

A Sequential Dehydrogenative Borylation/Hydrogenation Route to Polyethyl Substituted Weakly Coordinating Carborane Anions

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SUPPORTING INFORMATION

Experimental and Spectroscopic data for $[(\text{PPh}_3)_2\text{Rh}(\text{nbd})][12\text{-Br-CB}_{11}\text{H}_{11}]$, $[(\text{PPh}_3)_2\text{Rh}(12\text{-Br-CB}_{11}\text{H}_{11})]$, $\text{Cs}[1\text{-}^i\text{Pr}_3\text{Si-CB}_{11}\text{H}_{11}]$ and $[(\text{PPh}_3)_2\text{Rh}(\text{nbd})][1\text{-}^i\text{Pr}_3\text{Si-CB}_{11}\text{H}_{11}]$

ESI-MS for complexes **2a/b**, **4a/b**, **6**, **7**, **7-D₆**, **11**, **12** (Figures S1-S7)

Bond lengths and Angles for complexes **2a**, **7**, **9**, **10** and **13** (Tables S1-S10)

[(PPh₃)₂Rh(nbd)][12-Br-CB₁₁H₁₁]:

Triphenylphosphine (163 mg, 0.620 mmol) was added to a suspension of [Rh(\square -Cl)(nbd)]₂ (72 mg, 0.155 mmol) in methanol (15 cm³) and the mixture stirred for 20 minutes. Cs[12-Br-CB₁₁H₁₁] (110 mg, 0.310 mmol) was added to form an orange precipitate and, to assure completion, the reaction was stirred for 2 hours. Methanol was pumped off and the residue dissolved in CH₂Cl₂ (10 cm³) to give a suspension that was cannula filtered. The volume of the clear solution was reduced to 3 cm³ and the compound was crystallised by layering hexanes to yield orange crystals (246 mg, 84 %) that were washed with pentane twice and dried *in vacuo*.

¹H NMR (\square /ppm CD₂Cl₂): 7.49-7.20 (m, 30H, PPh₃), 4.46 (s, 4H, C₇H₈), 3.98 (s, 2H, C₇H₈), 2.29 (br s, 1H, C_{cage}-H), 1.55 (s, 2H, C₇H₈).

¹H{¹¹B} NMR (\square /ppm CD₂Cl₂): 7.49-7.20 (m, 30H, PPh₃), 4.46 (s, 4H, C₇H₈), 3.98 (s, 2H, C₇H₈), 2.29 (br s, 1H, C_{cage}-H), 1.85 (br s, 5H, B-H), 1.66 (br s, 5H, B-H), 1.55 (s, 2H, C₇H₈).

¹¹B NMR (\square /ppm CD₂Cl₂): -2.27 (s, 1B, B(12)-Br), -11.72 (d, 5B, B(7-11)-H, *J*(BH) = 139 Hz), -16.10 (d, 5B, B(2-6)-H, *J*(BH) = 153 Hz).

¹¹B{¹H} NMR (\square /ppm CD₂Cl₂): -2.27 (s, 1B, B(12)-Br), -11.72 (s, 5B, B(7-11)-H), -16.10 (s, 5B, B(2-6)-H).

³¹P{¹H} NMR (\square /ppm CD₂Cl₂): 30.5 (d, *J*(RhP) = 155 Hz).

[(PPh₃)₂Rh(12-Br-CB₁₁H₁₁)]

¹H NMR (\square /ppm CD₂Cl₂): 7.57-7.06 (m, 30H, PPh₃), 2.61 (br s, 1H, C_{cage}-H), -0.42 (br q, 5H, B-H).

¹H{¹¹B} NMR (\square /ppm CD₂Cl₂): 7.57-7.06 (m, 30H, PPh₃), 2.61 (br s, 1H, C_{cage}-H), 1.77 (br s, 5H, B-H), -0.42 (br s, 5H, B-H).

¹¹B{¹H} NMR (\square /ppm CD₂Cl₂): -0.58 (s, 1B, B(12)-Br), -13.77 (s, 5B, B(7-11)-H), -16.56 (s, 5B, B(2-6)-H).

³¹P{¹H} NMR (\square /ppm CD₂Cl₂): 45.0 (d, *J*(RhP) = 195 Hz).

Cs[1-ⁱPr₃Si-CB₁₁H₁₁]:

Butyllithium (1.45 ml, 3.63 mmol of a 2.5 M solution in hexane) was added to a solution of Cs[CB₁₁H₁₂] (1.002 g, 3.63 mmol) in THF (15 ml) at -70 °C. The new solution was allowed to warm up to room temperature and the resulting white suspension stirred overnight. ⁱPr₃SiCl (0.86 ml, 3.63 mmol) in THF (10 ml) was added and the mixture stirred for 20 hours. The new solution was filtered and the solvent removed to give a residue which was dissolved in water. A white precipitate was obtained after addition of excess of CsCl (3.056 g, 18.15 mmol). The solid was filtered, washed with water, dried and dissolved in ethanol. This was removed by rotary evaporation and the solid vacuum dried.

Yield: 66 %

¹H NMR (δ /ppm d₆-acetone): 1.24 (sept., 3H, Si(CH(CH₃)₂)₃); 1.17 (d, 18H, Si(CH(CH₃)₂)₃).

¹H{¹¹B} NMR (δ /ppm d₆-acetone): 1.94 (br s, 1H, B-H); 1.88 (br s, 5H, B-H); 1.67 (br s, 5H, B-H); 1.24 (2 sept., 3H, Si(CH(CH₃)₂)₃); 1.17 (d, 18H, Si(CH(CH₃)₂)₃).

¹¹B NMR (δ /ppm d₆-acetone): -1.93 (d, 1B, B(12)-H, J (B-H) = 134.0 Hz); -10.89 (d, 5B, B(2-11)-H, J (B-H) = 151.0 Hz); -12.71 (d, 5B, B(2-11)-H, J (B-H) = 166.1 Hz).

¹¹B{¹H} NMR (δ /ppm d₆-acetone): -1.94(s, 1B, B(12)-H); -10.89 (s, 5B, B(12)-H); -12.71 (s, 5B, B(2-11)-H).

[(PPh₃)₂Rh(nbd)][1-ⁱPr₃Si-CB₁₁H₁₁]

[Rh(\square -Cl)(nbd)]₂ (50 mg, 0.108 mmol), nbd (26 \square l, 28 mmol) and Cs[1-ⁱPr₃Si-CB₁₁H₁₁] (94 mg, 0.216 mmol) were stirred in THF (15 ml) for 3 hours. PPh₃ (115 mg, 0.435 mmol) was added to the reaction which was stirred overnight. THF was pumped off and the residue dissolved in CH₂Cl₂ and cannula filtered. The compound was crystallised by addition of hexanes to yield 189

mg (0.185 mmol) of $[(\text{PPh}_3)_2\text{Rh}(\text{nbd})][1-\text{iPr}_3\text{Si-CB}_{11}\text{H}_{11}]$. The orange crystals were washed with hexane twice and dried *in vacuo*.

Yield: 85 %

^1H NMR (δ/ppm CDCl_3): 7.34 (m, 30H, PPh_3), 4.48 (s, 4H, C_7H_8), 4.08 (s, 2H, C_7H_8), 1.52 (s, 2H, C_7H_8), 1.27 (sept, 3H, $\text{Si(CH(CH}_3)_2)_3$), 1.16 (d, 18H, $\text{Si(CH(CH}_3)_2)_3$).

$^1\text{H}\{\text{B}\}$ NMR (δ/ppm CDCl_3): 7.34 (m, 30H, PPh_3), 4.48 (s, 4H, C_7H_8), 4.09 (s, 2H, C_7H_8), 2.30 (br s, 1H, $B(12)\text{-H}$), 2.08 (br s, 5H, $B(2\text{-}6)\text{-H}$), 1.96 (br s, 5H, $B(7\text{-}11)\text{-H}$), 1.52 (s, 2H, C_7H_8), 1.27 (sept, 3H, $\text{Si(CH(CH}_3)_2)_3$), 1.16 (d, 18H, $\text{Si(CH(CH}_3)_2)_3$).

^{11}B NMR (δ/ppm CDCl_3): -2.04 (d, 1B, $B(12)\text{-H}$, $J(\text{B-H}) = 133.9$ Hz)), -10.75 (d, 5B, $B(7\text{-}11)\text{-H}$, $J(\text{B-H}) = 147.7$ Hz)), -12.29 (d, 5B, $B(2\text{-}6)\text{-H}$, $J(\text{B-H}) = 138.0$ Hz)).

$^{11}\text{B}\{\text{H}\}$ NMR (δ/ppm CDCl_3): -2.04 (s, 1B, $B(12)\text{-H}$), -10.75 (s, 5B, $B(7\text{-}12)\text{-H}$), -12.29 (s, 5B, $B(2\text{-}6)\text{-H}$).

$^{31}\text{P}\{\text{H}\}$ NMR (δ/ppm CDCl_3): 30.59 (d, $J(\text{RhP}) = 155.4$ Hz)

Table 1. Bond lengths [Å] for **2a**.

| | |
|-------------|------------|
| Rh-C(7) | 2.1812(17) |
| Rh-C(8) | 2.2003(16) |
| Rh-C(5) | 2.2108(17) |
| Rh-C(4) | 2.2249(17) |
| Rh-P(2) | 2.3056(4) |
| Rh-P(1) | 2.3409(4) |
| P(1)-C(17) | 1.8215(17) |
| P(1)-C(11) | 1.8312(17) |
| P(1)-C(23) | 1.8385(17) |
| P(2)-C(29) | 1.8195(17) |
| P(2)-C(41) | 1.8264(17) |
| P(2)-C(35) | 1.8293(17) |
| C(4)-C(5) | 1.371(3) |
| C(4)-C(9) | 1.533(2) |
| C(5)-C(6) | 1.539(3) |
| C(6)-C(7) | 1.542(3) |
| C(6)-C(10) | 1.544(3) |
| C(7)-C(8) | 1.383(3) |
| C(8)-C(9) | 1.531(2) |
| C(9)-C(10) | 1.541(3) |
| C(11)-C(16) | 1.393(2) |
| C(11)-C(12) | 1.400(2) |
| C(12)-C(13) | 1.391(2) |
| C(13)-C(14) | 1.382(3) |
| C(14)-C(15) | 1.379(3) |
| C(15)-C(16) | 1.397(3) |
| C(17)-C(22) | 1.396(2) |
| C(17)-C(18) | 1.401(2) |
| C(18)-C(19) | 1.386(2) |
| C(19)-C(20) | 1.390(3) |
| C(20)-C(21) | 1.382(3) |
| C(21)-C(22) | 1.392(3) |
| C(23)-C(28) | 1.395(2) |
| C(23)-C(24) | 1.397(2) |
| C(24)-C(25) | 1.393(3) |
| C(25)-C(26) | 1.384(3) |
| C(26)-C(27) | 1.382(3) |
| C(27)-C(28) | 1.394(2) |
| C(29)-C(30) | 1.387(3) |
| C(29)-C(34) | 1.401(3) |
| C(30)-C(31) | 1.398(3) |
| C(31)-C(32) | 1.383(3) |
| C(32)-C(33) | 1.377(3) |
| C(33)-C(34) | 1.386(3) |
| C(35)-C(40) | 1.382(3) |
| C(35)-C(36) | 1.398(2) |
| C(36)-C(37) | 1.390(3) |
| C(37)-C(38) | 1.385(3) |
| C(38)-C(39) | 1.380(3) |
| C(39)-C(40) | 1.395(3) |
| C(41)-C(42) | 1.390(2) |
| C(41)-C(46) | 1.400(2) |
| C(42)-C(43) | 1.401(3) |
| C(43)-C(44) | 1.379(3) |

| | |
|-------------|-----------|
| C(44)-C(45) | 1.382 (3) |
| C(45)-C(46) | 1.392 (2) |
| C(1)-B(4) | 1.656 (5) |
| C(1)-B(5) | 1.690 (6) |
| C(1)-B(3) | 1.706 (5) |
| C(1)-B(2) | 1.711 (4) |
| C(1)-B(6) | 1.719 (6) |
| B(2)-B(6) | 1.738 (6) |
| B(2)-B(11) | 1.751 (5) |
| B(2)-B(7) | 1.785 (5) |
| B(2)-B(3) | 1.820 (7) |
| B(3)-B(4) | 1.734 (6) |
| B(3)-B(8) | 1.773 (6) |
| B(3)-B(7) | 1.778 (5) |
| B(4)-B(8) | 1.731 (5) |
| B(4)-B(5) | 1.738 (6) |
| B(4)-B(9) | 1.753 (5) |
| B(5)-B(6) | 1.727 (5) |
| B(5)-B(9) | 1.750 (6) |
| B(5)-B(10) | 1.784 (5) |
| B(6)-B(11) | 1.754 (5) |
| B(6)-B(10) | 1.766 (6) |
| B(7)-B(12) | 1.767 (4) |
| B(7)-B(11) | 1.774 (6) |
| B(7)-B(8) | 1.829 (6) |
| B(8)-B(9) | 1.761 (5) |
| B(8)-B(12) | 1.782 (4) |
| B(9)-B(10) | 1.758 (5) |
| B(9)-B(12) | 1.795 (4) |
| B(10)-B(11) | 1.743 (5) |
| B(10)-B(12) | 1.798 (4) |
| B(11)-B(12) | 1.782 (4) |
| B(12)-C(2) | 1.583 (4) |
| C(2)-C(3) | 1.323 (4) |

Table 2. Bond angles [deg] for **2a**.

| | |
|-------------------|------------|
| C(7)-Rh-C(8) | 36.79(7) |
| C(7)-Rh-C(5) | 66.05(7) |
| C(8)-Rh-C(5) | 77.37(7) |
| C(7)-Rh-C(4) | 77.20(7) |
| C(8)-Rh-C(4) | 64.89(6) |
| C(5)-Rh-C(4) | 36.02(7) |
| C(7)-Rh-P(2) | 100.92(5) |
| C(8)-Rh-P(2) | 94.12(5) |
| C(5)-Rh-P(2) | 166.58(5) |
| C(4)-Rh-P(2) | 147.84(5) |
| C(7)-Rh-P(1) | 147.91(5) |
| C(8)-Rh-P(1) | 165.32(5) |
| C(5)-Rh-P(1) | 93.35(5) |
| C(4)-Rh-P(1) | 100.94(5) |
| P(2)-Rh-P(1) | 96.924(15) |
| C(17)-P(1)-C(11) | 105.74(8) |
| C(17)-P(1)-C(23) | 102.97(8) |
| C(11)-P(1)-C(23) | 103.83(7) |
| C(17)-P(1)-Rh | 109.03(5) |
| C(11)-P(1)-Rh | 111.37(5) |
| C(23)-P(1)-Rh | 122.50(5) |
| C(29)-P(2)-C(41) | 108.75(8) |
| C(29)-P(2)-C(35) | 100.85(7) |
| C(41)-P(2)-C(35) | 103.37(8) |
| C(29)-P(2)-Rh | 121.04(6) |
| C(41)-P(2)-Rh | 108.31(6) |
| C(35)-P(2)-Rh | 113.03(6) |
| C(5)-C(4)-C(9) | 107.10(15) |
| C(5)-C(4)-Rh | 71.43(10) |
| C(9)-C(4)-Rh | 96.17(10) |
| C(4)-C(5)-C(6) | 106.31(16) |
| C(4)-C(5)-Rh | 72.55(10) |
| C(6)-C(5)-Rh | 95.25(11) |
| C(5)-C(6)-C(7) | 101.97(14) |
| C(5)-C(6)-C(10) | 100.24(15) |
| C(7)-C(6)-C(10) | 99.64(16) |
| C(8)-C(7)-C(6) | 106.41(16) |
| C(8)-C(7)-Rh | 72.36(10) |
| C(6)-C(7)-Rh | 96.36(11) |
| C(7)-C(8)-C(9) | 106.56(16) |
| C(7)-C(8)-Rh | 70.86(10) |
| C(9)-C(8)-Rh | 97.23(10) |
| C(8)-C(9)-C(4) | 101.57(13) |
| C(8)-C(9)-C(10) | 100.21(15) |
| C(4)-C(9)-C(10) | 100.28(15) |
| C(9)-C(10)-C(6) | 93.90(14) |
| C(16)-C(11)-C(12) | 118.81(16) |
| C(16)-C(11)-P(1) | 122.48(14) |
| C(12)-C(11)-P(1) | 118.68(13) |
| C(13)-C(12)-C(11) | 120.59(18) |
| C(14)-C(13)-C(12) | 119.92(18) |
| C(15)-C(14)-C(13) | 120.14(18) |
| C(14)-C(15)-C(16) | 120.4(2) |
| C(11)-C(16)-C(15) | 120.11(19) |

| | |
|-------------------|------------|
| C(22)-C(17)-C(18) | 119.01(16) |
| C(22)-C(17)-P(1) | 119.65(13) |
| C(18)-C(17)-P(1) | 121.26(13) |
| C(19)-C(18)-C(17) | 120.25(17) |
| C(18)-C(19)-C(20) | 120.18(18) |
| C(21)-C(20)-C(19) | 120.09(18) |
| C(20)-C(21)-C(22) | 120.03(18) |
| C(21)-C(22)-C(17) | 120.41(17) |
| C(28)-C(23)-C(24) | 118.55(16) |
| C(28)-C(23)-P(1) | 120.71(13) |
| C(24)-C(23)-P(1) | 120.67(12) |
| C(25)-C(24)-C(23) | 120.40(17) |
| C(26)-C(25)-C(24) | 120.53(17) |
| C(27)-C(26)-C(25) | 119.55(17) |
| C(26)-C(27)-C(28) | 120.29(17) |
| C(27)-C(28)-C(23) | 120.68(17) |
| C(30)-C(29)-C(34) | 119.50(16) |
| C(30)-C(29)-P(2) | 119.90(14) |
| C(34)-C(29)-P(2) | 120.52(14) |
| C(29)-C(30)-C(31) | 120.2(2) |
| C(32)-C(31)-C(30) | 119.7(2) |
| C(33)-C(32)-C(31) | 120.38(18) |
| C(32)-C(33)-C(34) | 120.5(2) |
| C(33)-C(34)-C(29) | 119.66(19) |
| C(40)-C(35)-C(36) | 118.90(16) |
| C(40)-C(35)-P(2) | 122.05(13) |
| C(36)-C(35)-P(2) | 118.91(14) |
| C(37)-C(36)-C(35) | 119.99(18) |
| C(38)-C(37)-C(36) | 120.55(18) |
| C(39)-C(38)-C(37) | 119.70(18) |
| C(38)-C(39)-C(40) | 119.9(2) |
| C(35)-C(40)-C(39) | 120.99(18) |
| C(42)-C(41)-C(46) | 119.14(16) |
| C(42)-C(41)-P(2) | 124.88(13) |
| C(46)-C(41)-P(2) | 115.97(13) |
| C(41)-C(42)-C(43) | 119.60(18) |
| C(44)-C(43)-C(42) | 120.81(19) |
| C(43)-C(44)-C(45) | 119.92(18) |
| C(44)-C(45)-C(46) | 119.89(18) |
| C(45)-C(46)-C(41) | 120.62(17) |
| B(4)-C(1)-B(5) | 62.6(2) |
| B(4)-C(1)-B(3) | 62.1(3) |
| B(5)-C(1)-B(3) | 113.9(3) |
| B(4)-C(1)-B(2) | 114.2(3) |
| B(5)-C(1)-B(2) | 111.9(3) |
| B(3)-C(1)-B(2) | 64.4(3) |
| B(4)-C(1)-B(6) | 112.3(3) |
| B(5)-C(1)-B(6) | 60.8(3) |
| B(3)-C(1)-B(6) | 113.8(3) |
| B(2)-C(1)-B(6) | 60.9(2) |
| C(1)-B(2)-B(6) | 59.8(2) |
| C(1)-B(2)-B(11) | 105.7(3) |
| B(6)-B(2)-B(11) | 60.4(2) |
| C(1)-B(2)-B(7) | 104.2(3) |
| B(6)-B(2)-B(7) | 108.4(3) |
| B(11)-B(2)-B(7) | 60.2(2) |
| C(1)-B(2)-B(3) | 57.7(2) |

| | |
|-----------------------|------------|
| B (6) -B (2) -B (3) | 107.5 (3) |
| B (11) -B (2) -B (3) | 107.1 (2) |
| B (7) -B (2) -B (3) | 59.1 (2) |
| C (1) -B (3) -B (4) | 57.6 (2) |
| C (1) -B (3) -B (8) | 104.5 (3) |
| B (4) -B (3) -B (8) | 59.2 (2) |
| C (1) -B (3) -B (7) | 104.8 (3) |
| B (4) -B (3) -B (7) | 107.8 (3) |
| B (8) -B (3) -B (7) | 62.0 (2) |
| C (1) -B (3) -B (2) | 58.0 (2) |
| B (4) -B (3) -B (2) | 105.4 (3) |
| B (8) -B (3) -B (2) | 108.2 (3) |
| B (7) -B (3) -B (2) | 59.5 (2) |
| C (1) -B (4) -B (8) | 108.6 (3) |
| C (1) -B (4) -B (3) | 60.4 (2) |
| B (8) -B (4) -B (3) | 61.5 (2) |
| C (1) -B (4) -B (5) | 59.7 (2) |
| B (8) -B (4) -B (5) | 110.0 (2) |
| B (3) -B (4) -B (5) | 110.2 (3) |
| C (1) -B (4) -B (9) | 107.0 (3) |
| B (8) -B (4) -B (9) | 60.7 (2) |
| B (3) -B (4) -B (9) | 109.9 (2) |
| B (5) -B (4) -B (9) | 60.2 (2) |
| C (1) -B (5) -B (6) | 60.4 (2) |
| C (1) -B (5) -B (4) | 57.8 (2) |
| B (6) -B (5) -B (4) | 108.0 (3) |
| C (1) -B (5) -B (9) | 105.6 (3) |
| B (6) -B (5) -B (9) | 108.5 (2) |
| B (4) -B (5) -B (9) | 60.4 (2) |
| C (1) -B (5) -B (10) | 106.6 (3) |
| B (6) -B (5) -B (10) | 60.4 (2) |
| B (4) -B (5) -B (10) | 107.7 (3) |
| B (9) -B (5) -B (10) | 59.7 (2) |
| C (1) -B (6) -B (5) | 58.7 (2) |
| C (1) -B (6) -B (2) | 59.4 (2) |
| B (5) -B (6) -B (2) | 108.9 (3) |
| C (1) -B (6) -B (11) | 105.2 (3) |
| B (5) -B (6) -B (11) | 108.5 (3) |
| B (2) -B (6) -B (11) | 60.2 (2) |
| C (1) -B (6) -B (10) | 106.1 (3) |
| B (5) -B (6) -B (10) | 61.4 (2) |
| B (2) -B (6) -B (10) | 108.7 (3) |
| B (11) -B (6) -B (10) | 59.4 (2) |
| B (12) -B (7) -B (11) | 60.43 (19) |
| B (12) -B (7) -B (3) | 107.7 (3) |
| B (11) -B (7) -B (3) | 107.9 (2) |
| B (12) -B (7) -B (2) | 108.0 (3) |
| B (11) -B (7) -B (2) | 58.9 (2) |
| B (3) -B (7) -B (2) | 61.4 (2) |
| B (12) -B (7) -B (8) | 59.40 (18) |
| B (11) -B (7) -B (8) | 106.7 (2) |
| B (3) -B (7) -B (8) | 58.9 (2) |
| B (2) -B (7) -B (8) | 107.3 (2) |
| B (4) -B (8) -B (9) | 60.3 (2) |
| B (4) -B (8) -B (3) | 59.3 (2) |
| B (9) -B (8) -B (3) | 107.8 (3) |
| B (4) -B (8) -B (12) | 108.3 (2) |

| | |
|-------------------|-----------|
| B(9)-B(8)-B(12) | 60.87(17) |
| B(3)-B(8)-B(12) | 107.3(3) |
| B(4)-B(8)-B(7) | 105.6(2) |
| B(9)-B(8)-B(7) | 106.5(2) |
| B(3)-B(8)-B(7) | 59.1(2) |
| B(12)-B(8)-B(7) | 58.58(19) |
| B(5)-B(9)-B(4) | 59.5(2) |
| B(5)-B(9)-B(10) | 61.1(2) |
| B(4)-B(9)-B(10) | 108.2(3) |
| B(5)-B(9)-B(8) | 108.0(3) |
| B(4)-B(9)-B(8) | 59.0(2) |
| B(10)-B(9)-B(8) | 109.4(3) |
| B(5)-B(9)-B(12) | 108.9(2) |
| B(4)-B(9)-B(12) | 106.7(3) |
| B(10)-B(9)-B(12) | 60.80(18) |
| B(8)-B(9)-B(12) | 60.15(19) |
| B(11)-B(10)-B(9) | 108.2(3) |
| B(11)-B(10)-B(6) | 60.0(2) |
| B(9)-B(10)-B(6) | 106.3(3) |
| B(11)-B(10)-B(5) | 106.4(3) |
| B(9)-B(10)-B(5) | 59.2(2) |
| B(6)-B(10)-B(5) | 58.2(2) |
| B(11)-B(10)-B(12) | 60.40(18) |
| B(9)-B(10)-B(12) | 60.60(18) |
| B(6)-B(10)-B(12) | 107.8(3) |
| B(5)-B(10)-B(12) | 107.3(3) |
| B(10)-B(11)-B(2) | 109.1(2) |
| B(10)-B(11)-B(6) | 60.7(2) |
| B(2)-B(11)-B(6) | 59.4(2) |
| B(10)-B(11)-B(7) | 109.2(2) |
| B(2)-B(11)-B(7) | 60.9(2) |
| B(6)-B(11)-B(7) | 108.2(3) |
| B(10)-B(11)-B(12) | 61.33(19) |
| B(2)-B(11)-B(12) | 108.9(2) |
| B(6)-B(11)-B(12) | 109.1(2) |
| B(7)-B(11)-B(12) | 59.58(19) |
| C(2)-B(12)-B(7) | 123.1(2) |
| C(2)-B(12)-B(8) | 122.6(2) |
| B(7)-B(12)-B(8) | 62.0(2) |
| C(2)-B(12)-B(11) | 122.7(2) |
| B(7)-B(12)-B(11) | 60.0(2) |
| B(8)-B(12)-B(11) | 108.3(2) |
| C(2)-B(12)-B(9) | 122.1(2) |
| B(7)-B(12)-B(9) | 107.7(2) |
| B(8)-B(12)-B(9) | 59.0(2) |
| B(11)-B(12)-B(9) | 104.9(2) |
| C(2)-B(12)-B(10) | 121.0(2) |
| B(7)-B(12)-B(10) | 107.0(2) |
| B(8)-B(12)-B(10) | 106.7(2) |
| B(11)-B(12)-B(10) | 58.3(2) |
| B(9)-B(12)-B(10) | 58.60(19) |
| C(3)-C(2)-B(12) | 127.0(3) |

Table 3. Bond lengths [Å] for **7**.

| | |
|---------------|-----------|
| Rh-C(7) | 2.173(3) |
| Rh-C(6) | 2.194(3) |
| Rh-C(3) | 2.210(3) |
| Rh-C(4) | 2.221(3) |
| Rh-P(1) | 2.3229(7) |
| Rh-P(2) | 2.3458(8) |
| P(1)-C(23) | 1.824(3) |
| P(1)-C(11) | 1.831(3) |
| P(1)-C(17) | 1.833(3) |
| P(2)-C(35) | 1.824(3) |
| P(2)-C(41) | 1.827(3) |
| P(2)-C(29) | 1.828(3) |
| C(2)-C(3) | 1.532(4) |
| C(2)-C(7) | 1.542(4) |
| C(2)-C(8) | 1.544(5) |
| C(3)-C(4) | 1.365(4) |
| C(4)-C(5) | 1.523(4) |
| C(5)-C(6) | 1.537(4) |
| C(5)-C(8) | 1.545(5) |
| C(6)-C(7) | 1.366(4) |
| C(11)-C(12) | 1.377(4) |
| C(11)-C(16) | 1.382(4) |
| C(12)-C(13) | 1.390(5) |
| C(13)-C(14) | 1.360(6) |
| C(14)-C(15) | 1.368(6) |
| C(15)-C(16) | 1.397(5) |
| C(17)-C(22) | 1.393(4) |
| C(17)-C(18) | 1.398(4) |
| C(18)-C(19) | 1.390(5) |
| C(19)-C(20) | 1.380(6) |
| C(20)-C(21) | 1.380(6) |
| C(21)-C(22) | 1.388(5) |
| C(23)-C(24A) | 1.32(3) |
| C(23)-C(24) | 1.379(6) |
| C(23)-C(28A) | 1.40(2) |
| C(23)-C(28) | 1.412(5) |
| C(26)-C(25) | 1.317(7) |
| C(26)-C(27A) | 1.35(3) |
| C(26)-C(27) | 1.413(6) |
| C(26)-C(25A) | 1.58(3) |
| C(24)-C(25) | 1.390(8) |
| | |
| C(27)-C(28) | 1.382(6) |
| C(24A)-C(25A) | 1.31(4) |
| C(27A)-C(28A) | 1.42(4) |
| C(29)-C(30) | 1.386(4) |
| C(29)-C(34) | 1.395(4) |
| C(30)-C(31) | 1.385(5) |
| C(31)-C(32) | 1.377(5) |
| C(32)-C(33) | 1.382(5) |
| C(33)-C(34) | 1.387(4) |
| C(35)-C(36) | 1.388(4) |
| C(35)-C(40) | 1.409(4) |
| C(36)-C(37) | 1.392(5) |

| | |
|------------------|------------|
| C (37) -C (38) | 1.378 (6) |
| C (38) -C (39) | 1.383 (5) |
| C (39) -C (40) | 1.382 (4) |
| C (41) -C (46) | 1.389 (5) |
| C (41) -C (42) | 1.391 (4) |
| C (42) -C (43) | 1.392 (5) |
| C (43) -C (44) | 1.379 (6) |
| C (44) -C (45) | 1.354 (6) |
| C (45) -C (46) | 1.394 (5) |
| C (1) -B (6) | 1.681 (7) |
| C (1) -B (3) | 1.722 (6) |
| C (1) -B (5) | 1.732 (7) |
| C (1) -B (2) | 1.743 (7) |
| C (1) -B (4) | 1.744 (8) |
| B (2) -C (51) | 1.630 (7) |
| B (2) -B (6) | 1.723 (8) |
| B (2) -B (11) | 1.753 (8) |
| B (2) -B (3) | 1.754 (7) |
| B (2) -B (7) | 1.779 (6) |
| B (3) -B (7) | 1.768 (6) |
| B (3) -B (4) | 1.782 (6) |
| B (3) -B (8) | 1.790 (6) |
| B (4) -C (53) | 1.572 (7) |
| B (4) -B (5) | 1.730 (7) |
| B (4) -B (8) | 1.791 (6) |
| B (4) -B (9) | 1.800 (7) |
| B (5) -B (9) | 1.735 (6) |
| B (5) -B (6) | 1.746 (7) |
| B (5) -B (10) | 1.776 (6) |
| B (6) -B (11) | 1.709 (6) |
| B (6) -B (10) | 1.718 (8) |
| B (7) -B (11) | 1.752 (6) |
| B (7) -B (12) | 1.769 (6) |
| B (7) -B (8) | 1.782 (6) |
| B (8) -C (55) | 1.589 (6) |
| B (8) -B (9) | 1.791 (6) |
| B (8) -B (12) | 1.802 (6) |
| B (9) -B (10) | 1.764 (7) |
| B (9) -B (12) | 1.776 (6) |
| B (10) -C (57) | 1.588 (16) |
| B (10) -C (57A) | 1.623 (16) |
| B (10) -B (11) | 1.766 (7) |
| B (10) -B (12) | 1.804 (6) |
| B (11) -B (12) | 1.767 (6) |
| B (12) -C (59) | 1.605 (5) |
| C (51) -C (52) | 1.333 (14) |
| C (51) -C (52A) | 1.461 (17) |
| C (53) -C (54A) | 1.534 (15) |
| C (53) -C (54) | 1.558 (11) |
| C (55) -C (56) | 1.533 (5) |
| C (57) -C (58) | 1.33 (2) |
| C (57A) -C (58A) | 1.57 (2) |
| C (59) -C (60) | 1.522 (6) |

Table 4. Bond angles [deg] for 7.

| | |
|-------------------|------------|
| C(7)-Rh-C(6) | 36.45(12) |
| C(7)-Rh-C(3) | 65.92(11) |
| C(6)-Rh-C(3) | 77.13(11) |
| C(7)-Rh-C(4) | 76.96(11) |
| C(6)-Rh-C(4) | 64.81(11) |
| C(3)-Rh-C(4) | 35.88(11) |
| C(7)-Rh-P(1) | 98.54(8) |
| C(6)-Rh-P(1) | 94.67(8) |
| C(3)-Rh-P(1) | 162.89(8) |
| C(4)-Rh-P(1) | 151.51(8) |
| C(7)-Rh-P(2) | 145.87(9) |
| C(6)-Rh-P(2) | 164.59(8) |
| C(3)-Rh-P(2) | 91.39(8) |
| C(4)-Rh-P(2) | 99.88(8) |
| P(1)-Rh-P(2) | 99.01(3) |
| C(23)-P(1)-C(11) | 109.65(14) |
| C(23)-P(1)-C(17) | 103.55(14) |
| C(11)-P(1)-C(17) | 102.41(13) |
| C(23)-P(1)-Rh | 111.36(10) |
| C(11)-P(1)-Rh | 116.03(10) |
| C(17)-P(1)-Rh | 112.81(9) |
| C(35)-P(2)-C(41) | 104.23(14) |
| C(35)-P(2)-C(29) | 104.39(14) |
| C(41)-P(2)-C(29) | 102.98(14) |
| C(35)-P(2)-Rh | 109.52(10) |
| C(41)-P(2)-Rh | 123.72(9) |
| C(29)-P(2)-Rh | 110.26(10) |
| C(3)-C(2)-C(7) | 101.8(2) |
| C(3)-C(2)-C(8) | 99.8(3) |
| C(7)-C(2)-C(8) | 99.7(3) |
| C(4)-C(3)-C(2) | 106.6(3) |
| C(4)-C(3)-Rh | 72.52(16) |
| C(2)-C(3)-Rh | 95.35(17) |
| C(3)-C(4)-C(5) | 107.3(3) |
| C(3)-C(4)-Rh | 71.60(16) |
| C(5)-C(4)-Rh | 96.52(18) |
| C(4)-C(5)-C(6) | 101.3(2) |
| C(4)-C(5)-C(8) | 100.0(3) |
| C(6)-C(5)-C(8) | 99.9(3) |
| C(7)-C(6)-C(5) | 106.8(3) |
| C(7)-C(6)-Rh | 70.92(18) |
| C(5)-C(6)-Rh | 97.19(19) |
| C(6)-C(7)-C(2) | 106.8(3) |
| C(6)-C(7)-Rh | 72.63(18) |
| C(2)-C(7)-Rh | 96.53(19) |
| C(2)-C(8)-C(5) | 93.8(2) |
| C(12)-C(11)-C(16) | 118.8(3) |
| C(12)-C(11)-P(1) | 117.0(2) |
| C(16)-C(11)-P(1) | 124.2(3) |
| C(11)-C(12)-C(13) | 120.6(3) |
| C(14)-C(13)-C(12) | 120.6(4) |
| C(13)-C(14)-C(15) | 119.4(3) |
| C(14)-C(15)-C(16) | 120.8(3) |
| C(11)-C(16)-C(15) | 119.8(3) |

| | |
|-----------------------|-----------|
| C(22) -C(17) -C(18) | 118.9(3) |
| C(22) -C(17) -P(1) | 120.6(2) |
| C(18) -C(17) -P(1) | 120.3(2) |
| C(19) -C(18) -C(17) | 120.2(3) |
| C(20) -C(19) -C(18) | 120.4(3) |
| C(19) -C(20) -C(21) | 119.7(3) |
| | |
| C(20) -C(21) -C(22) | 120.6(4) |
| C(21) -C(22) -C(17) | 120.2(3) |
| C(24A) -C(23) -C(24) | 30.9(14) |
| C(24A) -C(23) -C(28A) | 121.3(16) |
| C(24) -C(23) -C(28A) | 96.5(9) |
| C(24A) -C(23) -C(28) | 114.7(13) |
| C(24) -C(23) -C(28) | 117.0(3) |
| C(28A) -C(23) -C(28) | 53.7(8) |
| C(24A) -C(23) -P(1) | 111.2(12) |
| C(24) -C(23) -P(1) | 119.9(3) |
| C(28A) -C(23) -P(1) | 121.9(9) |
| C(28) -C(23) -P(1) | 122.9(2) |
| C(25) -C(26) -C(27A) | 93.7(12) |
| C(25) -C(26) -C(27) | 120.9(4) |
| C(27A) -C(26) -C(27) | 56.0(11) |
| C(25) -C(26) -C(25A) | 26.8(11) |
| C(27A) -C(26) -C(25A) | 105.5(18) |
| C(27) -C(26) -C(25A) | 107.5(11) |
| C(23) -C(24) -C(25) | 122.4(5) |
| C(26) -C(25) -C(24) | 119.9(5) |
| C(28) -C(27) -C(26) | 119.4(4) |
| C(27) -C(28) -C(23) | 120.2(4) |
| C(25A) -C(24A) -C(23) | 118(3) |
| C(24A) -C(25A) -C(26) | 122(3) |
| C(26) -C(27A) -C(28A) | 124(2) |
| C(23) -C(28A) -C(27A) | 115.3(19) |
| C(30) -C(29) -C(34) | 119.4(3) |
| C(30) -C(29) -P(2) | 121.1(2) |
| C(34) -C(29) -P(2) | 119.6(2) |
| C(31) -C(30) -C(29) | 120.2(3) |
| C(32) -C(31) -C(30) | 120.2(3) |
| C(31) -C(32) -C(33) | 120.2(3) |
| C(32) -C(33) -C(34) | 120.0(3) |
| C(33) -C(34) -C(29) | 120.0(3) |
| C(36) -C(35) -C(40) | 118.5(3) |
| C(36) -C(35) -P(2) | 123.2(2) |
| C(40) -C(35) -P(2) | 118.2(2) |
| C(35) -C(36) -C(37) | 120.4(3) |
| C(38) -C(37) -C(36) | 120.4(3) |
| C(37) -C(38) -C(39) | 120.0(3) |
| C(40) -C(39) -C(38) | 120.2(3) |
| C(39) -C(40) -C(35) | 120.5(3) |
| C(46) -C(41) -C(42) | 118.5(3) |
| C(46) -C(41) -P(2) | 123.3(3) |
| C(42) -C(41) -P(2) | 118.2(2) |
| C(41) -C(42) -C(43) | 120.4(3) |
| | |
| C(44) -C(43) -C(42) | 120.1(4) |
| C(45) -C(44) -C(43) | 119.8(4) |
| C(44) -C(45) -C(46) | 120.9(4) |

| | |
|------------------------|-----------|
| C (41) -C (46) -C (45) | 120.1 (4) |
| B (6) -C (1) -B (3) | 108.4 (3) |
| B (6) -C (1) -B (5) | 61.5 (3) |
| B (3) -C (1) -B (5) | 109.7 (3) |
| B (6) -C (1) -B (2) | 60.4 (3) |
| B (3) -C (1) -B (2) | 60.8 (3) |
| B (5) -C (1) -B (2) | 111.3 (4) |
| B (6) -C (1) -B (4) | 109.2 (4) |
| B (3) -C (1) -B (4) | 61.9 (3) |
| B (5) -C (1) -B (4) | 59.7 (3) |
| B (2) -C (1) -B (4) | 111.6 (3) |
| C (51) -B (2) -B (6) | 120.5 (4) |
| C (51) -B (2) -C (1) | 121.5 (4) |
| B (6) -B (2) -C (1) | 58.0 (3) |
| C (51) -B (2) -B (11) | 122.1 (4) |
| B (6) -B (2) -B (11) | 58.9 (3) |
| C (1) -B (2) -B (11) | 105.6 (4) |
| C (51) -B (2) -B (3) | 124.7 (5) |
| B (6) -B (2) -B (3) | 105.0 (3) |
| C (1) -B (2) -B (3) | 59.0 (3) |
| B (11) -B (2) -B (3) | 107.2 (3) |
| C (51) -B (2) -B (7) | 125.9 (4) |
| B (6) -B (2) -B (7) | 105.3 (3) |
| C (1) -B (2) -B (7) | 106.0 (3) |
| B (11) -B (2) -B (7) | 59.5 (2) |
| B (3) -B (2) -B (7) | 60.1 (3) |
| C (1) -B (3) -B (2) | 60.2 (3) |
| C (1) -B (3) -B (7) | 107.5 (3) |
| B (2) -B (3) -B (7) | 60.7 (3) |
| C (1) -B (3) -B (4) | 59.7 (3) |
| B (2) -B (3) -B (4) | 109.4 (3) |
| B (7) -B (3) -B (4) | 108.4 (3) |
| C (1) -B (3) -B (8) | 107.4 (3) |
| B (2) -B (3) -B (8) | 109.4 (3) |
| B (7) -B (3) -B (8) | 60.1 (2) |
| B (4) -B (3) -B (8) | 60.2 (3) |
| C (53) -B (4) -B (5) | 120.7 (4) |
| C (53) -B (4) -C (1) | 122.3 (4) |
| B (5) -B (4) -C (1) | 59.8 (3) |
| C (53) -B (4) -B (3) | 123.0 (4) |
| B (5) -B (4) -B (3) | 107.1 (4) |
| C (1) -B (4) -B (3) | 58.4 (3) |
| C (53) -B (4) -B (8) | 123.3 (4) |
| B (5) -B (4) -B (8) | 107.6 (3) |
| C (1) -B (4) -B (8) | 106.3 (3) |
| B (3) -B (4) -B (8) | 60.1 (2) |
| C (53) -B (4) -B (9) | 123.4 (4) |
| B (5) -B (4) -B (9) | 58.8 (3) |
| C (1) -B (4) -B (9) | 105.3 (3) |
| B (3) -B (4) -B (9) | 106.6 (3) |
| B (8) -B (4) -B (9) | 59.8 (2) |
| B (4) -B (5) -C (1) | 60.5 (3) |
| B (4) -B (5) -B (9) | 62.6 (3) |
| C (1) -B (5) -B (9) | 108.8 (3) |
| B (4) -B (5) -B (6) | 106.9 (3) |
| C (1) -B (5) -B (6) | 57.8 (3) |
| B (9) -B (5) -B (6) | 105.8 (3) |

| | |
|-------------------------|------------|
| B (4) -B (5) -B (10) | 110.8 (3) |
| C (1) -B (5) -B (10) | 106.5 (3) |
| B (9) -B (5) -B (10) | 60.3 (3) |
| B (6) -B (5) -B (10) | 58.4 (3) |
| C (1) -B (6) -B (11) | 110.5 (4) |
| C (1) -B (6) -B (10) | 111.6 (4) |
| B (11) -B (6) -B (10) | 62.0 (3) |
| C (1) -B (6) -B (2) | 61.6 (3) |
| B (11) -B (6) -B (2) | 61.4 (3) |
| B (10) -B (6) -B (2) | 113.1 (3) |
| C (1) -B (6) -B (5) | 60.7 (3) |
| B (11) -B (6) -B (5) | 110.9 (3) |
| B (10) -B (6) -B (5) | 61.7 (3) |
| B (2) -B (6) -B (5) | 111.6 (4) |
| B (11) -B (7) -B (3) | 106.6 (3) |
| B (11) -B (7) -B (12) | 60.2 (3) |
| B (3) -B (7) -B (12) | 109.0 (3) |
| B (11) -B (7) -B (2) | 59.5 (3) |
| B (3) -B (7) -B (2) | 59.3 (3) |
| B (12) -B (7) -B (2) | 108.8 (3) |
| B (11) -B (7) -B (8) | 108.3 (3) |
| B (3) -B (7) -B (8) | 60.6 (2) |
| B (12) -B (7) -B (8) | 61.0 (2) |
| B (2) -B (7) -B (8) | 108.6 (3) |
| C (55) -B (8) -B (7) | 124.6 (3) |
| C (55) -B (8) -B (3) | 122.1 (3) |
| B (7) -B (8) -B (3) | 59.3 (2) |
| C (55) -B (8) -B (9) | 121.8 (3) |
| B (7) -B (8) -B (9) | 106.1 (3) |
| B (3) -B (8) -B (9) | 106.6 (3) |
| C (55) -B (8) -B (4) | 119.2 (3) |
| B (7) -B (8) -B (4) | 107.3 (3) |
| B (3) -B (8) -B (4) | 59.7 (3) |
| B (9) -B (8) -B (4) | 60.3 (2) |
| C (55) -B (8) -B (12) | 124.0 (3) |
| B (7) -B (8) -B (12) | 59.1 (2) |
| B (3) -B (8) -B (12) | 106.5 (3) |
| B (9) -B (8) -B (12) | 59.3 (2) |
| B (4) -B (8) -B (12) | 107.9 (3) |
| B (5) -B (9) -B (10) | 61.0 (3) |
| B (5) -B (9) -B (12) | 109.6 (3) |
| B (10) -B (9) -B (12) | 61.2 (2) |
| B (5) -B (9) -B (8) | 107.4 (3) |
| B (10) -B (9) -B (8) | 109.4 (3) |
| B (12) -B (9) -B (8) | 60.7 (2) |
| B (5) -B (9) -B (4) | 58.6 (3) |
| B (10) -B (9) -B (4) | 108.1 (3) |
| B (12) -B (9) -B (4) | 108.7 (3) |
| B (8) -B (9) -B (4) | 59.9 (2) |
| C (57) -B (10) -C (57A) | 15.5 (13) |
| C (57) -B (10) -B (6) | 116.1 (10) |
| C (57A) -B (10) -B (6) | 127.7 (6) |
| C (57) -B (10) -B (9) | 131.9 (12) |
| C (57A) -B (10) -B (9) | 116.5 (6) |
| B (6) -B (10) -B (9) | 105.7 (3) |
| C (57) -B (10) -B (11) | 114.6 (11) |
| C (57A) -B (10) -B (11) | 128.1 (7) |

| | |
|--------------------------|------------|
| B (6) -B (10) -B (11) | 58.7 (3) |
| B (9) -B (10) -B (11) | 106.6 (3) |
| C (57) -B (10) -B (5) | 125.4 (8) |
| C (57A) -B (10) -B (5) | 119.3 (7) |
| B (6) -B (10) -B (5) | 59.9 (3) |
| B (9) -B (10) -B (5) | 58.7 (3) |
| B (11) -B (10) -B (5) | 107.0 (4) |
| C (57) -B (10) -B (12) | 124.4 (7) |
| C (57A) -B (10) -B (12) | 121.4 (7) |
| B (6) -B (10) -B (12) | 105.6 (3) |
| B (9) -B (10) -B (12) | 59.7 (2) |
| B (11) -B (10) -B (12) | 59.3 (2) |
| B (5) -B (10) -B (12) | 106.5 (3) |
| B (6) -B (11) -B (7) | 107.1 (3) |
| B (6) -B (11) -B (2) | 59.7 (3) |
| B (7) -B (11) -B (2) | 61.0 (3) |
| B (6) -B (11) -B (10) | 59.3 (3) |
| B (7) -B (11) -B (10) | 109.5 (3) |
| B (2) -B (11) -B (10) | 109.5 (3) |
| B (6) -B (11) -B (12) | 107.6 (3) |
| B (7) -B (11) -B (12) | 60.3 (2) |
| B (2) -B (11) -B (12) | 110.1 (3) |
| B (10) -B (11) -B (12) | 61.4 (3) |
| C (59) -B (12) -B (11) | 122.9 (3) |
| C (59) -B (12) -B (7) | 123.1 (3) |
| B (11) -B (12) -B (7) | 59.4 (3) |
| C (59) -B (12) -B (9) | 121.9 (3) |
| B (11) -B (12) -B (9) | 106.1 (3) |
| B (7) -B (12) -B (9) | 107.3 (3) |
| C (59) -B (12) -B (8) | 122.6 (3) |
| B (11) -B (12) -B (8) | 106.8 (3) |
| B (7) -B (12) -B (8) | 59.9 (2) |
| B (9) -B (12) -B (8) | 60.1 (2) |
| C (59) -B (12) -B (10) | 121.4 (3) |
| B (11) -B (12) -B (10) | 59.3 (3) |
| B (7) -B (12) -B (10) | 107.1 (3) |
| B (9) -B (12) -B (10) | 59.1 (3) |
| B (8) -B (12) -B (10) | 107.2 (3) |
| C (52) -C (51) -C (52A) | 43.5 (9) |
| C (52) -C (51) -B (2) | 118.3 (8) |
| C (52A) -C (51) -B (2) | 115.9 (7) |
| C (54A) -C (53) -C (54) | 36.0 (6) |
| C (54A) -C (53) -B (4) | 109.5 (7) |
| C (54) -C (53) -B (4) | 117.7 (5) |
| C (56) -C (55) -B (8) | 115.7 (3) |
| C (58) -C (57) -B (10) | 119.2 (14) |
| C (58A) -C (57A) -B (10) | 111.3 (10) |
| C (60) -C (59) -B (12) | 115.2 (4) |

Table 5. Bond lengths [Å] for **9**.

| | |
|-------------|------------|
| Rh-P(1) | 2.2241(12) |
| Rh-P(2) | 2.2295(11) |
| Rh-B(12) | 2.384(5) |
| Rh-B(7) | 2.387(5) |
| Rh-H(7) | 1.87(5) |
| Rh-H(12) | 1.80(4) |
| P(1)-C(23) | 1.817(5) |
| P(1)-C(17) | 1.821(5) |
| P(1)-C(11) | 1.831(5) |
| C(11)-C(16) | 1.394(7) |
| C(11)-C(12) | 1.408(7) |
| C(12)-C(13) | 1.381(7) |
| C(13)-C(14) | 1.361(11) |
| C(14)-C(15) | 1.375(12) |
| C(15)-C(16) | 1.405(8) |
| C(17)-C(22) | 1.398(7) |
| C(17)-C(18) | 1.408(6) |
| C(18)-C(19) | 1.378(7) |
| C(19)-C(20) | 1.388(8) |
| C(20)-C(21) | 1.376(8) |
| C(21)-C(22) | 1.394(7) |
| C(23)-C(28) | 1.403(7) |
| C(23)-C(24) | 1.405(7) |
| C(24)-C(25) | 1.381(7) |
| C(25)-C(26) | 1.367(9) |
| C(26)-C(27) | 1.404(9) |
| C(27)-C(28) | 1.379(7) |
| P(2)-C(29) | 1.817(4) |
| P(2)-C(35) | 1.827(4) |
| P(2)-C(41) | 1.833(4) |
| C(29)-C(30) | 1.389(6) |
| C(29)-C(34) | 1.398(6) |
| C(30)-C(31) | 1.384(7) |
| C(31)-C(32) | 1.390(7) |
| C(32)-C(33) | 1.369(7) |
| C(33)-C(34) | 1.386(7) |
| C(35)-C(40) | 1.402(6) |
| | |
| C(35)-C(36) | 1.403(6) |
| C(36)-C(37) | 1.393(6) |
| C(37)-C(38) | 1.377(7) |
| C(38)-C(39) | 1.384(7) |
| C(39)-C(40) | 1.379(7) |
| C(41)-C(46) | 1.392(6) |
| C(41)-C(42) | 1.398(6) |
| C(42)-C(43) | 1.395(7) |
| C(43)-C(44) | 1.374(8) |
| C(44)-C(45) | 1.381(8) |
| C(45)-C(46) | 1.406(7) |
| C(1)-B(3) | 1.714(6) |
| C(1)-B(2) | 1.733(7) |
| C(1)-B(6) | 1.733(7) |
| C(1)-B(5) | 1.738(6) |
| C(1)-B(4) | 1.739(6) |

| | |
|-------------|-----------|
| C(1)-Si | 1.930 (4) |
| B(2)-B(7) | 1.755 (7) |
| B(2)-B(11) | 1.782 (7) |
| B(2)-B(3) | 1.786 (8) |
| B(2)-B(6) | 1.791 (8) |
| B(2)-H(2) | 1.1200 |
| B(3)-B(4) | 1.766 (7) |
| B(3)-B(8) | 1.782 (7) |
| B(3)-B(7) | 1.788 (8) |
| B(3)-H(3) | 1.1200 |
| B(4)-B(8) | 1.758 (7) |
| B(4)-B(5) | 1.767 (7) |
| B(4)-B(9) | 1.776 (7) |
| B(5)-B(10) | 1.762 (7) |
| B(5)-B(6) | 1.766 (7) |
| B(5)-B(9) | 1.767 (7) |
| B(6)-B(11) | 1.779 (8) |
| B(6)-B(10) | 1.781 (7) |
| B(7)-B(12) | 1.720 (6) |
| B(7)-B(11) | 1.777 (7) |
| B(7)-B(8) | 1.786 (8) |
| B(7)-H(7) | 1.04 (6) |
| B(8)-B(9) | 1.777 (7) |
| B(8)-B(12) | 1.781 (7) |
| B(9)-B(12) | 1.761 (7) |
| B(9)-B(10) | 1.789 (7) |
| B(10)-B(12) | 1.760 (7) |
| B(10)-B(11) | 1.785 (7) |
| B(11)-B(12) | 1.778 (7) |
| B(12)-H(12) | 1.23 (4) |
| Si-C(5) | 1.888 (6) |
| Si-C(8) | 1.902 (5) |
| Si-C(2) | 1.902 (6) |
| C(2)-C(4) | 1.520 (9) |
| C(2)-C(3) | 1.561 (8) |
| C(5)-C(7) | 1.552 (8) |
| C(5)-C(6) | 1.569 (9) |
| C(8)-C(9) | 1.535 (8) |
| C(8)-C(10) | 1.545 (8) |

Table 6. Bond angles [deg] for **9**.

| | |
|-------------------|------------|
| P(1)-Rh-P(2) | 95.47(4) |
| P(1)-Rh-B(12) | 155.22(11) |
| P(2)-Rh-B(12) | 109.31(11) |
| P(1)-Rh-B(7) | 112.95(12) |
| P(2)-Rh-B(7) | 151.59(12) |
| | |
| B(12)-Rh-B(7) | 42.28(16) |
| P(1)-Rh-H(7) | 88.3(16) |
| P(2)-Rh-H(7) | 176.2(16) |
| B(12)-Rh-H(7) | 66.9(17) |
| B(7)-Rh-H(7) | 24.7(16) |
| | |
| P(1)-Rh-H(12) | 173.6(13) |
| P(2)-Rh-H(12) | 79.1(13) |
| B(12)-Rh-H(12) | 30.4(13) |
| B(7)-Rh-H(12) | 72.5(13) |
| H(7)-Rh-H(12) | 97(2) |
| C(23)-P(1)-C(17) | 108.7(2) |
| C(23)-P(1)-C(11) | 100.1(2) |
| C(17)-P(1)-C(11) | 102.7(2) |
| C(23)-P(1)-Rh | 116.28(16) |
| C(17)-P(1)-Rh | 115.70(14) |
| C(11)-P(1)-Rh | 111.40(16) |
| C(16)-C(11)-C(12) | 118.6(5) |
| C(16)-C(11)-P(1) | 123.6(4) |
| C(12)-C(11)-P(1) | 117.6(4) |
| C(13)-C(12)-C(11) | 121.1(6) |
| C(14)-C(13)-C(12) | 119.9(7) |
| C(13)-C(14)-C(15) | 120.5(6) |
| C(14)-C(15)-C(16) | 120.9(7) |
| C(11)-C(16)-C(15) | 118.9(6) |
| C(22)-C(17)-C(18) | 118.5(4) |
| C(22)-C(17)-P(1) | 125.2(4) |
| C(18)-C(17)-P(1) | 116.2(4) |
| C(19)-C(18)-C(17) | 120.7(5) |
| C(18)-C(19)-C(20) | 120.2(5) |
| C(21)-C(20)-C(19) | 120.0(5) |
| C(20)-C(21)-C(22) | 120.5(5) |
| C(21)-C(22)-C(17) | 120.0(5) |
| C(28)-C(23)-C(24) | 118.1(5) |
| C(28)-C(23)-P(1) | 119.6(4) |
| C(24)-C(23)-P(1) | 122.2(4) |
| C(25)-C(24)-C(23) | 120.7(5) |
| C(26)-C(25)-C(24) | 120.2(5) |
| C(25)-C(26)-C(27) | 120.9(5) |
| C(28)-C(27)-C(26) | 118.9(6) |
| C(27)-C(28)-C(23) | 121.3(5) |
| C(29)-P(2)-C(35) | 101.31(19) |
| C(29)-P(2)-C(41) | 102.8(2) |
| C(35)-P(2)-C(41) | 103.89(19) |
| C(29)-P(2)-Rh | 124.71(13) |
| C(35)-P(2)-Rh | 112.34(14) |
| C(41)-P(2)-Rh | 109.63(14) |
| C(30)-C(29)-C(34) | 118.6(4) |

| | |
|------------------------|-----------|
| C (30) -C (29) -P (2) | 121.8 (3) |
| C (34) -C (29) -P (2) | 119.7 (3) |
| C (31) -C (30) -C (29) | 120.7 (4) |
| C (30) -C (31) -C (32) | 119.9 (5) |
| C (33) -C (32) -C (31) | 120.1 (5) |
| C (32) -C (33) -C (34) | 120.2 (4) |
| C (33) -C (34) -C (29) | 120.6 (4) |
| C (40) -C (35) -C (36) | 118.2 (4) |
| C (40) -C (35) -P (2) | 119.8 (3) |
| C (36) -C (35) -P (2) | 122.0 (3) |
| C (37) -C (36) -C (35) | 120.5 (4) |
| C (38) -C (37) -C (36) | 120.2 (4) |
| C (37) -C (38) -C (39) | 119.9 (4) |
| C (40) -C (39) -C (38) | 120.6 (5) |
| C (39) -C (40) -C (35) | 120.6 (4) |
| C (46) -C (41) -C (42) | 118.3 (4) |
| C (46) -C (41) -P (2) | 119.6 (3) |
| C (42) -C (41) -P (2) | 122.1 (3) |
| C (43) -C (42) -C (41) | 120.8 (4) |
| C (44) -C (43) -C (42) | 120.3 (5) |
| C (43) -C (44) -C (45) | 120.0 (4) |
| C (44) -C (45) -C (46) | 120.1 (5) |
| C (41) -C (46) -C (45) | 120.5 (5) |
| B (3) -C (1) -B (2) | 62.4 (3) |
| B (3) -C (1) -B (6) | 113.3 (4) |
| B (2) -C (1) -B (6) | 62.2 (3) |
| B (3) -C (1) -B (5) | 111.5 (3) |
| B (2) -C (1) -B (5) | 111.5 (3) |
| B (6) -C (1) -B (5) | 61.2 (3) |
| B (3) -C (1) -B (4) | 61.5 (3) |
| B (2) -C (1) -B (4) | 112.2 (3) |
| B (6) -C (1) -B (4) | 111.9 (3) |
| B (5) -C (1) -B (4) | 61.1 (3) |
| B (3) -C (1) -Si | 120.4 (3) |
| B (2) -C (1) -Si | 118.0 (3) |
| B (6) -C (1) -Si | 116.7 (3) |
| B (5) -C (1) -Si | 119.8 (3) |
| B (4) -C (1) -Si | 121.5 (3) |
| C (1) -B (2) -B (7) | 105.0 (4) |
| C (1) -B (2) -B (11) | 106.1 (3) |
| B (7) -B (2) -B (11) | 60.3 (3) |
| C (1) -B (2) -B (3) | 58.3 (3) |
| B (7) -B (2) -B (3) | 60.7 (3) |
| B (11) -B (2) -B (3) | 109.4 (4) |
| C (1) -B (2) -B (6) | 58.9 (3) |
| B (7) -B (2) -B (6) | 106.9 (3) |
| B (11) -B (2) -B (6) | 59.7 (3) |
| B (3) -B (2) -B (6) | 107.3 (4) |
| C (1) -B (3) -B (4) | 59.9 (3) |
| C (1) -B (3) -B (8) | 106.3 (3) |
| B (4) -B (3) -B (8) | 59.4 (3) |
| C (1) -B (3) -B (2) | 59.3 (3) |
| B (4) -B (3) -B (2) | 108.4 (3) |
| B (8) -B (3) -B (2) | 108.1 (3) |
| C (1) -B (3) -B (7) | 104.4 (3) |
| B (4) -B (3) -B (7) | 106.5 (3) |
| B (8) -B (3) -B (7) | 60.0 (3) |

| | |
|-----------------------|-----------|
| B (2) -B (3) -B (7) | 58.8 (3) |
| C (1) -B (4) -B (8) | 106.3 (4) |
| C (1) -B (4) -B (3) | 58.6 (3) |
| B (8) -B (4) -B (3) | 60.8 (3) |
| C (1) -B (4) -B (5) | 59.4 (3) |
| B (8) -B (4) -B (5) | 108.2 (4) |
| B (3) -B (4) -B (5) | 107.8 (4) |
| C (1) -B (4) -B (9) | 106.4 (3) |
| B (8) -B (4) -B (9) | 60.4 (3) |
| B (3) -B (4) -B (9) | 108.8 (4) |
| B (5) -B (4) -B (9) | 59.8 (3) |
| C (1) -B (5) -B (10) | 106.7 (3) |
| C (1) -B (5) -B (6) | 59.3 (3) |
| B (10) -B (5) -B (6) | 60.6 (3) |
| C (1) -B (5) -B (9) | 106.8 (3) |
| B (10) -B (5) -B (9) | 60.9 (3) |
| B (6) -B (5) -B (9) | 109.6 (4) |
| C (1) -B (5) -B (4) | 59.5 (3) |
| B (10) -B (5) -B (4) | 109.3 (4) |
| B (6) -B (5) -B (4) | 109.0 (3) |
| B (9) -B (5) -B (4) | 60.3 (3) |
| C (1) -B (6) -B (5) | 59.6 (3) |
| C (1) -B (6) -B (11) | 106.2 (4) |
| B (5) -B (6) -B (11) | 107.9 (4) |
| C (1) -B (6) -B (10) | 106.1 (3) |
| B (5) -B (6) -B (10) | 59.6 (3) |
| B (11) -B (6) -B (10) | 60.2 (3) |
| C (1) -B (6) -B (2) | 58.9 (3) |
| B (5) -B (6) -B (2) | 107.5 (4) |
| B (11) -B (6) -B (2) | 59.9 (3) |
| B (10) -B (6) -B (2) | 107.6 (4) |
| B (12) -B (7) -B (2) | 109.2 (4) |
| B (12) -B (7) -B (11) | 61.1 (3) |
| B (2) -B (7) -B (11) | 60.6 (3) |
| B (12) -B (7) -B (8) | 61.0 (3) |
| B (2) -B (7) -B (8) | 109.4 (4) |
| B (11) -B (7) -B (8) | 110.8 (4) |
| B (12) -B (7) -B (3) | 108.5 (4) |
| B (2) -B (7) -B (3) | 60.5 (3) |
| B (11) -B (7) -B (3) | 109.5 (4) |
| B (8) -B (7) -B (3) | 59.8 (3) |
| B (12) -B (7) -Rh | 68.8 (2) |
| B (2) -B (7) -Rh | 150.3 (4) |
| B (11) -B (7) -Rh | 96.1 (3) |
| | |
| B (8) -B (7) -Rh | 95.6 (3) |
| B (3) -B (7) -Rh | 149.2 (4) |
| B (12) -B (7) -H (7) | 117 (3) |
| B (2) -B (7) -H (7) | 123 (3) |
| B (11) -B (7) -H (7) | 117 (3) |
| B (8) -B (7) -H (7) | 121 (3) |
| B (3) -B (7) -H (7) | 126 (3) |
| Rh-B (7) -H (7) | 48 (3) |
| B (4) -B (8) -B (9) | 60.3 (3) |
| B (4) -B (8) -B (12) | 106.5 (3) |
| B (9) -B (8) -B (12) | 59.3 (3) |
| B (4) -B (8) -B (3) | 59.8 (3) |

| | |
|-------------------|-----------|
| B(9)-B(8)-B(3) | 108.0(4) |
| B(12)-B(8)-B(3) | 106.1(4) |
| B(4)-B(8)-B(7) | 106.9(4) |
| B(9)-B(8)-B(7) | 106.0(3) |
| B(12)-B(8)-B(7) | 57.7(3) |
| B(3)-B(8)-B(7) | 60.2(3) |
| B(12)-B(9)-B(5) | 105.9(3) |
| B(12)-B(9)-B(4) | 106.6(3) |
| B(5)-B(9)-B(4) | 59.8(3) |
| B(12)-B(9)-B(8) | 60.4(3) |
| B(5)-B(9)-B(8) | 107.3(3) |
| B(4)-B(9)-B(8) | 59.3(3) |
| B(12)-B(9)-B(10) | 59.4(3) |
| B(5)-B(9)-B(10) | 59.4(3) |
| B(4)-B(9)-B(10) | 107.6(3) |
| B(8)-B(9)-B(10) | 108.6(4) |
| B(12)-B(10)-B(5) | 106.2(3) |
| B(12)-B(10)-B(6) | 106.8(3) |
| B(5)-B(10)-B(6) | 59.8(3) |
| B(12)-B(10)-B(11) | 60.2(3) |
| B(5)-B(10)-B(11) | 107.8(3) |
| B(6)-B(10)-B(11) | 59.9(3) |
| B(12)-B(10)-B(9) | 59.5(3) |
| B(5)-B(10)-B(9) | 59.7(3) |
| B(6)-B(10)-B(9) | 108.0(3) |
| B(11)-B(10)-B(9) | 108.8(3) |
| B(7)-B(11)-B(12) | 57.9(3) |
| B(7)-B(11)-B(6) | 106.5(4) |
| B(12)-B(11)-B(6) | 106.1(4) |
| B(7)-B(11)-B(2) | 59.1(3) |
| B(12)-B(11)-B(2) | 105.4(4) |
| B(6)-B(11)-B(2) | 60.4(3) |
| B(7)-B(11)-B(10) | 105.8(4) |
| B(12)-B(11)-B(10) | 59.2(3) |
| B(6)-B(11)-B(10) | 59.9(3) |
| B(2)-B(11)-B(10) | 107.8(4) |
| B(7)-B(12)-B(10) | 109.5(3) |
| B(7)-B(12)-B(9) | 109.7(3) |
| B(10)-B(12)-B(9) | 61.1(3) |
| B(7)-B(12)-B(11) | 61.0(3) |
| B(10)-B(12)-B(11) | 60.6(3) |
| B(9)-B(12)-B(11) | 110.4(4) |
| B(7)-B(12)-B(8) | 61.3(3) |
| B(10)-B(12)-B(8) | 109.8(4) |
| B(9)-B(12)-B(8) | 60.2(3) |
| B(11)-B(12)-B(8) | 111.0(3) |
| B(7)-B(12)-Rh | 69.0(2) |
| B(10)-B(12)-Rh | 149.9(3) |
| B(9)-B(12)-Rh | 148.9(3) |
| B(11)-B(12)-Rh | 96.1(3) |
| B(8)-B(12)-Rh | 95.9(3) |
| B(7)-B(12)-H(12) | 116.5(19) |
| B(10)-B(12)-H(12) | 121.9(19) |
| B(9)-B(12)-H(12) | 126.1(19) |
| B(11)-B(12)-H(12) | 115(2) |
| B(8)-B(12)-H(12) | 122.4(19) |
| Rh-B(12)-H(12) | 47.7(18) |

| | |
|-----------------|----------|
| C(5)-Si-C(8) | 107.7(3) |
| C(5)-Si-C(2) | 113.7(3) |
| C(8)-Si-C(2) | 104.0(2) |
| C(5)-Si-C(1) | 106.4(2) |
| C(8)-Si-C(1) | 113.1(2) |
| C(2)-Si-C(1) | 112.1(2) |
| C(4)-C(2)-C(3) | 108.7(5) |
| C(4)-C(2)-Si | 121.7(4) |
| C(3)-C(2)-Si | 109.8(5) |
| C(7)-C(5)-C(6) | 108.7(5) |
| C(7)-C(5)-Si | 115.8(4) |
| C(6)-C(5)-Si | 113.4(5) |
| C(9)-C(8)-C(10) | 109.7(5) |
| C(9)-C(8)-Si | 116.2(4) |
| C(10)-C(8)-Si | 116.8(4) |

Table 7. Bond lengths [Å] for **10**.

| | |
|-------------|-----------|
| Rh-P(2) | 2.2129(9) |
| Rh-P(1) | 2.2457(8) |
| Rh-B(7) | 2.401(4) |
| Rh-B(8) | 2.405(4) |
| Rh-H(7) | 1.93(3) |
| Rh-H(8) | 1.93(3) |
| P(1)-C(17) | 1.822(3) |
| P(1)-C(11) | 1.825(3) |
| P(1)-C(23) | 1.832(3) |
| P(2)-C(35) | 1.824(3) |
| P(2)-C(41) | 1.825(3) |
| P(2)-C(29) | 1.834(3) |
| C(11)-C(12) | 1.397(5) |
| C(11)-C(16) | 1.400(5) |
| C(12)-C(13) | 1.404(5) |
| C(13)-C(14) | 1.370(7) |
| C(14)-C(15) | 1.372(6) |
| C(15)-C(16) | 1.382(5) |
| C(17)-C(18) | 1.401(4) |
| C(17)-C(22) | 1.403(5) |
| C(18)-C(19) | 1.388(5) |
| C(19)-C(20) | 1.372(5) |
| C(20)-C(21) | 1.378(5) |
| C(21)-C(22) | 1.385(5) |
| C(23)-C(24) | 1.398(4) |
| C(23)-C(28) | 1.402(5) |
| C(24)-C(25) | 1.388(5) |
| C(25)-C(26) | 1.378(6) |
| C(26)-C(27) | 1.376(6) |
| C(27)-C(28) | 1.383(5) |
| C(29)-C(34) | 1.389(5) |
| C(29)-C(30) | 1.410(5) |
| C(30)-C(31) | 1.388(5) |
| C(31)-C(32) | 1.387(7) |
| C(32)-C(33) | 1.377(7) |
| C(33)-C(34) | 1.400(6) |
| C(35)-C(36) | 1.393(5) |
| C(35)-C(40) | 1.399(5) |
| C(36)-C(37) | 1.386(5) |
| C(37)-C(38) | 1.378(6) |
| C(38)-C(39) | 1.380(6) |
| C(39)-C(40) | 1.391(5) |
| C(41)-C(42) | 1.390(5) |
| C(41)-C(46) | 1.403(5) |
| C(42)-C(43) | 1.407(6) |
| C(43)-C(44) | 1.370(7) |
| C(44)-C(45) | 1.370(7) |
| C(45)-C(46) | 1.377(5) |
| C(1)-C(2) | 1.518(5) |
| C(1)-B(6) | 1.693(6) |
| C(1)-B(3) | 1.702(5) |
| C(1)-B(5) | 1.705(5) |
| C(1)-B(2) | 1.723(6) |
| C(1)-B(4) | 1.728(5) |

| | |
|-------------|----------|
| B(2)-B(3) | 1.757(6) |
| B(2)-B(6) | 1.759(6) |
| B(2)-B(7) | 1.766(5) |
| B(2)-B(11) | 1.805(6) |
| B(3)-B(7) | 1.777(6) |
| B(3)-B(4) | 1.778(6) |
| B(3)-B(8) | 1.779(5) |
| B(4)-B(5) | 1.756(6) |
| B(4)-B(8) | 1.769(6) |
| B(4)-B(9) | 1.785(6) |
| B(5)-B(10) | 1.754(7) |
| B(5)-B(6) | 1.767(7) |
| B(5)-B(9) | 1.783(6) |
| B(6)-B(10) | 1.755(6) |
| B(6)-B(11) | 1.779(7) |
| B(7)-B(8) | 1.732(6) |
| B(7)-H(7) | 1.08(3) |
| B(8)-H(8) | 1.15(3) |
| B(7)-B(11) | 1.787(5) |
| B(7)-B(12) | 1.792(5) |
| B(8)-B(12) | 1.783(6) |
| B(8)-B(9) | 1.786(5) |
| B(9)-C(3) | 1.596(5) |
| B(9)-B(10) | 1.794(6) |
| B(9)-B(12) | 1.804(7) |
| C(3)-C(4) | 1.512(5) |
| B(10)-B(12) | 1.774(6) |
| B(10)-B(11) | 1.796(7) |
| B(11)-C(5) | 1.590(6) |
| B(11)-B(12) | 1.813(6) |
| C(5)-C(6) | 1.505(6) |
| B(12)-C(7) | 1.597(5) |
| C(7)-C(8) | 1.481(6) |

Table 8. Bond angles [deg] for **10**.

| | |
|-------------------|------------|
| P(2)-Rh-P(1) | 95.77(3) |
| P(2)-Rh-B(7) | 111.71(10) |
| P(1)-Rh-B(7) | 152.43(10) |
| P(2)-Rh-B(8) | 153.47(9) |
| P(1)-Rh-B(8) | 110.20(10) |
| B(7)-Rh-B(8) | 42.24(14) |
| P(2)-Rh-H(7) | 86.7(10) |
| P(1)-Rh-H(7) | 174.7(8) |
| B(7)-Rh-H(7) | 25.9(10) |
| B(8)-Rh-H(7) | 67.9(10) |
| P(2)-Rh-H(8) | 178.0(8) |
| P(1)-Rh-H(8) | 82.9(9) |
| B(7)-Rh-H(8) | 69.7(9) |
| B(8)-Rh-H(8) | 28.1(8) |
| H(7)-Rh-H(8) | 94.5(13) |
| C(17)-P(1)-C(11) | 104.90(15) |
| C(17)-P(1)-C(23) | 100.16(15) |
| C(11)-P(1)-C(23) | 102.81(14) |
| C(17)-P(1)-Rh | 115.69(10) |
| C(11)-P(1)-Rh | 104.50(10) |
| C(23)-P(1)-Rh | 126.47(11) |
| C(35)-P(2)-C(41) | 110.38(16) |
| C(35)-P(2)-C(29) | 98.12(15) |
| C(41)-P(2)-C(29) | 103.07(16) |
| C(35)-P(2)-Rh | 116.58(11) |
| C(41)-P(2)-Rh | 112.29(11) |
| C(29)-P(2)-Rh | 114.82(12) |
| C(12)-C(11)-C(16) | 118.9(3) |
| C(12)-C(11)-P(1) | 123.7(3) |
| C(16)-C(11)-P(1) | 117.4(3) |
| C(11)-C(12)-C(13) | 119.4(4) |
| C(14)-C(13)-C(12) | 120.4(4) |
| C(13)-C(14)-C(15) | 120.6(4) |
| C(14)-C(15)-C(16) | 120.1(4) |
| C(15)-C(16)-C(11) | 120.6(4) |
| C(18)-C(17)-C(22) | 118.3(3) |
| C(18)-C(17)-P(1) | 120.6(3) |
| C(22)-C(17)-P(1) | 121.0(2) |
| C(19)-C(18)-C(17) | 120.6(3) |
| C(20)-C(19)-C(18) | 120.1(3) |
| C(19)-C(20)-C(21) | 120.3(4) |
| C(20)-C(21)-C(22) | 120.5(3) |
| C(21)-C(22)-C(17) | 120.2(3) |
| C(24)-C(23)-C(28) | 118.0(3) |
| C(24)-C(23)-P(1) | 119.0(2) |
| C(28)-C(23)-P(1) | 123.0(2) |
| C(25)-C(24)-C(23) | 120.7(3) |
| C(26)-C(25)-C(24) | 120.2(3) |
| C(27)-C(26)-C(25) | 119.8(3) |
| C(26)-C(27)-C(28) | 120.7(4) |
| C(27)-C(28)-C(23) | 120.5(3) |
| C(34)-C(29)-C(30) | 118.7(3) |
| C(34)-C(29)-P(2) | 124.0(3) |
| C(30)-C(29)-P(2) | 117.2(3) |

| | |
|------------------------|-----------|
| C (31) -C (30) -C (29) | 120.3 (4) |
| C (32) -C (31) -C (30) | 119.8 (4) |
| C (33) -C (32) -C (31) | 121.0 (4) |
| C (32) -C (33) -C (34) | 119.3 (5) |
| C (29) -C (34) -C (33) | 120.9 (4) |
| C (36) -C (35) -C (40) | 118.9 (3) |
| C (36) -C (35) -P (2) | 118.3 (3) |
| C (40) -C (35) -P (2) | 122.5 (3) |
| C (37) -C (36) -C (35) | 120.3 (3) |
| C (38) -C (37) -C (36) | 120.3 (4) |
| C (37) -C (38) -C (39) | 120.2 (3) |
| C (38) -C (39) -C (40) | 120.1 (4) |
| C (39) -C (40) -C (35) | 120.1 (4) |
| | |
| C (42) -C (41) -C (46) | 118.7 (3) |
| C (42) -C (41) -P (2) | 125.6 (3) |
| C (46) -C (41) -P (2) | 115.6 (3) |
| C (41) -C (42) -C (43) | 119.3 (4) |
| C (44) -C (43) -C (42) | 120.4 (4) |
| C (45) -C (44) -C (43) | 120.8 (4) |
| C (44) -C (45) -C (46) | 119.6 (4) |
| C (45) -C (46) -C (41) | 121.2 (4) |
| C (2) -C (1) -B (6) | 119.0 (3) |
| C (2) -C (1) -B (3) | 118.3 (3) |
| B (6) -C (1) -B (3) | 112.7 (3) |
| C (2) -C (1) -B (5) | 119.0 (3) |
| B (6) -C (1) -B (5) | 62.7 (3) |
| B (3) -C (1) -B (5) | 113.1 (3) |
| C (2) -C (1) -B (2) | 118.3 (3) |
| B (6) -C (1) -B (2) | 62.0 (3) |
| B (3) -C (1) -B (2) | 61.7 (2) |
| B (5) -C (1) -B (2) | 113.6 (3) |
| C (2) -C (1) -B (4) | 118.9 (3) |
| B (6) -C (1) -B (4) | 112.9 (3) |
| B (3) -C (1) -B (4) | 62.4 (2) |
| B (5) -C (1) -B (4) | 61.5 (2) |
| B (2) -C (1) -B (4) | 113.1 (3) |
| C (1) -B (2) -B (3) | 58.6 (2) |
| C (1) -B (2) -B (6) | 58.2 (2) |
| B (3) -B (2) -B (6) | 107.0 (3) |
| C (1) -B (2) -B (7) | 104.7 (3) |
| B (3) -B (2) -B (7) | 60.6 (2) |
| B (6) -B (2) -B (7) | 106.4 (3) |
| C (1) -B (2) -B (11) | 105.7 (3) |
| B (3) -B (2) -B (11) | 109.4 (3) |
| B (6) -B (2) -B (11) | 59.9 (2) |
| B (7) -B (2) -B (11) | 60.1 (2) |
| C (1) -B (3) -B (2) | 59.7 (2) |
| C (1) -B (3) -B (7) | 105.0 (3) |
| B (2) -B (3) -B (7) | 59.9 (2) |
| C (1) -B (3) -B (4) | 59.5 (2) |
| B (2) -B (3) -B (4) | 109.0 (3) |
| B (7) -B (3) -B (4) | 106.6 (3) |
| C (1) -B (3) -B (8) | 104.9 (3) |
| B (2) -B (3) -B (8) | 107.0 (3) |
| B (7) -B (3) -B (8) | 58.3 (2) |
| B (4) -B (3) -B (8) | 59.6 (2) |

| | |
|-----------------------|------------|
| C (1) -B (4) -B (5) | 58.6 (2) |
| C (1) -B (4) -B (8) | 104.3 (3) |
| B (5) -B (4) -B (8) | 107.1 (3) |
| C (1) -B (4) -B (3) | 58.1 (2) |
| B (5) -B (4) -B (3) | 107.1 (3) |
| B (8) -B (4) -B (3) | 60.2 (2) |
| C (1) -B (4) -B (9) | 106.2 (3) |
| B (5) -B (4) -B (9) | 60.5 (2) |
| B (8) -B (4) -B (9) | 60.3 (2) |
| B (3) -B (4) -B (9) | 109.4 (3) |
| C (1) -B (5) -B (10) | 105.6 (3) |
| C (1) -B (5) -B (4) | 59.9 (2) |
| B (10) -B (5) -B (4) | 108.7 (3) |
| C (1) -B (5) -B (6) | 58.3 (2) |
| B (10) -B (5) -B (6) | 59.8 (3) |
| B (4) -B (5) -B (6) | 108.0 (3) |
| C (1) -B (5) -B (9) | 107.3 (3) |
| B (10) -B (5) -B (9) | 61.0 (3) |
| B (4) -B (5) -B (9) | 60.6 (2) |
| B (6) -B (5) -B (9) | 109.0 (3) |
| C (1) -B (6) -B (10) | 106.1 (3) |
| C (1) -B (6) -B (2) | 59.9 (2) |
| B (10) -B (6) -B (2) | 109.4 (3) |
| C (1) -B (6) -B (5) | 59.0 (2) |
| B (10) -B (6) -B (5) | 59.7 (3) |
| B (2) -B (6) -B (5) | 108.8 (3) |
| C (1) -B (6) -B (11) | 108.1 (3) |
| B (10) -B (6) -B (11) | 61.1 (3) |
| B (2) -B (6) -B (11) | 61.3 (2) |
| B (5) -B (6) -B (11) | 109.6 (3) |
| B (8) -B (7) -B (2) | 108.8 (3) |
| B (8) -B (7) -B (3) | 60.9 (2) |
| B (2) -B (7) -B (3) | 59.4 (2) |
| B (8) -B (7) -B (11) | 109.8 (3) |
| B (2) -B (7) -B (11) | 61.0 (2) |
| B (3) -B (7) -B (11) | 109.3 (3) |
| B (8) -B (7) -B (12) | 60.8 (2) |
| B (2) -B (7) -B (12) | 109.7 (3) |
| B (3) -B (7) -B (12) | 109.9 (3) |
| B (11) -B (7) -B (12) | 60.9 (2) |
| B (8) -B (7) -Rh | 69.02 (18) |
| B (2) -B (7) -Rh | 135.0 (2) |
| B (3) -B (7) -Rh | 84.50 (19) |
| B (11) -B (7) -Rh | 163.9 (2) |
| B (12) -B (7) -Rh | 107.3 (2) |
| B (7) -B (8) -B (4) | 109.1 (3) |
| B (7) -B (8) -B (3) | 60.8 (2) |
| B (4) -B (8) -B (3) | 60.1 (2) |
| B (7) -B (8) -B (12) | 61.3 (2) |
| B (4) -B (8) -B (12) | 109.2 (3) |
| B (3) -B (8) -B (12) | 110.2 (3) |
| B (7) -B (8) -B (9) | 110.0 (3) |
| B (4) -B (8) -B (9) | 60.3 (2) |
| B (3) -B (8) -B (9) | 109.3 (3) |
| B (12) -B (8) -B (9) | 60.7 (2) |
| B (7) -B (8) -Rh | 68.74 (19) |
| B (4) -B (8) -Rh | 135.7 (2) |

| | |
|------------------------|------------|
| B (3) -B (8) -Rh | 84.32 (19) |
| B (12) -B (8) -Rh | 107.4 (2) |
| B (9) -B (8) -Rh | 164.0 (3) |
| C (3) -B (9) -B (5) | 123.4 (3) |
| C (3) -B (9) -B (4) | 123.4 (4) |
| B (5) -B (9) -B (4) | 59.0 (2) |
| C (3) -B (9) -B (8) | 123.9 (3) |
| B (5) -B (9) -B (8) | 105.2 (3) |
| B (4) -B (9) -B (8) | 59.4 (2) |
| C (3) -B (9) -B (10) | 122.7 (3) |
| B (5) -B (9) -B (10) | 58.7 (3) |
| B (4) -B (9) -B (10) | 105.7 (3) |
| B (8) -B (9) -B (10) | 105.0 (3) |
| C (3) -B (9) -B (12) | 121.2 (3) |
| B (5) -B (9) -B (12) | 106.4 (3) |
| B (4) -B (9) -B (12) | 107.6 (3) |
| B (8) -B (9) -B (12) | 59.6 (2) |
| B (10) -B (9) -B (12) | 59.1 (3) |
| C (4) -C (3) -B (9) | 114.8 (3) |
| B (5) -B (10) -B (6) | 60.5 (3) |
| B (5) -B (10) -B (12) | 109.0 (3) |
| B (6) -B (10) -B (12) | 108.7 (3) |
| B (5) -B (10) -B (9) | 60.3 (2) |
| B (6) -B (10) -B (9) | 109.0 (3) |
| B (12) -B (10) -B (9) | 60.7 (2) |
| B (5) -B (10) -B (11) | 109.5 (3) |
| B (6) -B (10) -B (11) | 60.1 (2) |
| B (12) -B (10) -B (11) | 61.0 (2) |
| B (9) -B (10) -B (11) | 110.3 (3) |
| C (5) -B (11) -B (6) | 121.0 (3) |
| C (5) -B (11) -B (7) | 125.6 (4) |
| B (6) -B (11) -B (7) | 104.7 (3) |
| C (5) -B (11) -B (10) | 122.7 (3) |
| B (6) -B (11) -B (10) | 58.8 (2) |
| B (7) -B (11) -B (10) | 105.0 (3) |
| C (5) -B (11) -B (2) | 121.8 (3) |
| B (6) -B (11) -B (2) | 58.8 (2) |
| B (7) -B (11) -B (2) | 58.9 (2) |
| B (10) -B (11) -B (2) | 105.6 (3) |
| C (5) -B (11) -B (12) | 124.2 (3) |
| B (6) -B (11) -B (12) | 105.9 (3) |
| B (7) -B (11) -B (12) | 59.7 (2) |
| B (10) -B (11) -B (12) | 58.9 (2) |
| B (2) -B (11) -B (12) | 107.0 (3) |
| C (6) -C (5) -B (11) | 115.3 (3) |
| C (7) -B (12) -B (10) | 121.1 (3) |
| C (7) -B (12) -B (8) | 123.4 (3) |
| B (10) -B (12) -B (8) | 105.9 (3) |
| C (7) -B (12) -B (7) | 126.1 (4) |
| B (10) -B (12) -B (7) | 105.7 (3) |
| B (8) -B (12) -B (7) | 57.9 (2) |
| C (7) -B (12) -B (9) | 118.6 (3) |
| B (10) -B (12) -B (9) | 60.2 (3) |
| B (8) -B (12) -B (9) | 59.7 (2) |
| B (7) -B (12) -B (9) | 106.5 (3) |
| C (7) -B (12) -B (11) | 123.1 (3) |
| B (10) -B (12) -B (11) | 60.1 (2) |

| | |
|-----------------------|------------|
| B (8) -B (12) -B (11) | 106.3 (3) |
| B (7) -B (12) -B (11) | 59.4 (2) |
| B (9) -B (12) -B (11) | 109.0 (3) |
| C (8) -C (7) -B (12) | 117.4 (3) |
| B (8) -B (7) -H (7) | 119.9 (16) |
| B (2) -B (7) -H (7) | 118.5 (16) |
| B (3) -B (7) -H (7) | 115.6 (16) |
| B (11) -B (7) -H (7) | 124.3 (17) |
| B (12) -B (7) -H (7) | 125.4 (16) |
| Rh-B (7) -H (7) | 51.6 (16) |
| B (7) -B (8) -H (8) | 119.1 (15) |
| B (4) -B (8) -H (8) | 122.1 (16) |
| B (3) -B (8) -H (8) | 119.5 (14) |
| B (12) -B (8) -H (8) | 120.8 (15) |
| B (9) -B (8) -H (8) | 122.5 (14) |
| Rh-B (8) -H (8) | 52.2 (15) |

Table 9. Bond lengths [Å] for **13**.

| | |
|-------------|------------|
| Rh-C(3) | 2.246(4) |
| Rh-C(4) | 2.249(5) |
| Rh-C(8) | 2.252(4) |
| Rh-C(5) | 2.273(4) |
| Rh-C(7) | 2.274(5) |
| Rh-C(6) | 2.287(4) |
| Rh-P(1) | 2.3770(11) |
| Rh-P(2) | 2.3864(11) |
| P(1)-C(21) | 1.829(5) |
| P(1)-C(31) | 1.830(5) |
| P(1)-C(11) | 1.833(5) |
| P(2)-C(41) | 1.830(4) |
| P(2)-C(61) | 1.831(4) |
| P(2)-C(51) | 1.841(4) |
| C(3)-C(4) | 1.375(7) |
| C(5)-C(6) | 1.362(7) |
| C(7)-C(8) | 1.375(7) |
| C(11)-C(12) | 1.395(7) |
| C(11)-C(16) | 1.397(7) |
| C(12)-C(13) | 1.375(7) |
| C(13)-C(14) | 1.381(8) |
| C(14)-C(15) | 1.373(8) |
| C(15)-C(16) | 1.385(7) |
| C(21)-C(22) | 1.397(6) |
| C(21)-C(26) | 1.410(7) |
| C(22)-C(23) | 1.383(7) |
| C(23)-C(24) | 1.376(8) |
| C(24)-C(25) | 1.389(7) |
| C(25)-C(26) | 1.375(7) |
| C(31)-C(32) | 1.386(7) |
| C(31)-C(36) | 1.408(7) |
| C(32)-C(33) | 1.391(7) |
| C(33)-C(34) | 1.385(8) |
| C(34)-C(35) | 1.377(8) |
| C(35)-C(36) | 1.373(7) |
| C(41)-C(46) | 1.403(6) |
| C(41)-C(42) | 1.406(6) |
| C(42)-C(43) | 1.384(7) |
| C(43)-C(44) | 1.375(7) |
| C(44)-C(45) | 1.387(7) |
| C(45)-C(46) | 1.380(7) |
| C(51)-C(56) | 1.393(6) |
| C(51)-C(52) | 1.400(6) |
| C(52)-C(53) | 1.377(6) |
| C(53)-C(54) | 1.375(8) |
| C(54)-C(55) | 1.378(7) |
| C(55)-C(56) | 1.388(7) |
| C(61)-C(62) | 1.404(6) |
| C(61)-C(66) | 1.405(6) |
| C(62)-C(63) | 1.374(7) |
| C(63)-C(64) | 1.383(7) |
| C(64)-C(65) | 1.382(7) |
| C(65)-C(66) | 1.382(6) |
| C(1)-B(3) | 1.692(7) |

| | |
|------------------|------------|
| C (1) -B (5) | 1.693 (8) |
| C (1) -B (2) | 1.705 (8) |
| C (1) -B (4) | 1.705 (7) |
| C (1) -B (6) | 1.708 (7) |
| B (2) -B (7) | 1.765 (7) |
| B (2) -B (8) | 1.768 (7) |
| B (2) -B (3) | 1.782 (8) |
| B (2) -B (6) | 1.783 (8) |
| B (3) -B (9) | 1.777 (7) |
| B (3) -B (4) | 1.779 (9) |
| B (3) -B (8) | 1.781 (8) |
| B (4) -B (10) | 1.774 (8) |
| B (4) -B (5) | 1.781 (8) |
| B (4) -B (9) | 1.792 (8) |
| B (5) -B (11) | 1.780 (7) |
| B (5) -B (10) | 1.780 (7) |
| B (5) -B (6) | 1.783 (8) |
| B (6) -B (7) | 1.770 (8) |
| B (6) -B (11) | 1.778 (7) |
| B (7) -B (8) | 1.772 (7) |
| B (7) -B (12) | 1.789 (7) |
| B (7) -B (11) | 1.799 (7) |
| B (7) -Br (7) | 1.955 (5) |
| B (8) -B (9) | 1.777 (7) |
| B (8) -B (12) | 1.787 (7) |
| B (8) -Br (8) | 1.949 (5) |
| B (9) -B (12) | 1.779 (7) |
| B (9) -B (10) | 1.783 (8) |
| B (9) -Br (9) | 1.945 (5) |
| B (10) -B (12) | 1.785 (7) |
| B (10) -B (11) | 1.793 (7) |
| B (10) -Br (10) | 1.951 (5) |
| B (11) -B (12) | 1.787 (7) |
| B (11) -Br (11) | 1.947 (5) |
| B (12) -Br (12) | 1.948 (5) |
| C (81) -Cl (1) | 1.740 (7) |
| C (81) -Cl (2A) | 1.776 (8) |
| C (82) -Cl (4B) | 1.695 (17) |
| C (82) -Cl (3) | 1.739 (9) |
| C (82) -Cl (4) | 1.768 (13) |
| C (83) -Cl (6B) | 1.612 (10) |
| C (83) -Cl (5) | 1.755 (10) |
| C (83) -Cl (6A) | 1.831 (11) |
| C (84A) -Cl (8A) | 1.582 (16) |
| C (84A) -Cl (7A) | 1.628 (15) |
| C (85) -Cl (10) | 1.53 (2) |
| C (85) -Cl (9A) | 1.68 (2) |
| C (85) -Cl (9B) | 1.99 (4) |
| C (86) -Cl (11) | 1.69 (3) |
| C (86) -Cl (12) | 1.69 (3) |

Table 10. Bond angles [deg] for **13**.

| | |
|------------------------|------------|
| C (3) -Rh-C (4) | 35.63(18) |
| C (3) -Rh-C (8) | 87.79(18) |
| C (4) -Rh-C (8) | 120.69(18) |
| C (3) -Rh-C (5) | 119.27(19) |
| C (4) -Rh-C (5) | 86.21(19) |
| C (8) -Rh-C (5) | 152.82(19) |
| C (3) -Rh-C (7) | 120.03(18) |
| C (4) -Rh-C (7) | 155.26(19) |
| C (8) -Rh-C (7) | 35.37(17) |
| C (5) -Rh-C (7) | 118.26(18) |
| C (3) -Rh-C (6) | 153.21(18) |
| C (4) -Rh-C (6) | 117.99(18) |
| C (8) -Rh-C (6) | 118.65(17) |
| C (5) -Rh-C (6) | 34.76(18) |
| C (7) -Rh-C (6) | 86.62(18) |
| C (3) -Rh-P (1) | 84.57(13) |
| C (4) -Rh-P (1) | 94.99(13) |
| C (8) -Rh-P (1) | 94.80(12) |
| C (5) -Rh-P (1) | 85.86(13) |
| C (7) -Rh-P (1) | 83.97(12) |
| C (6) -Rh-P (1) | 96.55(12) |
| C (3) -Rh-P (2) | 93.76(13) |
| C (4) -Rh-P (2) | 84.11(13) |
| C (8) -Rh-P (2) | 84.28(12) |
| C (5) -Rh-P (2) | 95.70(13) |
| C (7) -Rh-P (2) | 96.16(12) |
| C (6) -Rh-P (2) | 85.32(12) |
| P (1) -Rh-P (2) | 178.13(4) |
| C (21) -P (1) -C (31) | 102.8(2) |
| C (21) -P (1) -C (11) | 102.9(2) |
| C (31) -P (1) -C (11) | 103.3(2) |
| C (21) -P (1) -Rh | 116.35(14) |
| C (31) -P (1) -Rh | 114.14(14) |
| C (11) -P (1) -Rh | 115.61(15) |
| C (41) -P (2) -C (61) | 103.30(19) |
| C (41) -P (2) -C (51) | 104.6(2) |
| C (61) -P (2) -C (51) | 102.21(19) |
| C (41) -P (2) -Rh | 115.19(14) |
| C (61) -P (2) -Rh | 114.99(14) |
| C (51) -P (2) -Rh | 114.90(14) |
| C (4) -C (3) -Rh | 72.3(3) |
| C (3) -C (4) -Rh | 72.1(3) |
| C (6) -C (5) -Rh | 73.2(3) |
| C (5) -C (6) -Rh | 72.1(3) |
| C (8) -C (7) -Rh | 71.5(3) |
| C (7) -C (8) -Rh | 73.2(3) |
| C (12) -C (11) -C (16) | 118.0(4) |
| C (12) -C (11) -P (1) | 120.2(4) |
| C (16) -C (11) -P (1) | 121.7(4) |
| C (13) -C (12) -C (11) | 120.8(5) |
| C (12) -C (13) -C (14) | 120.4(6) |
| C (15) -C (14) -C (13) | 119.8(5) |
| C (14) -C (15) -C (16) | 120.2(5) |
| C (15) -C (16) -C (11) | 120.7(5) |

| | |
|------------------------|-----------|
| C (22) -C (21) -C (26) | 117.7 (4) |
| C (22) -C (21) -P (1) | 122.2 (4) |
| C (26) -C (21) -P (1) | 120.0 (3) |
| C (23) -C (22) -C (21) | 120.8 (5) |
| C (24) -C (23) -C (22) | 120.2 (5) |
| C (23) -C (24) -C (25) | 120.4 (5) |
| C (26) -C (25) -C (24) | 119.5 (5) |
| C (25) -C (26) -C (21) | 121.2 (4) |
| C (32) -C (31) -C (36) | 117.4 (4) |
| C (32) -C (31) -P (1) | 122.5 (4) |
| C (36) -C (31) -P (1) | 120.1 (4) |
| C (31) -C (32) -C (33) | 121.2 (5) |
| C (34) -C (33) -C (32) | 119.8 (5) |
| C (35) -C (34) -C (33) | 119.9 (5) |
| C (36) -C (35) -C (34) | 120.0 (5) |
| C (35) -C (36) -C (31) | 121.6 (5) |
| C (46) -C (41) -C (42) | 117.7 (4) |
| C (46) -C (41) -P (2) | 120.7 (3) |
| C (42) -C (41) -P (2) | 121.6 (3) |
| C (43) -C (42) -C (41) | 120.8 (4) |
| C (44) -C (43) -C (42) | 120.3 (4) |
| C (43) -C (44) -C (45) | 120.1 (4) |
| C (46) -C (45) -C (44) | 120.1 (5) |
| C (45) -C (46) -C (41) | 121.0 (4) |
| C (56) -C (51) -C (52) | 118.8 (4) |
| C (56) -C (51) -P (2) | 121.9 (3) |
| C (52) -C (51) -P (2) | 119.2 (3) |
| C (53) -C (52) -C (51) | 120.4 (5) |
| C (54) -C (53) -C (52) | 120.1 (5) |
| C (53) -C (54) -C (55) | 120.4 (5) |
| C (54) -C (55) -C (56) | 120.1 (5) |
| C (55) -C (56) -C (51) | 120.1 (4) |
| C (62) -C (61) -C (66) | 117.8 (4) |
| C (62) -C (61) -P (2) | 120.2 (3) |
| C (66) -C (61) -P (2) | 122.0 (3) |
| C (63) -C (62) -C (61) | 120.8 (4) |
| C (62) -C (63) -C (64) | 120.7 (4) |
| C (65) -C (64) -C (63) | 119.5 (4) |
| C (66) -C (65) -C (64) | 120.5 (4) |
| C (65) -C (66) -C (61) | 120.7 (4) |
| B (3) -C (1) -B (5) | 115.8 (4) |
| B (3) -C (1) -B (2) | 63.3 (3) |
| B (5) -C (1) -B (2) | 115.8 (4) |
| B (3) -C (1) -B (4) | 63.2 (3) |
| B (5) -C (1) -B (4) | 63.2 (3) |
| B (2) -C (1) -B (4) | 116.0 (4) |
| B (3) -C (1) -B (6) | 115.8 (4) |
| B (5) -C (1) -B (6) | 63.2 (3) |
| B (2) -C (1) -B (6) | 63.0 (3) |
| B (4) -C (1) -B (6) | 116.0 (4) |
| C (1) -B (2) -B (7) | 104.1 (4) |
| C (1) -B (2) -B (8) | 104.0 (4) |
| B (7) -B (2) -B (8) | 60.2 (3) |
| C (1) -B (2) -B (3) | 58.0 (3) |
| B (7) -B (2) -B (3) | 108.2 (4) |
| B (8) -B (2) -B (3) | 60.2 (3) |
| C (1) -B (2) -B (6) | 58.6 (3) |

| | |
|-----------------------|-----------|
| B (7) -B (2) -B (6) | 59.9 (3) |
| B (8) -B (2) -B (6) | 108.0 (4) |
| B (3) -B (2) -B (6) | 107.8 (4) |
| C (1) -B (3) -B (9) | 104.5 (4) |
| C (1) -B (3) -B (4) | 58.8 (3) |
| B (9) -B (3) -B (4) | 60.5 (3) |
| C (1) -B (3) -B (8) | 103.9 (4) |
| B (9) -B (3) -B (8) | 59.9 (3) |
| B (4) -B (3) -B (8) | 108.4 (4) |
| C (1) -B (3) -B (2) | 58.7 (3) |
| B (9) -B (3) -B (2) | 107.8 (4) |
| B (4) -B (3) -B (2) | 108.6 (4) |
| B (8) -B (3) -B (2) | 59.5 (3) |
| C (1) -B (4) -B (10) | 103.8 (4) |
| C (1) -B (4) -B (3) | 58.1 (3) |
| B (10) -B (4) -B (3) | 107.8 (4) |
| C (1) -B (4) -B (5) | 58.1 (3) |
| B (10) -B (4) -B (5) | 60.1 (3) |
| B (3) -B (4) -B (5) | 107.3 (4) |
| C (1) -B (4) -B (9) | 103.3 (4) |
| B (10) -B (4) -B (9) | 60.0 (3) |
| B (3) -B (4) -B (9) | 59.7 (3) |
| B (5) -B (4) -B (9) | 107.6 (4) |
| C (1) -B (5) -B (11) | 104.4 (4) |
| C (1) -B (5) -B (10) | 104.0 (4) |
| B (11) -B (5) -B (10) | 60.5 (3) |
| C (1) -B (5) -B (4) | 58.7 (3) |
| B (11) -B (5) -B (4) | 108.6 (4) |
| B (10) -B (5) -B (4) | 59.7 (3) |
| C (1) -B (5) -B (6) | 58.8 (3) |
| B (11) -B (5) -B (6) | 59.8 (3) |
| B (10) -B (5) -B (6) | 108.1 (4) |
| B (4) -B (5) -B (6) | 108.6 (4) |
| C (1) -B (6) -B (7) | 103.7 (4) |
| C (1) -B (6) -B (11) | 103.9 (4) |
| B (7) -B (6) -B (11) | 60.9 (3) |
| C (1) -B (6) -B (5) | 58.0 (3) |
| B (7) -B (6) -B (5) | 108.3 (4) |
| B (11) -B (6) -B (5) | 60.0 (3) |
| C (1) -B (6) -B (2) | 58.4 (3) |
| B (7) -B (6) -B (2) | 59.6 (3) |
| B (11) -B (6) -B (2) | 108.4 (4) |
| B (5) -B (6) -B (2) | 107.7 (4) |
| B (2) -B (7) -B (6) | 60.6 (3) |
| B (2) -B (7) -B (8) | 60.0 (3) |
| B (6) -B (7) -B (8) | 108.4 (4) |
| B (2) -B (7) -B (12) | 108.2 (3) |
| B (6) -B (7) -B (12) | 107.8 (4) |
| B (8) -B (7) -B (12) | 60.2 (3) |
| B (2) -B (7) -B (11) | 108.3 (4) |
| B (6) -B (7) -B (11) | 59.7 (3) |
| B (8) -B (7) -B (11) | 108.1 (3) |
| B (12) -B (7) -B (11) | 59.8 (3) |
| B (2) -B (7) -Br (7) | 121.4 (3) |
| B (6) -B (7) -Br (7) | 121.5 (3) |
| B (8) -B (7) -Br (7) | 121.7 (3) |
| B (12) -B (7) -Br (7) | 121.9 (3) |

| | |
|-------------------------|-----------|
| B (11) -B (7) -Br (7) | 121.7 (3) |
| B (2) -B (8) -B (7) | 59.8 (3) |
| B (2) -B (8) -B (9) | 108.5 (4) |
| B (7) -B (8) -B (9) | 108.4 (4) |
| B (2) -B (8) -B (3) | 60.3 (3) |
| B (7) -B (8) -B (3) | 108.0 (4) |
| B (9) -B (8) -B (3) | 59.9 (3) |
| B (2) -B (8) -B (12) | 108.1 (3) |
| B (7) -B (8) -B (12) | 60.3 (3) |
| B (9) -B (8) -B (12) | 59.9 (3) |
| B (3) -B (8) -B (12) | 107.7 (4) |
| B (2) -B (8) -Br (8) | 121.5 (3) |
| B (7) -B (8) -Br (8) | 121.7 (3) |
| B (9) -B (8) -Br (8) | 121.4 (3) |
| B (3) -B (8) -Br (8) | 121.7 (3) |
| B (12) -B (8) -Br (8) | 121.9 (3) |
| B (3) -B (9) -B (8) | 60.2 (3) |
| B (3) -B (9) -B (12) | 108.2 (3) |
| B (8) -B (9) -B (12) | 60.3 (3) |
| B (3) -B (9) -B (10) | 107.5 (4) |
| B (8) -B (9) -B (10) | 108.2 (3) |
| B (12) -B (9) -B (10) | 60.1 (3) |
| B (3) -B (9) -B (4) | 59.8 (3) |
| B (8) -B (9) -B (4) | 108.1 (4) |
| B (12) -B (9) -B (4) | 107.9 (4) |
| B (10) -B (9) -B (4) | 59.5 (3) |
| B (3) -B (9) -Br (9) | 121.3 (3) |
| B (8) -B (9) -Br (9) | 120.9 (3) |
| B (12) -B (9) -Br (9) | 121.7 (3) |
| B (10) -B (9) -Br (9) | 122.6 (3) |
| B (4) -B (9) -Br (9) | 122.2 (3) |
| B (4) -B (10) -B (5) | 60.2 (3) |
| B (4) -B (10) -B (9) | 60.5 (3) |
| B (5) -B (10) -B (9) | 108.1 (4) |
| B (4) -B (10) -B (12) | 108.4 (4) |
| B (5) -B (10) -B (12) | 107.6 (4) |
| B (9) -B (10) -B (12) | 59.8 (3) |
| B (4) -B (10) -B (11) | 108.4 (4) |
| B (5) -B (10) -B (11) | 59.8 (3) |
| B (9) -B (10) -B (11) | 107.9 (4) |
| B (12) -B (10) -B (11) | 59.9 (3) |
| B (4) -B (10) -Br (10) | 120.9 (3) |
| B (5) -B (10) -Br (10) | 120.8 (4) |
| B (9) -B (10) -Br (10) | 122.6 (3) |
| B (12) -B (10) -Br (10) | 122.7 (3) |
| B (11) -B (10) -Br (10) | 121.3 (3) |
| B (6) -B (11) -B (5) | 60.2 (3) |
| B (6) -B (11) -B (12) | 107.5 (3) |
| B (5) -B (11) -B (12) | 107.5 (3) |
| B (6) -B (11) -B (10) | 107.8 (4) |
| B (5) -B (11) -B (10) | 59.8 (3) |
| B (12) -B (11) -B (10) | 59.8 (3) |
| B (6) -B (11) -B (7) | 59.3 (3) |
| B (5) -B (11) -B (7) | 107.2 (4) |
| B (12) -B (11) -B (7) | 59.8 (3) |
| B (10) -B (11) -B (7) | 107.3 (3) |
| B (6) -B (11) -Br (11) | 121.8 (3) |

| | |
|---------------------------|------------|
| B (5) -B (11) -Br (11) | 121.2 (3) |
| B (12) -B (11) -Br (11) | 122.5 (3) |
| B (10) -B (11) -Br (11) | 121.5 (3) |
| B (7) -B (11) -Br (11) | 123.1 (3) |
| B (9) -B (12) -B (10) | 60.0 (3) |
| B (9) -B (12) -B (8) | 59.8 (3) |
| B (10) -B (12) -B (8) | 107.7 (3) |
| B (9) -B (12) -B (11) | 108.4 (3) |
| B (10) -B (12) -B (11) | 60.3 (3) |
| B (8) -B (12) -B (11) | 108.0 (3) |
| B (9) -B (12) -B (7) | 107.6 (3) |
| B (10) -B (12) -B (7) | 108.1 (3) |
| B (8) -B (12) -B (7) | 59.4 (3) |
| B (11) -B (12) -B (7) | 60.4 (3) |
| B (9) -B (12) -Br (12) | 121.8 (3) |
| B (10) -B (12) -Br (12) | 122.2 (3) |
| B (8) -B (12) -Br (12) | 121.7 (3) |
| B (11) -B (12) -Br (12) | 121.6 (3) |
| B (7) -B (12) -Br (12) | 121.5 (3) |
| C1 (1) -C (81) -C1 (2A) | 111.1 (4) |
| C1 (4B) -C (82) -C1 (3) | 117.3 (7) |
| C1 (4B) -C (82) -C1 (4) | 19.1 (8) |
| C1 (3) -C (82) -C1 (4) | 111.0 (5) |
| C1 (6B) -C (83) -C1 (5) | 107.9 (6) |
| C1 (6B) -C (83) -C1 (6A) | 67.5 (5) |
| C1 (5) -C (83) -C1 (6A) | 115.9 (5) |
| C1 (8A) -C (84A) -C1 (7A) | 132.7 (11) |
| C1 (10) -C (85) -C1 (9A) | 113.5 (15) |
| C1 (10) -C (85) -C1 (9B) | 126.7 (16) |
| C1 (9A) -C (85) -C1 (9B) | 58.1 (14) |
| C1 (11) -C (86) -C1 (12) | 111 (2) |

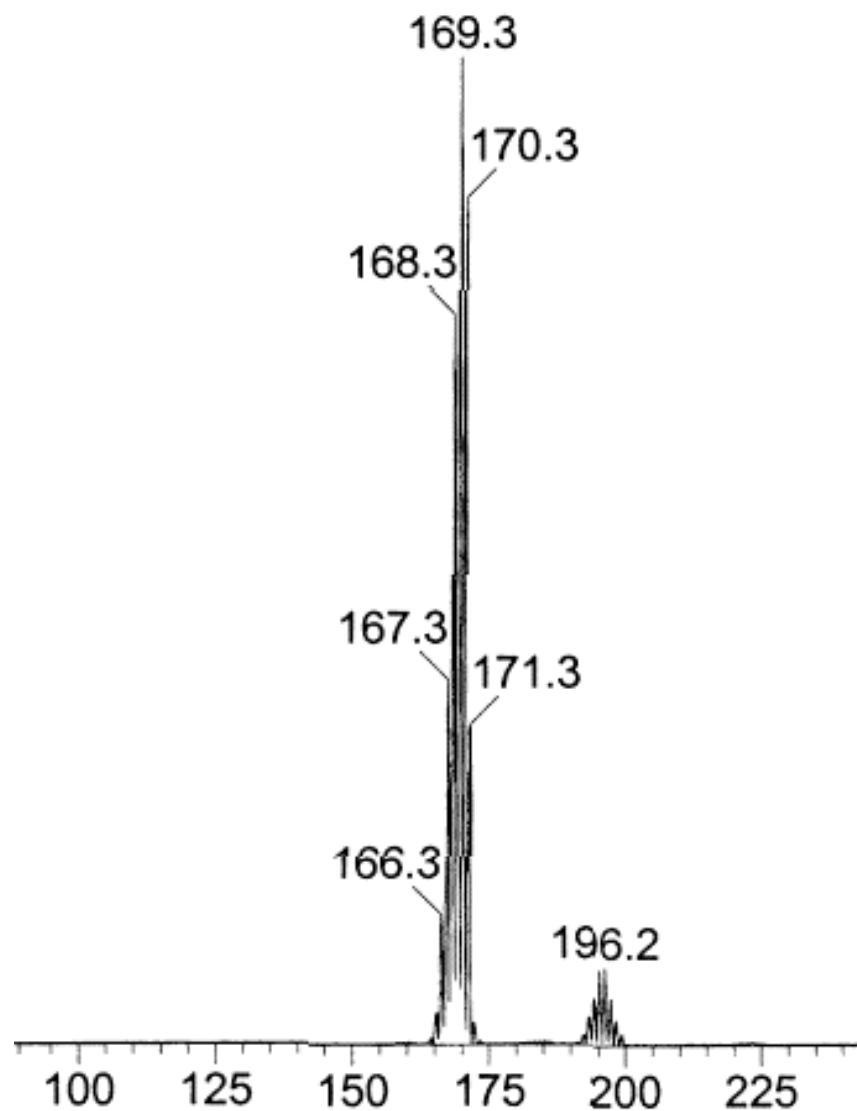


Figure S1. ESI-MS (negative mode) of **2a/b**

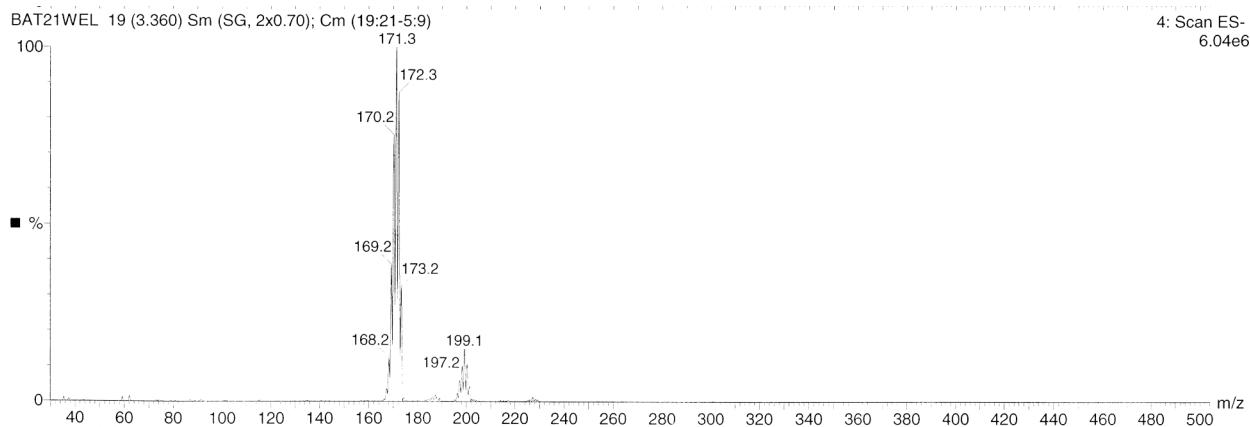


Figure S2. ESI-MS (negative mode) of **4a/b**

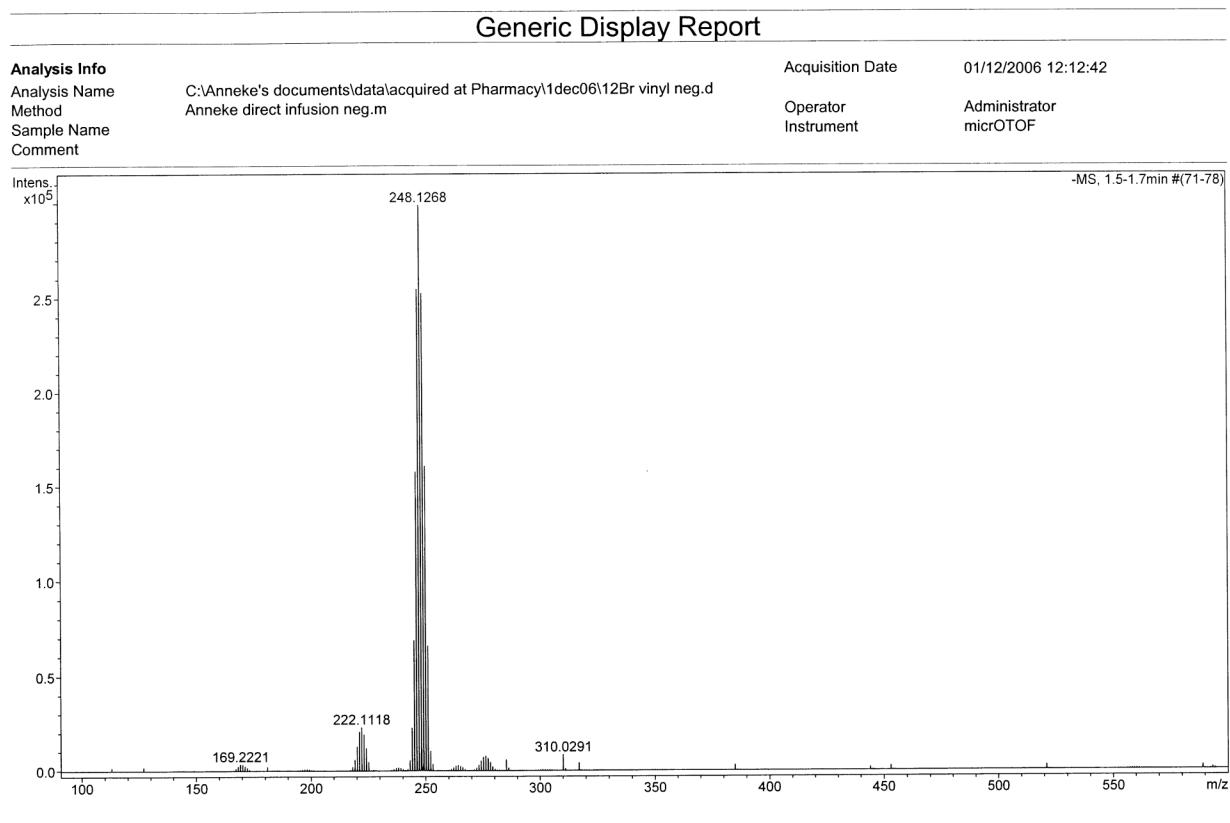


Figure S3. ESI-MS (negative mode) of 6.

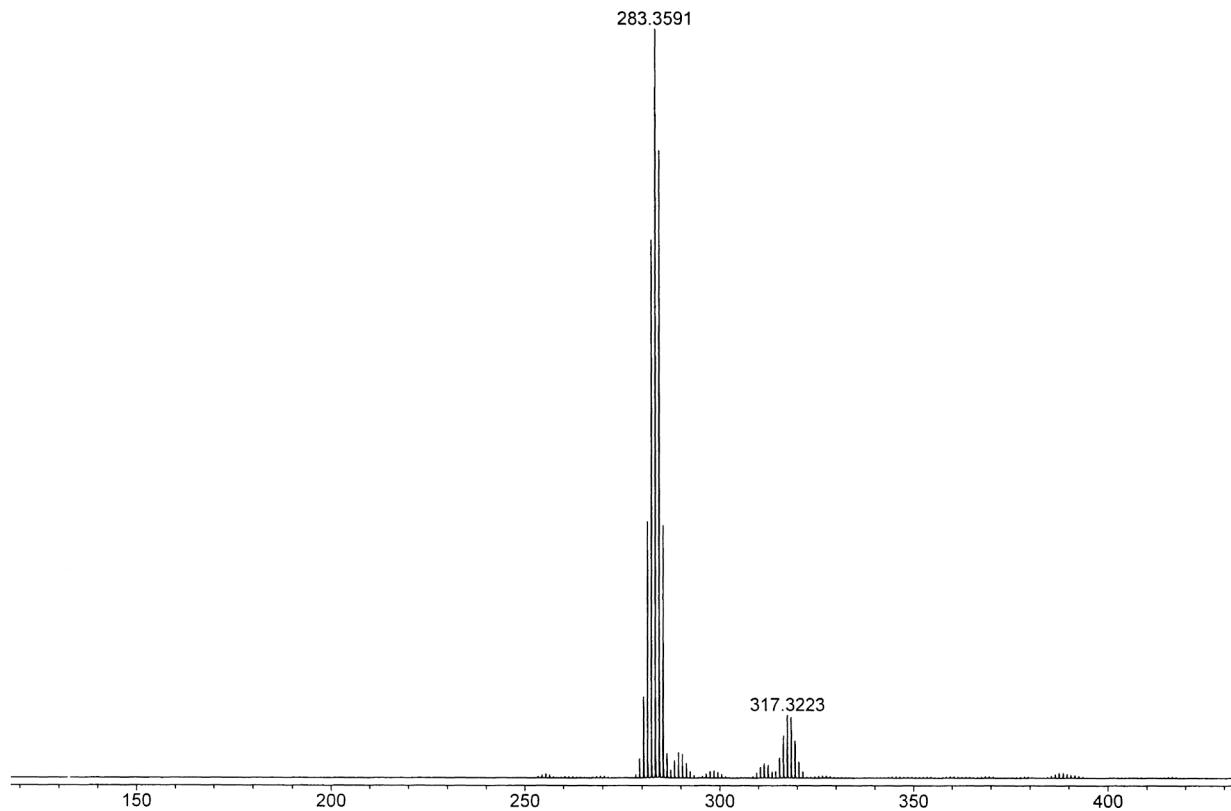


Figure S4. ESI-MS (negative mode) of 7

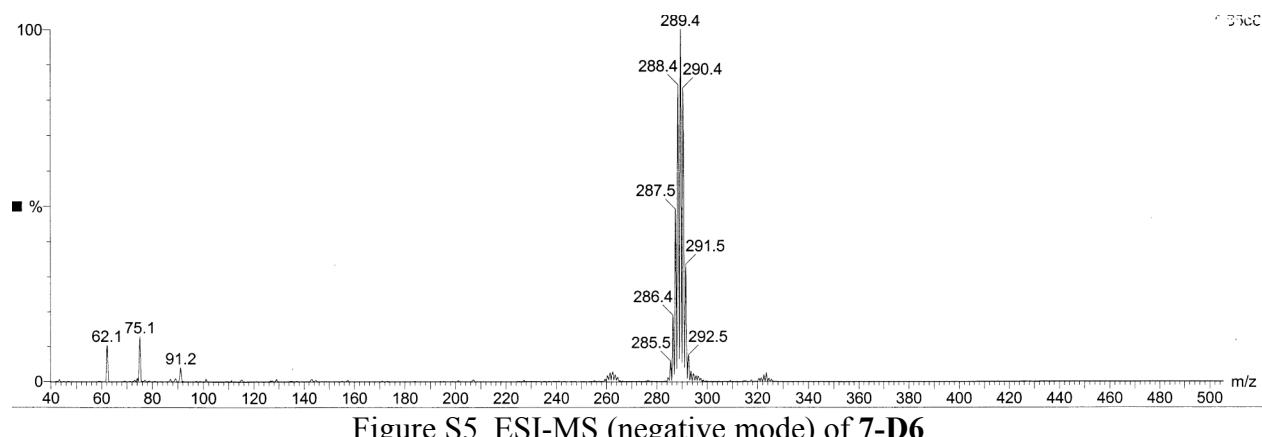


Figure S5. ESI-MS (negative mode) of 7-D6

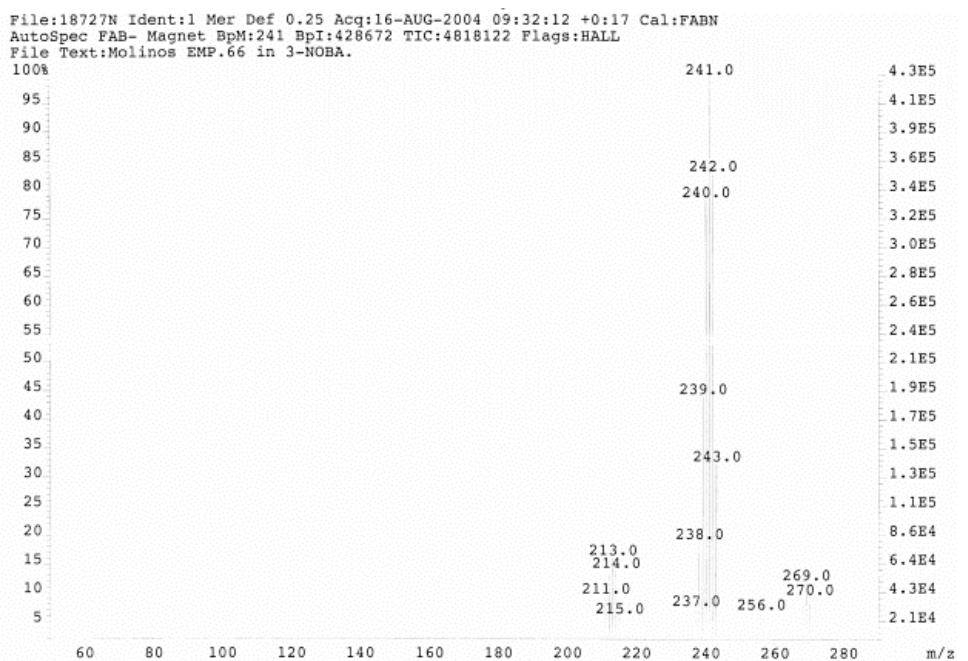


Figure S6. FAB-MS (negative mode) of **11**

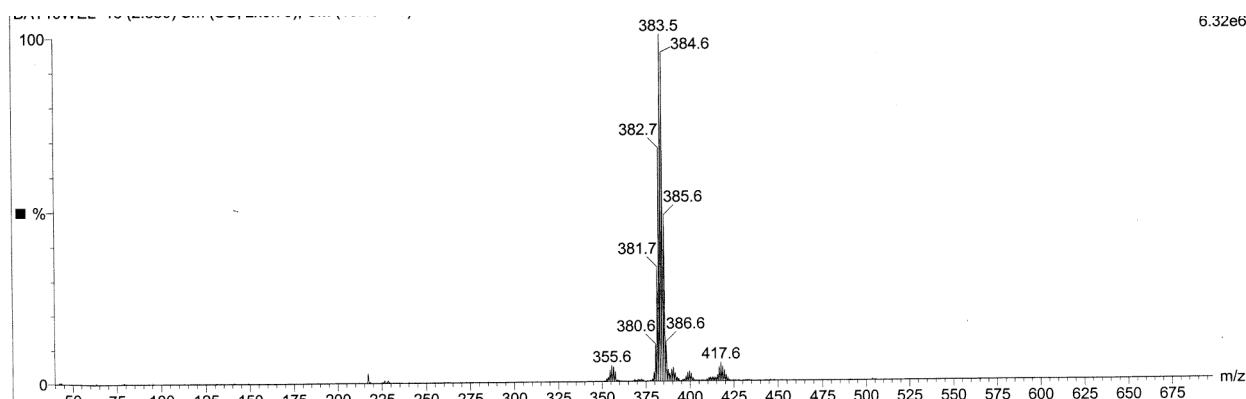


Figure S7. ESI-MS (negative mode) of **12**