAPTS•H₃ no H-bond

P	0.01297400	-0.04639700	2.04683200
C	-1.89640800	3.74857600	0.20550500
C	-0.74309800	1.42075700	1.26929100
C	-0.63768100	3.31337500	-0.22134900
C	-0.06649600	2.15449200	0.29087200
C	-2.00709100	1.85864400	1.72930500
C	-2.56324200	3.01956000	1.18784000
H	-3.56072400	3.35394600	1.50847900
H	0.91488500	1.82728000	-0.08407200
C	-2.35263800	-3.53110700	0.12819900
C	-0.86151600	-1.41190100	1.21376400
C	-2.60681000	-2.20920300	-0.25010300
C	-1.86535400	-1.15889600	0.27593700
C	-0.60297500	-2.74118700	1.62154600
C	-1.35070200	-3.78102200	1.06508300
H	-1.14338500	-4.82309200	1.34992100
H	-2.08809100	-0.13128400	-0.04670300
C	4.26218900	-0.23997900	0.22261200
C	1.65777900	-0.09265800	1.26023900
C	3.25443900	-1.08677100	-0.24914600
C	1.95900800	-1.00858900	0.24885700

C	2.66960100	0.75760000	1.76388300
C	3.95843700	0.66964300	1.23435000
H	4.75207000	1.34026400	1.59538400
H	1.18276400	-1.67238300	-0.16103500
O	1.63467300	3.60864900	-1.46016000
O	-0.44239300	4.15284700	-2.72890400
O	0.38864600	5.66794800	-0.84863800
S	0.16457400	4.33632100	-1.42318100
O	2.37374300	-3.15954100	-1.56024700
O	3.92472200	-1.61965300	-2.76339800
O	4.76727500	-3.14992400	-0.90060700
S	3.74750100	-2.26463600	-1.47607600
O	-4.04952700	-0.31977700	-1.31248800
O	-3.66220000	-2.33036900	-2.71902000
O	-5.17380100	-2.45170100	-0.66744800
S	-3.97915300	-1.95957200	-1.34237300
C	-2.77189700	1.06310700	2.73102700
C	2.35562600	1.76993600	2.81232500
C	0.48127800	-3.03611600	2.60084900
H	-2.10873300	0.67593500	3.52973100
H	-3.23625300	0.17582900	2.25481600
H	-3.58044900	1.65351600	3.19422900
H	0.44132100	-2.33868300	3.46138000
H	1.48091800	-2.89622500	2.14192700
H	0.42308600	-4.06992600	2.98162300
H	1.75248500	1.32495400	3.62853300
H	1.74278700	2.59472300	2.39581000
H	3.26885800	2.21128800	3.24629400
O	5.48662700	-0.30776100	-0.35235500
O	-3.05963600	-4.52069200	-0.46690800
O	-2.43736400	4.83816200	-0.38984300
C	-2.54138200	5.99268800	0.43379300
C	-3.97662900	-5.20724200	0.37646700
C	6.51411000	-0.85246400	0.46648700
H	-1.53091500	6.40840400	0.61912800
H	-3.04376000	5.76109500	1.39408600
H	-3.14363700	6.72490100	-0.12677000
H	-4.82920700	-4.54101600	0.61529300
H	-3.48758200	-5.55455800	1.30835700
H	-4.33601900	-6.07781600	-0.19456900
H	6.35203100	-1.94190900	0.58938600
H	6.54917400	-0.35479000	1.45622900
H	7.46343600	-0.67891000	-0.06443000
H	2.60552000	-4.06031300	-1.22804700
H	2.28399500	4.26768100	-1.11444600
H	-3.86335300	-0.00970400	-2.23261700

TMAPTS•Na₃

P	-0.32558	-0.99138	2.91646
C	3.49737	-1.46722	0.42708
C	1.1958	-1.4775	2.00975
C	2.2651	-1.79571	-0.14486
C	1.13305	-1.82723	0.66028
C	2.44448	-1.21181	2.60599
C	3.58601	-1.23074	1.79625
H	4.56848	-0.96709	2.21504
H	0.17173	-2.04129	0.16845
C	-0.72595	3.21301	1.10609
C	-0.2792	0.78927	2.4312
C	0.42061	2.46718	0.81807
C	0.64111	1.2751	1.49906
C	-1.38114	1.59095	2.79697
C	-1.57496	2.80403	2.13021
H	-2.46952	3.41058	2.33475
H	1.52367	0.68856	1.20484
C	-3.39219	-2.32109	-0.33476
C	-1.59714	-1.49317	1.68329
C	-2.78352	-1.05614	-0.40892
C	-1.91688	-0.66485	0.60334
C	-2.18509	-2.77037	1.75675
C	-3.08434	-3.14395	0.75289
H	-3.55754	-4.13641	0.77448
H	-1.45209	0.32293	0.48726
O	0.57846	-2.22074	-2.07969
O	2.2884	-0.52503	-2.41385
O	2.98732	-2.93126	-2.42674
S	2.02559	-1.94174	-1.92078
O	-1.96279	1.17059	-1.44153
O	-2.1922	-0.72166	-2.94755
O	-4.26352	0.4305	-2.07309
S	-2.86922	0.01645	-1.85025
O	2.716	2.06406	-0.35464
O	0.68495	2.32492	-1.76286
O	1.656	4.31301	-0.62977
S	1.47103	2.85318	-0.58264
C	2.54544	-0.77745	4.03039
C	-1.81932	-3.73274	2.83767
C	-2.41112	1.09708	3.75597
H	1.86272	-1.35398	4.68132
H	2.25483	0.2874	4.13515
H	3.57487	-0.87867	4.41506
H	-1.95167	0.57305	4.61452

H	-3.078	0.36348	3.25922
H	-3.04226	1.91865	4.13617
H	-1.717	-3.22604	3.8158
H	-0.84133	-4.20831	2.62586
H	-2.56428	-4.54142	2.9328
O	-4.20735	-2.81094	-1.2976
O	-1.10207	4.27461	0.30766
O	4.60573	-1.23871	-0.36415
C	5.37749	-2.41631	-0.64148
C	-0.63877	5.54834	0.7699
C	-5.52488	-2.26808	-1.32623
H	4.77553	-3.12167	-1.24638
H	5.70488	-2.8781	0.30978
H	6.26055	-2.08772	-1.21328
H	0.46355	5.59165	0.68748
H	-0.97243	5.71137	1.81259
H	-1.09439	6.30977	0.11611
H	-5.50607	-1.17382	-1.49872
H	-6.05661	-2.505	-0.3816
H	-6.03889	-2.76155	-2.1669
NA	-1.39125	3.19735	-1.70369
NA	3.85834	0.64142	-1.50422
NA	-0.01586	0.0621	-2.44

Pd(TMAPTS³⁻)

P	0.00286	0.00291	0.79176
C	-0.65322	4.39739	-0.4244
C	-0.40424	1.66308	0.15783
C	0.50763	3.71871	-0.80834
C	0.58437	2.34956	-0.56235
C	-1.5554	2.36273	0.59657
C	-1.65971	3.71191	0.25372
H	-2.56474	4.2717	0.53623
H	1.48814	1.83083	-0.91653
C	-3.50697	-2.7662	-0.31926
C	-1.24795	-1.18194	0.19558
C	-3.51059	-1.42247	-0.70656
C	-2.3565	-0.6711	-0.49513
C	-1.26576	-2.52757	0.63806
C	-2.39116	-3.29332	0.32879
H	-2.41522	-4.35628	0.61479
H	-2.36906	0.36993	-0.85191
C	4.125	-1.65813	-0.419
C	1.63808	-0.49065	0.15462
C	2.95333	-2.33254	-0.77696
C	1.73162	-1.70744	-0.5363

C	2.82332	0.16709	0.56575
C	4.04085	-0.42646	0.22798
H	4.98075	0.08365	0.4901
H	0.82712	-2.23781	-0.87046
O	3.03835	3.5293	-1.32353
O	1.68384	5.0166	-2.81693
O	2.17059	5.69804	-0.46356
S	1.97805	4.57266	-1.43253
O	1.51865	-4.43965	-1.2384
O	3.47829	-4.04734	-2.74863
O	3.83304	-4.75656	-0.38035
S	2.95212	-4.04706	-1.36181
O	-4.6268	0.86319	-1.19594
O	-5.27268	-1.05492	-2.67207
O	-6.04812	-0.97242	-0.2993
S	-5.00116	-0.57729	-1.29429
C	-2.64304	1.73948	1.40383
C	2.83369	1.44119	1.34007
C	-0.1602	-3.15577	1.41673
H	-2.23547	0.93627	2.06325
H	-3.42992	1.29902	0.75033
H	-3.13022	2.50103	2.04178
H	0.35035	-2.40009	2.06001
H	0.59595	-3.61893	0.74301
H	-0.55847	-3.95665	2.06809
H	1.93962	1.50681	2.00475
H	2.84021	2.32567	0.66323
H	3.74179	1.49889	1.96953
O	5.3681	-2.17139	-0.69066
O	-4.57381	-3.59356	-0.56366
O	-0.83882	5.72833	-0.70102
C	-0.50127	6.57627	0.37924
C	-5.44748	-3.71982	0.54108
C	5.93688	-2.86487	0.40281
H	0.59297	6.51584	0.56375
H	-1.07647	6.30486	1.29374
H	-0.77414	7.60321	0.07221
H	-5.93626	-2.74086	0.73482
H	-4.90058	-4.07899	1.44257
H	-6.20905	-4.47012	0.25755
H	5.33479	-3.77516	0.612
H	5.99719	-2.2101	1.30197
H	6.95976	-3.15333	0.09651
Pd	0.02702	0.0236	2.95613

[Pd(TMAPTS)₂]⁶⁻

P	0.03712	-2.30908	0.14203
C	4.03963	-3.55343	2.09753
C	1.60601	-2.93544	0.84426
C	2.84861	-4.06253	2.63178
C	1.64739	-3.75111	1.98725
C	2.81251	-2.42642	0.30853
C	4.00421	-2.76055	0.95308
H	4.96146	-2.38793	0.55743
H	0.72232	-4.16484	2.42345
C	-0.30967	-3.97072	-4.15981
C	-0.16022	-3.09491	-1.49791
C	0.727	-4.44239	-3.34356
C	0.7787	-4.00149	-2.01764
C	-1.20608	-2.62422	-2.32671
C	-1.25382	-3.08726	-3.6422
H	-2.05898	-2.74712	-4.31132
H	1.60168	-4.3879	-1.39259
C	-3.56223	-3.61301	2.73763
C	-1.30972	-2.949	1.20142
C	-3.39016	-4.21462	1.48377
C	-2.25637	-3.87769	0.73799
C	-1.489	-2.34527	2.46854
C	-2.61594	-2.70594	3.20834
H	-2.78126	-2.26198	4.20194
H	-2.13907	-4.36625	-0.24426
O	1.40403	-5.3553	4.38552
O	3.65957	-6.28425	3.83245
O	3.4655	-4.20159	5.18402
S	2.84227	-5.07816	4.13773
O	-4.08104	-5.73482	-0.52778
O	-4.66978	-6.52008	1.77273
O	-5.88911	-4.59938	0.76028
S	-4.61021	-5.38233	0.81475
O	2.91685	-5.77481	-2.83226
O	1.27985	-6.80274	-4.41972
O	2.62596	-4.82823	-5.12088
S	1.99668	-5.57407	-3.98108
C	2.84059	-1.54373	-0.88945
C	-0.53685	-1.33872	3.01261
C	-2.22336	-1.64917	-1.8468
H	2.09498	-0.70858	-0.77819
H	2.54381	-2.08967	-1.80735
H	3.8424	-1.10633	-1.04873
H	-1.72154	-0.77222	-1.34984
H	-2.88383	-2.09218	-1.07476

H	-2.85137	-1.27569	-2.67537
H	-0.32347	-0.54479	2.24299
H	0.44494	-1.79264	3.25534
H	-0.93418	-0.85334	3.92201
O	-4.64075	-3.88707	3.54667
O	-0.44638	-4.35287	-5.47433
O	5.26949	-3.81144	2.65758
C	5.61919	-2.87039	3.65591
C	0.27991	-3.51992	-6.35946
C	-5.74876	-3.04775	3.27727
H	4.91125	-2.94933	4.50999
H	5.62717	-1.83711	3.2407
H	6.64092	-3.13308	3.99231
H	1.36938	-3.6205	-6.15966
H	-0.04564	-2.45939	-6.26227
H	0.05382	-3.87546	-7.38346
H	-6.12363	-3.23996	2.24797
H	-5.47436	-1.97625	3.40659
H	-6.531	-3.31258	4.01486
Pd	0.00678	-0.00114	0.00516
P	-0.02707	2.30632	-0.13966
C	4.23098	3.70052	-1.28705
C	1.62412	2.99093	-0.52823
C	3.14877	4.16826	-2.04445
C	1.85731	3.81145	-1.64445
C	2.72132	2.52285	0.23318
C	4.00257	2.90253	-0.16864
H	4.87767	2.56318	0.40646
H	1.02055	4.19377	-2.25352
C	-1.26508	3.95601	4.00045
C	-0.56774	3.0849	1.42546
C	-0.10719	4.46572	3.39797
C	0.21821	4.02616	2.111
C	-1.73727	2.57626	2.03858
C	-2.05721	3.03741	3.3161
H	-2.96452	2.66804	3.81819
H	1.13275	4.44194	1.65503
C	-3.10075	3.46505	-3.39525
C	-1.16468	2.89468	-1.44557
C	-3.19924	4.07448	-2.13714
C	-2.21949	3.78456	-1.18255
C	-1.06962	2.28444	-2.71879
C	-2.04514	2.59792	-3.6661
H	-1.99654	2.14694	-4.66908
H	-2.31447	4.27876	-0.20065
O	2.02452	5.4155	-4.04794

O	4.09625	6.4222	-3.07314
O	4.2411	4.33955	-4.43066
S	3.3969	5.18884	-3.52648
O	-4.32239	5.57398	-0.31351
O	-4.49074	6.32371	-2.69358
O	-5.80383	4.35883	-1.90913
S	-4.5702	5.19369	-1.72794
O	2.09024	5.8786	3.31287
O	0.1384	6.84573	4.54248
O	1.39311	4.92336	5.50833
S	0.97157	5.64451	4.26182
C	2.54891	1.6345	1.41502
C	0.01079	1.31898	-3.05991
C	-2.60616	1.56532	1.37662
H	1.88024	0.76549	1.15833
H	2.04769	2.15966	2.25265
H	3.51754	1.24336	1.77442
H	-1.98586	0.70726	0.99503
H	-3.11737	1.98377	0.48662
H	-3.37154	1.17093	2.06875
H	0.1039	0.53486	-2.25734
H	1.001	1.8143	-3.11203
H	-0.18266	0.8168	-4.02477
O	-4.01226	3.693	-4.40012
O	-1.66942	4.3338	5.26004
O	5.53618	4.00495	-1.59765
C	6.10698	3.0823	-2.50741
C	-1.10081	3.52881	6.27651
C	-5.11884	2.81168	-4.33945
H	5.57535	3.13953	-3.48263
H	6.07251	2.04795	-2.09623
H	7.16412	3.38386	-2.64014
H	0.00237	3.6687	6.29225
H	-1.3634	2.45707	6.12623
H	-1.53485	3.87693	7.23386
H	-5.69154	2.99185	-3.40319
H	-4.78433	1.75136	-4.4027
H	-5.7544	3.04352	-5.21604

Pd(TMAPTS•Na₃)

Pd	-3.96154	-2.23634	1.02018
P	-2.0919	-1.20993	0.44532
C	-0.76085	-2.17937	-0.34478
C	-1.08671	-0.4305	1.76952
C	-2.21647	0.24479	-0.66082
C	0.01397	-1.57225	-1.33559

C	-0.32777	-3.38812	0.24212
C	0.30452	-0.5633	1.76585
C	-1.68924	0.54609	2.59509
C	-1.30583	1.29498	-0.50001
C	-3.12968	0.29071	-1.73474
C	1.27077	-2.06021	-1.66808
H	-0.30034	-0.63232	-1.8149
C	0.9152	-3.90121	-0.14733
C	-1.08973	-4.05619	1.33518
C	1.11988	0.33393	2.44467
H	0.80773	-1.32106	1.1488
C	-0.85655	1.41457	3.30742
C	-3.16339	0.75462	2.61596
C	-1.25765	2.38012	-1.36348
H	-0.55535	1.28302	0.30182
C	-3.09581	1.40799	-2.57581
C	-4.09142	-0.81481	-2.01066
C	1.73405	-3.22352	-1.0459
S	2.31724	-1.02523	-2.70121
H	1.31107	-4.80947	0.33046
H	-2.18507	-4.04154	1.12885
H	-0.96415	-3.5171	2.29511
H	-0.75661	-5.09771	1.48605
C	0.52893	1.3616	3.18593
S	2.87904	0.30252	2.10211
H	-1.29245	2.23359	3.89838
H	-3.70592	-0.21875	2.61996
H	-3.49674	1.27685	1.69683
H	-3.47931	1.35793	3.48442
C	-2.17694	2.44981	-2.42347
S	0.12606	3.5106	-1.16857
H	-3.78876	1.47821	-3.42668
H	-4.59074	-1.15467	-1.07037
H	-3.57423	-1.70891	-2.40933
H	-4.86036	-0.51199	-2.74199
O	3.04199	-3.63691	-1.20046
O	1.45445	0.12327	-3.06869
O	3.37328	-0.52615	-1.72401
O	2.86012	-1.8641	-3.77871
O	1.28478	2.4039	3.68413
O	3.14201	-1.07256	1.58694
O	3.03879	1.34318	1.01531
O	3.5966	0.65389	3.33865
O	-2.16983	3.44386	-3.34174
O	0.83087	2.94216	0.05736
O	1.00951	3.28356	-2.34071

O	-0.38651	4.87378	-0.95884
C	3.25601	-4.49286	-2.33265
Na	4.10883	-1.84475	-0.18093
C	1.7362	2.21232	5.02979
C	-2.74382	4.67604	-2.91316
Na	2.10644	3.27282	1.72008
H	3.05426	-3.93291	-3.26638
H	2.60851	-5.38672	-2.24954
H	4.31361	-4.80123	-2.2989
H	2.467	1.38246	5.05856
H	0.87009	2.0113	5.68885
H	2.22234	3.15188	5.33911
H	-2.19354	5.09274	-2.04651
H	-3.81574	4.53373	-2.66423
H	-2.65661	5.36629	-3.76774
Na	2.24643	1.52888	-1.32191

Pd(TMAPTS•H₃)

P	2.277693	0.003408	0.008549
C	-0.365676	-0.749945	3.716370
C	1.398363	-0.109979	1.611145
C	-0.718144	0.208910	2.753252
C	0.174920	0.548764	1.747420
C	1.778676	-1.070402	2.574373
C	0.900034	-1.332416	3.631521
H	1.155416	-2.090401	4.386025
H	-0.149039	1.294212	1.009962
C	-0.333880	-2.850642	-2.509383
C	1.412446	-1.334856	-0.894476
C	-0.698026	-2.492697	-1.201584
C	0.186772	-1.786151	-0.400251
C	1.805334	-1.694409	-2.202546
C	0.934938	-2.484586	-2.962020
H	1.199896	-2.763162	-3.992196
H	-0.146044	-1.520995	0.611256
C	-0.346564	3.598055	-1.215678
C	1.408323	1.450344	-0.703408
C	-0.704084	2.284295	-1.557994
C	0.184087	1.241133	-1.341290
C	1.796411	2.765659	-0.365509
C	0.921059	3.813780	-0.672722
H	1.181933	4.846991	-0.401522
H	-0.143997	0.229811	-1.612887
O	-2.253261	2.001098	1.638349
O	-3.143483	-0.291093	1.878727
O	-2.912642	1.207128	3.895123

S	-2.394840	0.772741	2.609673
O	-2.234539	0.421188	-2.549704
O	-3.137231	1.787114	-0.699385
O	-2.888728	2.771049	-3.008531
S	-2.379340	1.879688	-1.981149
O	-2.245756	-2.416830	0.897348
O	-3.133457	-1.505090	-1.221857
O	-2.882370	-3.994736	-0.908697
S	-2.377334	-2.657627	-0.650745
C	3.037190	-1.855231	2.447867
C	3.059483	3.052019	0.368413
C	3.069980	-1.195337	-2.808481
H	3.871401	-1.213163	2.074115
H	2.925940	-2.656007	1.690679
H	3.320792	-2.329077	3.403249
H	3.896096	-1.189200	-2.056674
H	2.962423	-0.141016	-3.130483
H	3.362675	-1.790606	-3.690385
H	3.880226	2.374190	0.028322
H	2.940660	2.847246	1.450425
H	3.366021	4.106228	0.256005
O	-1.225807	4.621127	-1.312987
O	-1.208266	-3.448105	-3.350608
O	-1.247990	-1.178467	4.647565
C	-1.274232	-0.412219	5.849923
C	-1.226914	-4.872625	-3.288147
C	-1.250007	5.277801	-2.578589
H	-1.619712	0.619322	5.645553
H	-0.273046	-0.402619	6.325424
H	-1.994633	-0.911317	6.516690
H	-1.579214	-5.213053	-2.295494
H	-0.221416	-5.283589	-3.508667
H	-1.938585	-5.204624	-4.060140
H	-1.594550	4.584868	-3.370050
H	-0.248464	5.684602	-2.823506
H	-1.970584	6.104858	-2.481600
H	-2.652519	-0.348753	-1.950630
H	-2.664507	1.866175	0.669720
H	-2.663639	-1.510830	1.259310
Pd	4.418709	0.005463	0.022670

Pd(TMAPTS•H3 no H-bond)

P	-0.001909	-0.006187	1.429248
C	-3.046447	-3.002606	-0.324119
C	-1.141929	-1.210605	0.687543
C	-3.013080	-1.674121	-0.760282

C	-2.063885	-0.785170	-0.273133
C	-1.168858	-2.547953	1.155862
C	-2.127234	-3.420365	0.636646
H	-2.152942	-4.468467	0.969124
H	-2.053198	0.249216	-0.648563
C	4.129185	-1.132051	-0.298688
C	1.617731	-0.387440	0.701481
C	2.964893	-1.760786	-0.751649
C	1.716997	-1.387034	-0.270506
C	2.786377	0.251408	1.186752
C	4.024874	-0.138482	0.673243
H	4.943451	0.358156	1.018786
H	0.818012	-1.887617	-0.660464
C	-1.071859	4.138481	-0.302168
C	-0.472717	1.589169	0.698532
C	0.054546	3.441673	-0.751512
C	0.350666	2.173951	-0.268035
C	-1.612081	2.282919	1.176862
C	-1.887101	3.552234	0.664306
H	-2.776349	4.102041	1.006028
H	1.235531	1.644741	-0.652330
O	-4.015209	0.415644	-1.946136
O	-3.996888	-1.724791	-3.228538
O	-5.586121	-1.380920	-1.259501
S	-4.279700	-1.203323	-1.904818
O	2.338956	3.248022	-1.981269
O	0.459654	4.322832	-3.224412
O	1.602885	5.513175	-1.276895
S	1.080018	4.298090	-1.913245
O	1.663344	-3.655289	-1.972716
O	3.513722	-2.548193	-3.229426
O	4.002286	-4.127283	-1.283273
S	3.197390	-3.075045	-1.915351
C	-0.200355	-3.026614	2.176431
C	-2.507034	1.681615	2.199491
C	2.709976	1.319383	2.217202
H	-0.173233	-2.306971	3.040189
H	0.835915	-3.038424	1.783784
H	-0.448450	-4.037680	2.541762
H	2.064590	0.975187	3.072310
H	2.207413	2.228001	1.830031
H	3.707006	1.603803	2.594476
H	-1.892913	1.288629	3.056233
H	-3.042151	0.795186	1.804355
H	-3.252357	2.403235	2.575032
O	-1.347714	5.342160	-0.856630

O	5.309892	-1.486742	-0.857253
O	-3.947055	-3.842229	-0.886073
C	-4.991088	-4.281214	-0.025998
C	6.207024	-2.182167	-0.000622
C	-1.182903	6.462038	0.004403
H	-5.679652	-3.437633	0.179723
H	-4.589984	-4.690149	0.922767
H	-5.530640	-5.074334	-0.567204
H	5.819511	-3.202651	0.190547
H	6.355981	-1.642201	0.955660
H	7.166521	-2.246790	-0.537489
H	-0.103661	6.626964	0.195002
H	-1.724693	6.321389	0.960979
H	-1.600190	7.331100	-0.528202
PD	-0.011099	-0.010103	3.588800
H	3.126485	3.728786	-1.628737
H	-4.815547	0.840992	-1.553673
H	1.695220	-4.571158	-1.604288

P(Mes)₃

P	0.000141	-0.002660	0.814637
C	3.990493	-2.103111	-0.281415
C	1.517637	-0.809502	0.221839
C	2.832759	-2.451683	-0.977101
C	1.601317	-1.825211	-0.757528
C	2.688410	-0.430386	0.925926
C	3.896888	-1.072741	0.656392
H	4.798976	-0.754324	1.201910
C	-0.168618	4.502254	-0.284588
C	-0.056444	1.714840	0.222562
C	0.703521	3.670461	-0.986923
C	0.774484	2.290938	-0.765892
C	-0.960519	2.542830	0.933609
C	-1.007234	3.910203	0.661754
H	-1.727569	4.534562	1.213180
C	-3.823654	-2.393458	-0.281782
C	-1.459905	-0.909259	0.220347
C	-3.540683	-1.218774	-0.979169
C	-2.378891	-0.471020	-0.760162
C	-1.722741	-2.110339	0.925380
C	-2.886823	-2.830560	0.656785
H	-3.065027	-3.770159	1.202841
H	2.890674	-3.236263	-1.747747
H	1.348335	4.110064	-1.763966
H	-4.246419	-0.873653	-1.751037
C	5.283125	-2.812197	-0.522754

H	6.142422	-2.118363	-0.490110
H	5.463906	-3.584839	0.249299
H	5.291778	-3.321561	-1.502546
C	2.664992	0.682359	1.922274
H	2.460561	1.661068	1.442388
H	1.853546	0.539006	2.663944
H	3.627875	0.762518	2.456542
C	0.456074	-2.224792	-1.631478
H	-0.307105	-2.825841	-1.099296
H	-0.085405	-1.344754	-2.028937
H	0.817531	-2.820986	-2.487942
C	-0.748213	-2.649939	1.920493
H	0.203144	-2.957191	1.440327
H	-0.469549	-1.878626	2.666422
H	-1.159057	-3.527668	2.449463
C	-2.144323	0.717133	-1.636466
H	-2.269341	1.680862	-1.105371
H	-1.113467	0.732876	-2.040252
H	-2.845754	0.708872	-2.489464
C	-5.087119	-3.152966	-0.523920
H	-4.928568	-4.243646	-0.447608
H	-5.861477	-2.886710	0.221261
H	-5.507478	-2.936677	-1.521983
C	-1.905969	1.970421	1.938644
H	-2.660642	1.311301	1.463316
H	-1.372384	1.332062	2.671415
H	-2.444682	2.766928	2.480998
C	-0.199812	5.976119	-0.527005
H	-1.229994	6.374053	-0.491367
H	0.381166	6.518774	0.243510
H	0.234525	6.237432	-1.508026
C	1.681145	1.493776	-1.646927
H	2.584532	1.127231	-1.121722
H	1.179305	0.588681	-2.040253
H	2.014132	2.102514	-2.506106

Pd(P(Mes)₃)

P	0.00636	0.00055	0.268
C	-2.36121	-3.83726	-0.87467
C	-0.8976	-1.47213	-0.3082
C	-2.62313	-2.6419	-1.54333
C	-1.9132	-1.46297	-1.29412
C	-0.5921	-2.6899	0.35859
C	-1.3261	-3.83856	0.06087
H	-1.06982	-4.77513	0.58007

C	4.51085	-0.08772	-0.8925
C	1.73195	-0.03153	-0.3131
C	3.61317	-0.92676	-1.55166
C	2.23809	-0.91525	-1.29655
C	2.62695	0.85491	0.34581
C	3.9877	0.80824	0.04069
H	4.66449	1.50845	0.55474
C	-2.20016	3.93996	-0.85293
C	-0.83499	1.51649	-0.28843
C	-1.03319	3.5879	-1.53053
C	-0.34385	2.39714	-1.28146
C	-2.03926	1.84348	0.39261
C	-2.69168	3.04047	0.09387
H	-3.62993	3.27274	0.62137
H	-3.40581	-2.62584	-2.31763
H	3.9939	-1.61287	-2.3242
H	-0.64762	4.25971	-2.31319
Pd	0.03384	-0.01936	2.56224
C	-3.1518	-5.07393	-1.15201
H	-2.49859	-5.95862	-1.2632
H	-3.852	-5.29484	-0.32362
H	-3.75213	-4.97527	-2.07339
C	0.50381	-2.79617	1.36104
H	1.48821	-2.48386	0.9606
H	0.31062	-2.08708	2.22351
H	0.59217	-3.82302	1.75681
C	-2.23747	-0.28162	-2.15218
H	-2.79505	0.50839	-1.61232
H	-1.32734	0.21104	-2.54448
H	-2.85125	-0.59754	-3.01423
C	-2.65338	0.94302	1.40745
H	-2.87666	-0.06629	1.00972
H	-1.92813	0.76113	2.25763
H	-3.58327	1.3733	1.81887
C	0.83855	2.10299	-2.14841
H	1.80387	2.20818	-1.61566
H	0.82525	1.06674	-2.53765
H	0.85568	2.79084	-3.01225
C	-2.90154	5.22917	-1.13113
H	-3.99775	5.09609	-1.17517
H	-2.70012	5.97275	-0.33616
H	-2.57252	5.67354	-2.08703
C	2.16603	1.85408	1.34906
H	1.4062	2.55192	0.94541
H	1.64407	1.33256	2.20837
H	3.00958	2.44385	1.74823

C	5.97678	-0.13861	-1.17463
H	6.40522	0.87397	-1.28812
H	6.52594	-0.62797	-0.34743
H	6.19482	-0.70666	-2.09595
C	1.3839	-1.8009	-2.14714
H	0.9813	-2.67316	-1.59644
H	0.50143	-1.26804	-2.55084
H	1.97031	-2.18269	-3.00136

P(2,4-*t*-Bu₂C₆H₃)₃

P	0.000000	0.000000	0.992400
C	0.755683	4.104433	-1.138480
C	0.211323	1.644767	0.179105
C	1.246609	2.905442	-1.648208
C	0.972646	1.706881	-0.993427
C	-0.286284	2.859087	0.730814
C	0.000000	4.039445	0.038893
H	-0.382117	4.983635	0.448275
H	1.376119	0.771891	-1.408906
C	-3.932384	-1.397776	-1.138480
C	-1.530071	-0.639373	0.179105
C	-3.139491	-0.373126	-1.648208
C	-1.964525	-0.011104	-0.993427
C	-2.332900	-1.677473	0.730814
C	-3.498262	-2.019723	0.038893
H	-4.124896	-2.822740	0.448275
H	-1.356536	0.805809	-1.408906
C	3.176702	-2.706657	-1.138480
C	1.318749	-1.005394	0.179105
C	1.892882	-2.532316	-1.648208
C	0.991879	-1.695776	-0.993427
C	2.619184	-1.181614	0.730814
C	3.498262	-2.019723	0.038893
H	4.507013	-2.160895	0.448275
H	-0.019583	-1.577699	-1.408906
C	-1.083248	2.950290	2.034062
C	3.096651	-0.537024	2.034062
C	-2.013402	-2.413266	2.034062
H	1.851279	2.889295	-2.564965
H	-3.427843	0.158607	-2.564965
H	1.576563	-3.047903	-2.564965
C	-3.028038	-3.508068	2.344771
H	-4.049588	-3.109746	2.495113
H	-3.063862	-4.285526	1.557623
H	-2.733945	-4.007840	3.286448
C	-0.645736	-3.088186	1.954803

H	-0.584349	-3.773554	1.088244
H	0.182214	-2.364163	1.860329
H	-0.462348	-3.674368	2.876592
C	-2.040516	-1.435834	3.212163
H	-3.027107	-0.941340	3.295012
H	-1.849760	-1.983055	4.155955
H	-1.266801	-0.650413	3.112796
C	-1.524057	4.376392	2.344771
H	-2.103919	4.371586	3.286448
H	-0.668325	5.061919	2.495113
H	-2.179443	4.796145	1.557623
C	-0.223211	2.485055	3.212163
H	-0.792496	2.593467	4.155955
H	0.070126	1.422289	3.112796
H	0.698329	3.092221	3.295012
C	-2.351580	2.103316	1.954803
H	-2.975819	2.392838	1.088244
H	-2.138532	1.024279	1.860329
H	-2.950922	2.237589	2.876592
C	4.552095	-0.868324	2.344771
H	4.717913	-1.952173	2.495113
H	5.243305	-0.510619	1.557623
H	4.837864	-0.363746	3.286448
C	2.997315	0.984870	1.954803
H	1.956318	1.339883	1.860329
H	3.413270	1.436779	2.876592
H	3.560168	1.380716	1.088244
C	2.263726	-1.049222	3.212163
H	2.328777	-2.150882	3.295012
H	2.642256	-0.610411	4.155955
H	1.196675	-0.771875	3.112796
C	4.211523	-3.604576	-1.790501
C	5.444869	-2.778596	-2.152668
H	5.896456	-2.302225	-1.262860
H	6.215653	-3.422927	-2.618012
H	5.188619	-1.975754	-2.868932
C	4.613498	-4.705198	-0.809518
H	3.740782	-5.323605	-0.528371
H	5.374271	-5.367855	-1.265407
H	5.042391	-4.288612	0.120644
C	3.680977	-4.257998	-3.056732
H	2.801628	-4.897918	-2.853172
H	3.393948	-3.508447	-3.818276
H	4.463966	-4.900795	-3.500579
C	1.015893	5.449574	-1.790501
C	-0.316100	6.104693	-2.152668

H	-0.954442	6.257594	-1.262860
H	-0.143484	7.094377	-2.618012
H	-0.883256	5.481353	-2.868932
C	1.768072	6.348005	-0.809518
H	2.739986	5.901415	-0.528371
H	1.961563	7.338183	-1.265407
H	1.192851	6.511145	0.120644
C	1.847046	5.316819	-3.056732
H	2.840908	4.875240	-2.853172
H	1.341430	4.693469	-3.818276
H	2.012230	6.316306	-3.500579
C	-5.227416	-1.844998	-1.790501
C	-5.128769	-3.326097	-2.152668
H	-4.942014	-3.955368	-1.262860
H	-6.072168	-3.671450	-2.618012
H	-4.305363	-3.505599	-2.868932
C	-6.381570	-1.642807	-0.809518
H	-6.480769	-0.577810	-0.528371
H	-7.335835	-1.970328	-1.265407
H	-6.235242	-2.222533	0.120644
C	-5.528023	-1.058821	-3.056732
H	-5.642536	0.022678	-2.853172
H	-4.735379	-1.185022	-3.818276
H	-6.476196	-1.415510	-3.500579

Pd(P(2,4-*t*-Bu₂C₆H₃)₃)

P	0.00544	-0.00209	-0.55224
C	-2.20566	-3.5911	1.47827
C	-0.99216	-1.34401	0.22161
C	-1.02889	-3.04875	1.98593
C	-0.44628	-1.9499	1.36123
C	-2.19685	-1.88402	-0.32217
C	-2.75062	-2.98401	0.3396
H	-3.6786	-3.41322	-0.05968
H	0.48705	-1.54117	1.77502
C	-2.01485	3.694	1.48406
C	-0.66231	1.5278	0.22713
C	-2.12802	2.40272	1.98999
C	-1.4609	1.35284	1.36537
C	-0.5311	2.84312	-0.31315
C	-1.21467	3.86796	0.34764
H	-1.12636	4.88675	-0.05027
H	-1.56825	0.33929	1.77851
C	4.21265	-0.1151	1.49027
C	1.66243	-0.19585	0.23013
C	3.15138	0.62871	1.99749

C	1.9089	0.57789	1.3722
C	2.73593	-0.96407	-0.31373
C	3.96356	-0.89098	0.35106
H	4.80173	-1.47548	-0.0485
H	1.08378	1.17604	1.78545
C	-2.92274	-1.35156	-1.56527
C	2.64444	-1.85638	-1.55993
C	0.29786	3.21511	-1.55097
H	-0.54962	-3.47411	2.87763
H	-2.7367	2.19796	2.8809
H	3.27898	1.25702	2.88909
C	0.36385	4.72787	-1.75695
H	-0.62659	5.17651	-1.96265
H	0.81767	5.25128	-0.89358
H	0.99847	4.93389	-2.63908
C	1.7438	2.75631	-1.3734
H	2.17796	3.14691	-0.43357
H	1.82599	1.65539	-1.34608
H	2.35995	3.11737	-2.22009
C	-0.31293	2.62608	-2.8476
H	-1.22793	2.02484	-2.66209
H	-0.6123	3.43306	-3.54467
H	0.43647	2.00489	-3.41288
C	-4.2684	-2.0429	-1.77834
H	-4.75462	-1.59897	-2.66711
H	-4.16685	-3.12714	-1.97578
H	-4.95384	-1.90148	-0.92077
C	-2.09706	-1.59333	-2.85397
H	-1.9576	-0.6428	-3.43912
H	-1.10516	-2.05168	-2.65303
H	-2.6244	-2.28758	-3.53701
C	-3.23926	0.13298	-1.39451
H	-3.78965	0.3229	-0.45353
H	-2.32336	0.75088	-1.37637
H	-3.86143	0.48356	-2.24122
C	3.92006	-2.67006	-1.77319
H	4.80497	-2.036	-1.97168
H	4.14448	-3.33352	-0.91597
H	3.78018	-3.31341	-2.66188
C	1.52113	-2.87732	-1.39422
H	0.52892	-2.39301	-1.36595
H	1.52483	-3.58232	-2.24843
H	1.63714	-3.45873	-0.45991
C	2.43973	-1.02056	-2.84823
H	2.37112	0.06965	-2.65138
H	3.28913	-1.15616	-3.54601

H	1.52779	-1.35489	-3.41685
C	5.59833	-0.11253	2.10794
C	5.96379	-1.53305	2.53682
H	5.95371	-2.23444	1.68188
H	6.97928	-1.55241	2.97766
H	5.25229	-1.91477	3.29265
C	6.6128	0.3759	1.07483
H	6.37741	1.40434	0.74304
H	7.63193	0.37666	1.50749
H	6.62875	-0.27014	0.1775
C	5.67639	0.79435	3.32619
H	5.44822	1.84675	3.07181
H	4.98071	0.47373	4.1247
H	6.69898	0.76818	3.74733
C	-2.90519	-4.78657	2.09783
C	-4.31682	-4.3822	2.52048
H	-4.9123	-4.01827	1.66267
H	-4.85014	-5.24774	2.95898
H	-4.28903	-3.57485	3.27591
C	-2.99346	-5.91125	1.06714
H	-1.9862	-6.22771	0.73802
H	-3.50867	-6.79033	1.50015
H	-3.55707	-5.60015	0.16808
C	-2.16669	-5.30925	3.32024
H	-1.14054	-5.64031	3.07165
H	-2.09878	-4.54695	4.11941
H	-2.70477	-6.18067	3.73822
C	-2.71346	4.89103	2.10159
C	-1.6722	5.93233	2.50973
H	-1.07276	6.2745	1.64576
H	-2.16709	6.82004	2.94887
H	-0.9726	5.52046	3.26086
C	-3.66336	5.50626	1.07468
H	-4.43715	4.77926	0.76485
H	-4.17224	6.3916	1.50262
H	-3.12708	5.83282	0.1644
C	-3.51808	4.50662	3.33306
H	-4.31226	3.77412	3.09428
H	-2.87772	4.07542	4.12578
H	-4.00957	5.40368	3.754
Pd	-0.00045	0.0072	-2.8206

TXP

P	0.000000	0.000000	1.126898
C	0.983713	4.129770	-0.771158
C	0.362313	1.599956	0.327168

C	1.650093	2.979403	-1.204033
C	1.342623	1.733616	-0.661739
C	-0.321946	2.750179	0.776655
C	0.000000	3.987077	0.213182
H	-0.542722	4.880800	0.560037
H	1.863408	0.833717	-1.023133
C	-4.068342	-1.212965	-0.771158
C	-1.566758	-0.486206	0.327168
C	-3.405286	-0.060679	-1.204033
C	-2.172667	0.295938	-0.661739
C	-2.220752	-1.653903	0.776655
C	-3.452910	-1.993538	0.213182
H	-3.955536	-2.910411	0.560037
H	-1.653724	1.196900	-1.023133
C	3.084630	-2.916805	-0.771158
C	1.204446	-1.113750	0.327168
C	1.755192	-2.918724	-1.204033
C	0.830044	-2.029554	-0.661739
C	2.542698	-1.096277	0.776655
C	3.452910	-1.993538	0.213182
H	4.498258	-1.970389	0.560037
H	-0.209684	-2.030617	-1.023133
C	-5.406471	-1.588379	-1.320943
C	1.327659	5.476331	-1.320943
C	4.078812	-3.887952	-1.320943
H	1.779950	5.401704	-2.325348
H	2.057770	5.996894	-0.671935
H	0.438590	6.127686	-1.393012
H	-5.567987	-1.159370	-2.325348
H	-6.222347	-1.216366	-0.671935
H	-5.526027	-2.684013	-1.393012
H	3.788038	-4.242333	-2.325348
H	4.164577	-4.780528	-0.671935
H	5.087437	-3.443673	-1.393012
C	-1.399772	2.644989	1.803385
C	2.990514	-0.110256	1.803385
C	-1.590742	-2.534733	1.803385
H	-1.080477	2.012124	2.654868
H	-2.303332	2.158395	1.384266
H	-1.694404	3.636204	2.189472
H	-1.202312	-1.941782	2.654868
H	-0.717559	-3.073941	1.384266
H	-2.301843	-3.285499	2.189472
H	2.282789	-0.070342	2.654868
H	3.020891	0.915547	1.384266
H	3.996247	-0.350706	2.189472

H	-3.860481	0.566021	-1.984807
H	1.440052	-3.626285	-1.984807
H	2.420428	3.060264	-1.984807

Pd(TXP)

P	0.	0.	0.40308
C	1.50207	4.00965	-1.37745
C	0.54056	1.57155	-0.33003
C	2.01966	2.78749	-1.82417
C	1.54606	1.58805	-1.30534
C	0.	2.79168	0.13302
C	0.49812	3.98228	-0.40644
H	0.07882	4.93468	-0.04595
H	1.95785	0.63322	-1.66631
C	-4.2235	-0.704	-1.37745
C	-1.63128	-0.31763	-0.33003
C	-3.42386	0.35533	-1.82417
C	-2.14832	0.5449	-1.30534
C	-2.41766	-1.39584	0.13302
C	-3.69782	-1.55976	-0.40644
H	-4.31297	-2.39908	-0.04595
H	-1.52731	1.37894	-1.66631
C	2.72143	-3.30566	-1.37745
C	1.09072	-1.25391	-0.33003
C	1.40421	-3.14282	-1.82417
C	0.60226	-2.13295	-1.30534
C	2.41766	-1.39584	0.13302
C	3.1997	-2.42253	-0.40644
H	4.23415	-2.5356	-0.04595
H	-0.43054	-2.01215	-1.66631
C	-5.59975	-0.90418	-1.92401
C	2.01683	5.30162	-1.92401
C	3.58292	-4.39743	-1.92401
H	1.91635	5.34281	-3.02438
H	3.09106	5.43344	-1.69645
H	1.47663	6.16693	-1.50291
H	-5.58518	-1.0118	-3.02438
H	-6.25103	-0.03979	-1.69645
H	-6.07903	-1.80467	-1.50291
H	3.66884	-4.33101	-3.02438
H	3.15997	-5.39366	-1.69645
H	4.60241	-4.36226	-1.50291
C	-1.06722	2.82554	1.16894
C	2.9806	-0.48853	1.16894
C	-1.91338	-2.33702	1.16894
H	-0.78308	2.16238	2.03197

H	-2.01988	2.40648	0.78853
H	-1.2552	3.85122	1.53117
H	-1.48114	-1.75935	2.03197
H	-1.07413	-2.95251	0.78853
H	-2.70765	-3.01265	1.53117
H	2.26421	-0.40303	2.03197
H	3.09402	0.54603	0.78853
H	3.96286	-0.83857	1.53117
Pd	0.	0.	2.56657
H	-3.80933	1.04165	-2.59234
H	1.00257	-3.81981	-2.59234
H	2.80677	2.77815	-2.59234

TMAP

P	0.000000	0.000000	1.185907
C	0.465290	4.218678	-0.665795
C	0.153930	1.634578	0.394433
C	1.280739	3.174786	-1.117232
C	1.117358	1.902456	-0.588903
C	-0.665527	2.686921	0.848578
C	-0.505311	3.968823	0.309271
H	-1.158600	4.774306	0.670341
H	1.751154	1.080130	-0.954503
C	-3.886127	-1.706386	-0.665795
C	-1.492551	-0.683981	0.394433
C	-3.389815	-0.478241	-1.117232
C	-2.206254	0.016432	-0.588903
C	-1.994178	-1.919823	0.848578
C	-3.184446	-2.422024	0.309271
H	-3.555370	-3.390530	0.670341
H	-1.810997	0.976479	-0.954503
C	3.420837	-2.512292	-0.665795
C	1.338621	-0.950597	0.394433
C	2.109076	-2.696545	-1.117232
C	1.088896	-1.918888	-0.588903
C	2.659705	-0.767097	0.848578
C	3.689757	-1.546799	0.309271
H	4.713970	-1.383776	0.670341
H	0.059843	-2.056609	-0.954503
C	-1.726668	2.438943	1.868464
C	2.975521	0.275867	1.868464
C	-1.248852	-2.714810	1.868464
H	-1.335114	1.832826	2.709160
H	-2.563773	1.853807	1.437339
H	-2.138863	3.380660	2.270516
H	-0.919717	-2.072656	2.709160

H	-0.323558	-3.147196	1.437339
H	-1.858306	-3.542640	2.270516
H	2.254831	0.239830	2.709160
H	2.887331	1.293389	1.437339
H	3.997169	0.161980	2.270516
O	4.366153	-3.308882	-1.223927
O	-5.048652	-2.126759	-1.223927
O	0.682499	5.435641	-1.223927
C	-0.128604	6.494708	-0.777601
C	-5.560280	-3.358728	-0.777601
C	5.688884	-3.135979	-0.777601
H	0.000000	6.678595	0.309082
H	-1.201775	6.303135	-0.984772
H	0.192178	7.388687	-1.335379
H	-5.783833	-3.339298	0.309082
H	-4.857787	-4.192335	-0.984772
H	-6.494880	-3.527913	-1.335379
H	5.783833	-3.339298	0.309082
H	6.059562	-2.110800	-0.984772
H	6.302702	-3.860775	-1.335379
H	2.033558	3.387831	-1.887195
H	1.917169	-3.455029	-1.887195
H	-3.950727	0.067197	-1.887195

Pd(TMAP)

Pd	0.000000	0.000000	2.680365
P	0.000000	0.000000	0.513883
C	0.535041	1.572644	-0.216130
C	-1.629470	-0.322963	-0.216130
C	1.094429	-1.249681	-0.216130
C	1.542151	1.593671	-1.192982
C	0.000000	2.792329	0.250843
C	-2.151235	0.538706	-1.192982
C	-2.418228	-1.396164	0.250843
C	0.609084	-2.132377	-1.192982
C	2.418228	-1.396164	0.250843
C	2.024439	2.786354	-1.708110
H	1.952169	0.640026	-1.558589
C	0.491678	3.993428	-0.273434
C	-1.068561	2.819976	1.285691
C	-3.425273	0.360039	-1.708110
H	-1.530363	1.370615	-1.558589
C	-3.704249	-1.570908	-0.273434
C	-1.907890	-2.335389	1.285691
C	1.400833	-3.146393	-1.708110
H	-0.421806	-2.010640	-1.558589

C	3.212571	-2.422520	-0.273434
C	2.976452	-0.484587	1.285691
C	1.498866	3.998167	-1.243310
H	2.810684	2.809164	-2.473556
H	0.065746	4.935107	0.097159
H	-0.784709	2.146454	2.141785
H	-2.020203	2.403809	0.899701
H	-1.257459	3.841479	1.659344
C	-4.211948	-0.701028	-1.243310
H	-3.838150	1.029541	-2.473556
H	-4.306801	-2.410616	0.097159
H	-1.466529	-1.752805	2.141785
H	-1.071658	-2.951451	0.899701
H	-2.698089	-3.009731	1.659344
C	2.713082	-3.297140	-1.243310
H	1.027466	-3.838706	-2.473556
H	4.241055	-2.524491	0.097159
H	2.251238	-0.393649	2.141785
H	3.091861	0.547643	0.899701
H	3.955548	-0.831748	1.659344
O	2.020414	5.124499	-1.786733
O	-5.448153	-0.812519	-1.786733
O	3.427739	-4.311980	-1.786733
C	1.514002	6.352155	-1.321349
C	-6.258129	-1.864914	-1.321349
C	4.744127	-4.487242	-1.321349
H	1.688303	6.479603	-0.233179
H	0.428065	6.450791	-1.526115
H	2.056799	7.139095	-1.868350
H	-6.455652	-1.777688	-0.233179
H	-5.800581	-2.854680	-1.526115
H	-7.211037	-1.788308	-1.868350
H	4.767349	-4.701915	-0.233179
H	5.372516	-3.596111	-1.526115
H	5.154239	-5.350787	-1.868350