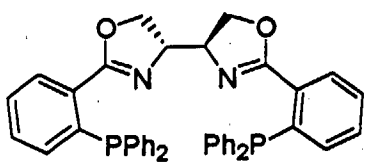
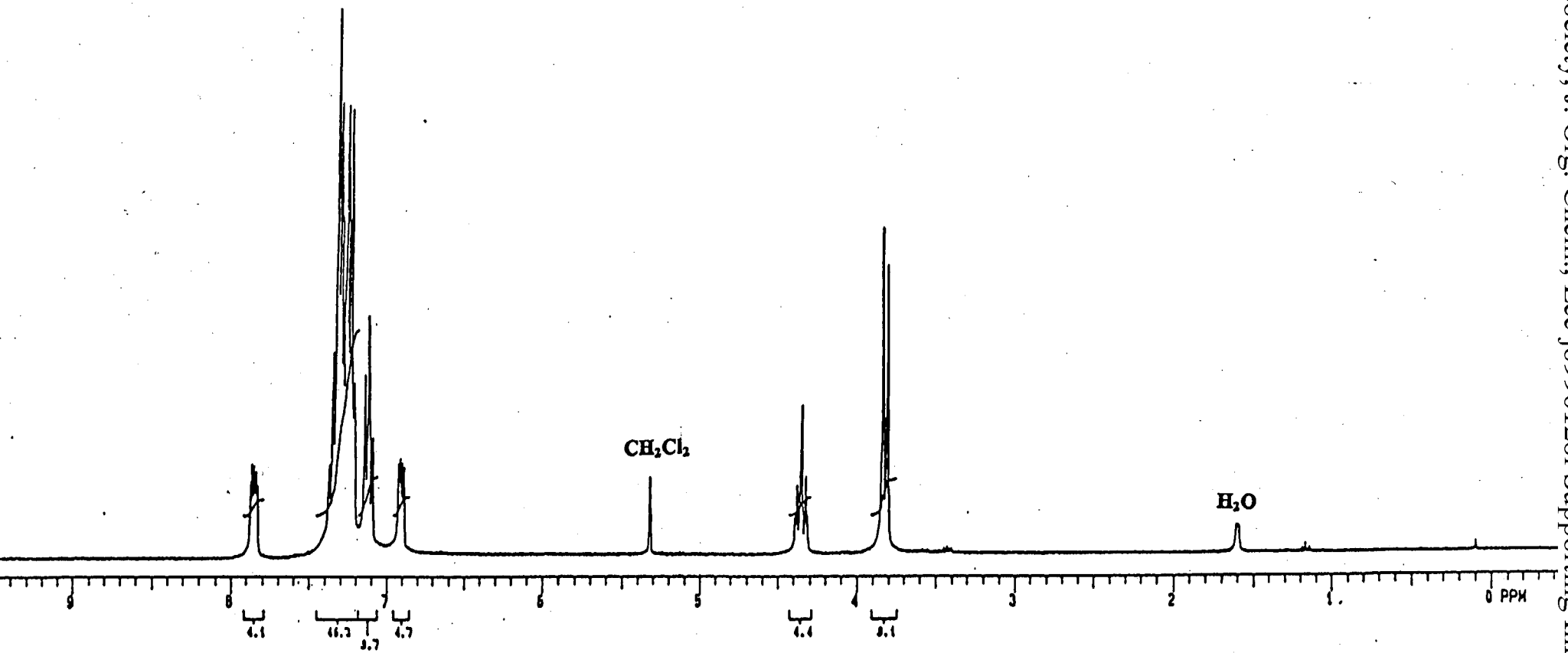
ang-gi Lee*, Chung Woo Lim, Choong Eui Song, Kwan Mook Kim, Chul Ho Jun

$^1$H NMR (300 MHz, $CD_2Cl_2$)




(*S*,*S*)-Phos-Biox 4

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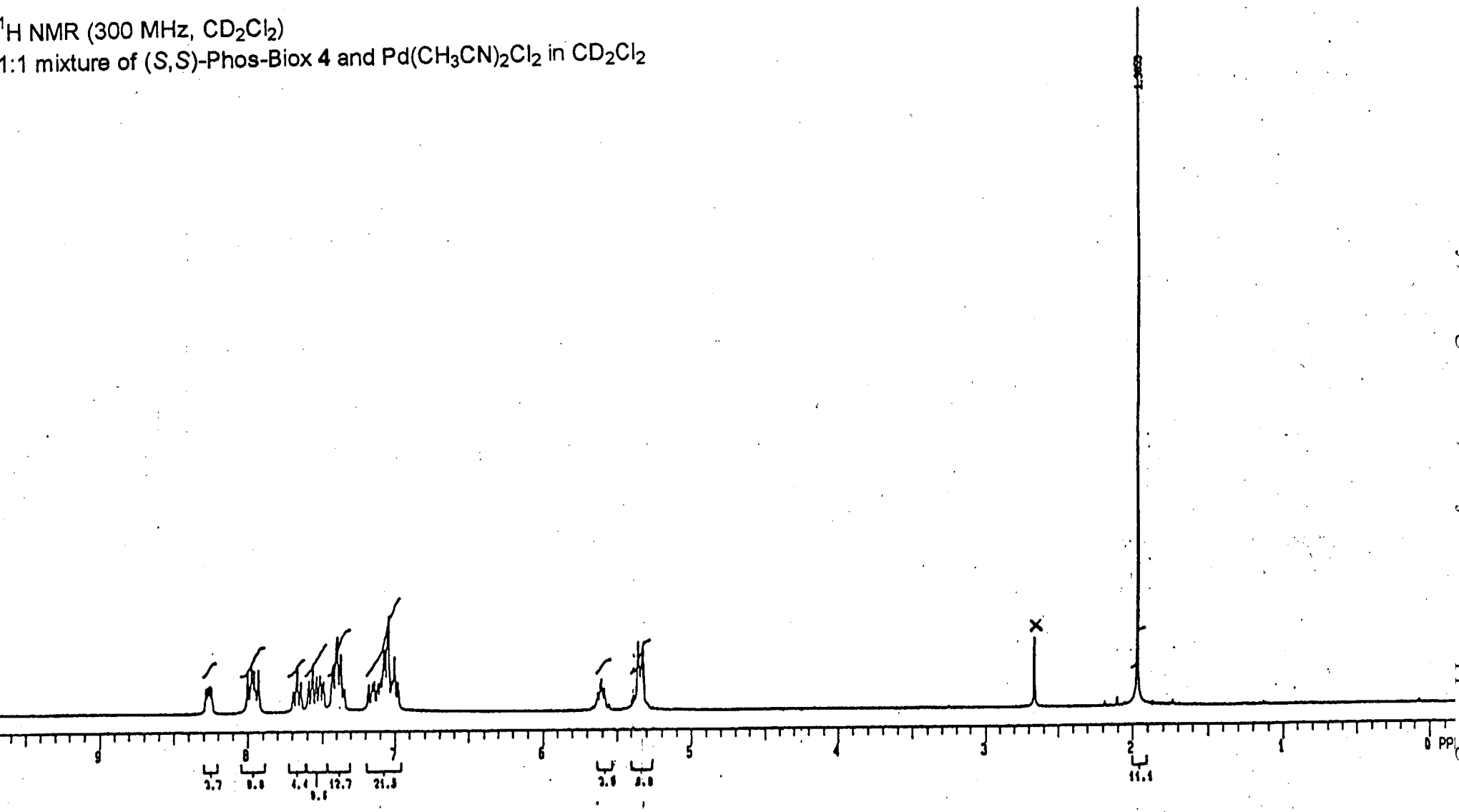
**pplementary Material.** $C_2$-Symmetric Bisphosphinobioxazoline as a Chiral Ligand. Highly Enantioselective.....
ng-gi Lee*, Chung Woo Lim, Choong Eui Song, Kwan Mook Kim, Chul Ho Jun

$^1$H NMR (300 MHz, $CD_2Cl_2$)
1:1 mixture of (*S*,*S*)-Phos-Biox **4** and $Pd(CH_3CN)_2Cl_2$ in $CD_2Cl_2$

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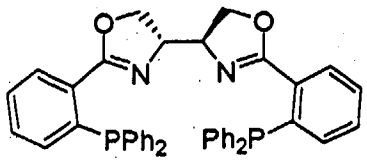
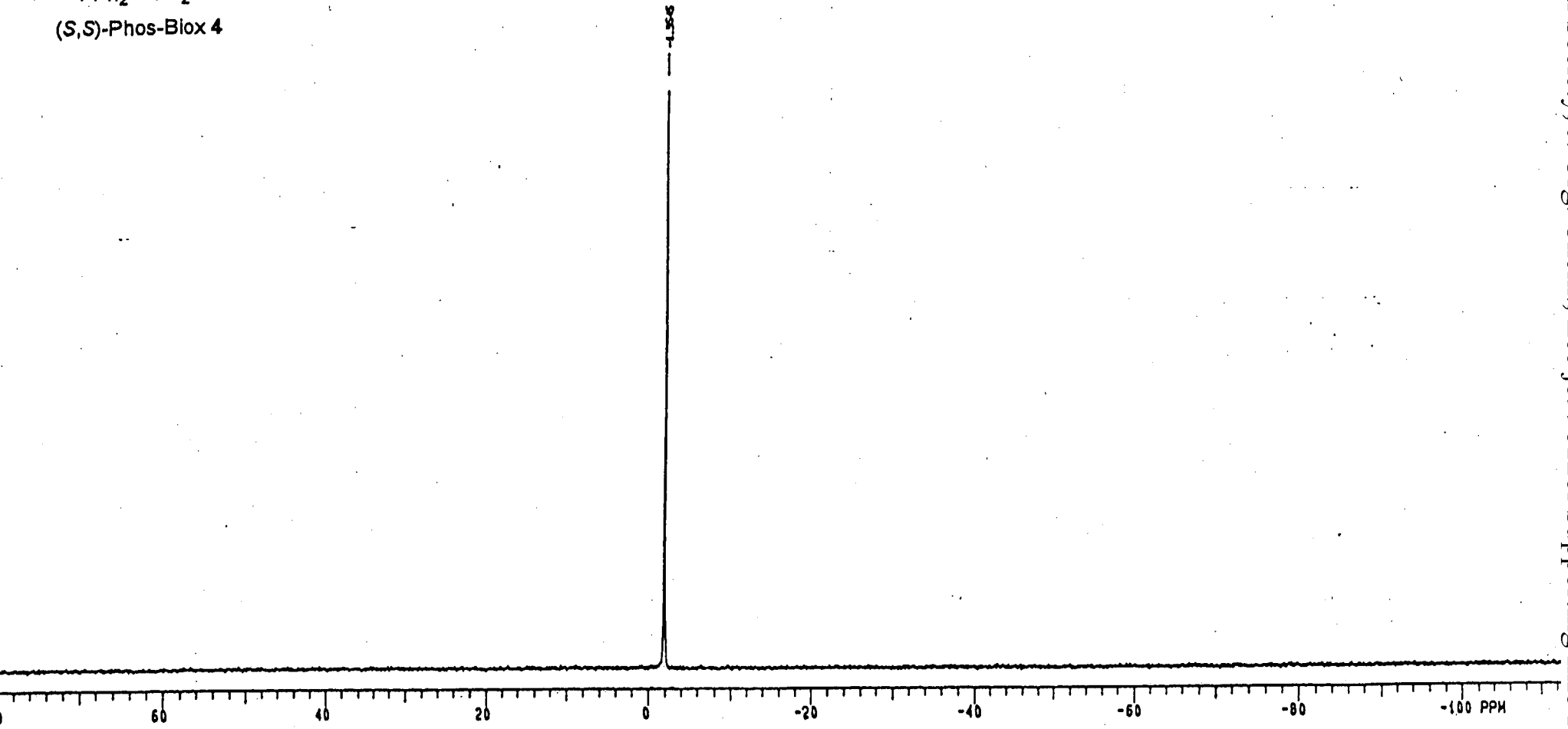
$^{31}P$ NMR(121 MHz, $CD_2Cl_2$)




(*S*,*S*)-Phos-Biox **4**

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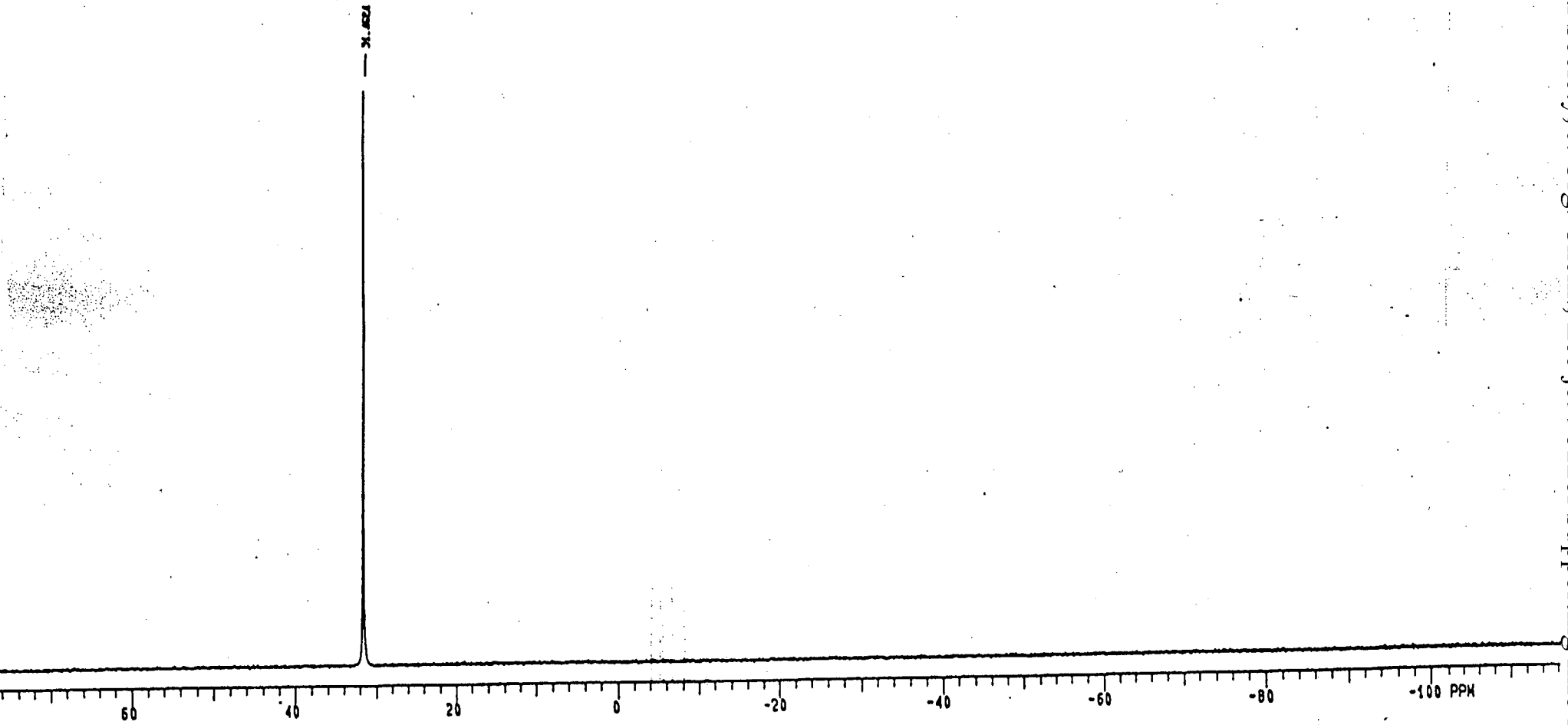
**upplementary Material.** $C_2$-Symmetric Bisphosphinobioxazoline as a Chiral Ligand. Highly Enantioselective.....
ang-gi Lee*, Chung Woo Lim, Choong Eui Song, Kwan Mook Kim, Chul Ho Jun

$^{31}P$ NMR(121 MHz, $CD_2Cl_2$)

1:1 mixture of (S,S)-Phos-Biox **4** and $Pd(CH_3CN)_2Cl_2$ in $CD_2Cl_2$

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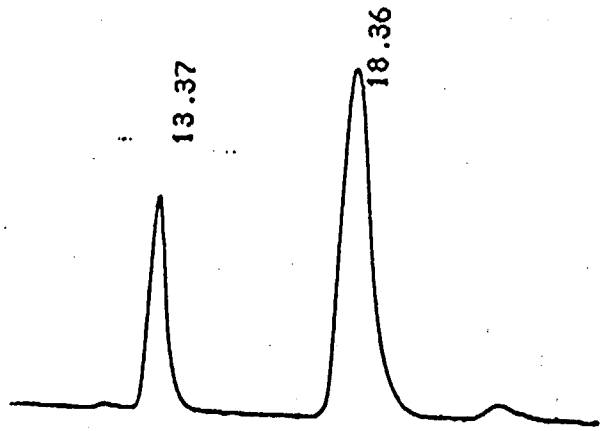
HPLC Chromatogram for racemic mixture of **13a** and **14a**
CHIRALCEL OJ column; 2-Propanol:n-hexane = 1:9, v/v;
flow rate: 1mL/min




HPLC Chromatogram of entry2 in Table 2

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Data for crystallographic analysis of **4** were measured on an Enraf-Nonius CAD-4 diffractormeter using graphite-monochromate Mo Kα(λ=0.71073 Å) and ϖ-2 scans in the range of θ; 1.57<θ<22.96. Structure was solved by direct methods and refined by least squares using the SHEL-X.

**Table S1a.** Crystal data and structure refinement of Phos-Biox **4**

| | |
|---|---|
| Empirical formula | $C_{42}H_{34}N_2O_2P_2$ |
| Formula weight | 660.65 |
| Temperature | 293(2) K |
| Wavelength | 0.71073 Å |
| Crystal system, space group | orthorhombic, P2(1)2(1)2(1) (No.19) |
| Unit cell dimensions | a = 10.4647(17) A alpha = 90.00(2) deg. |
| | b = 18.104(6) A beta = 90.00(2) deg. |
| | c = 18.635(5) A gamma = 90.00(2) deg. |
| Volume | 3530.5(15) $A^3$ |
| Z, Calculated density | 4, 1.243 $g/cm^3$ |
| Absorption coefficient | 0.162 $mm^{-1}$ |
| F(000) | 1384 |
| Crystal size | 0.35 x 0.40 x 0.60 mm |
| Theta range for data collection | 1.57 to 22.96 deg. |
| Index ranges | 0≤ h≤ 11, 0≤ k≤ 19, 0≤ l≤ 20 |
| Reflections collected / unique | 2545 / 2545 [R(int) = 0.0000] |
| Completeness to 2θ = 22.96 | 91.7% |
| Refinement method | Full-matrix least-squares on $F^2$ |
| Data / restraints / parameters | 2545 / 0 / 433 |
| Goodness-of-fit on $F^2$ | 1.091 |
| Final R indices [I>2σ (I)] | R1 = 0.0398, $wR_2$ = 0.1002 |
| R indices (all data) | R1 = 0.0401, $wR_2$ = 0.1006 |
| Absolute structure parameter | 0.05(12) |
| Largest diff. peak and hole | 0.277 and -0.312 $e.A^{-3}$ |

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**Table S1b.** Atomic coordinates ( x $10^4$) and equivalent isotropic displacement parameters (Å$^2$ x $10^3$) for **4**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| P(1) | 2578(1) | 167(1) | 788(1) | 42(1) |
| P(2) | -793(1) | 138(1) | -514(1) | 42(1) |
| O(1) | -26(3) | 2035(1) | 361(1) | 55(1) |
| O(2) | 3270(3) | 584(2) | -1156(2) | 57(1) |
| N(1) | 2013(3) | 1649(2) | 307(2) | 44(1) |
| N(2) | 1275(3) | 1035(2) | -1052(2) | 46(1) |
| C(1) | 947(3) | 1614(2) | 618(2) | 39(1) |
| C(2) | 1843(4) | 2125(2) | -328(2) | 44(1) |
| C(3) | 473(4) | 2405(2) | -261(2) | 58(1) |
| C(4) | 641(3) | 1162(2) | 1252(2) | 41(1) |
| C(5) | -332(4) | 1391(3) | 1705(2) | 57(1) |
| C(6) | -681(4) | 983(3) | 2300(2) | 70(1) |
| C(7) | -69(4) | 325(3) | 2425(2) | 63(1) |
| C(8) | 891(4) | 87(2) | 1982(2) | 52(1) |
| C(9) | 1300(3) | 493(2) | 1391(2) | 39(1) |
| C(10) | 2849(4) | -760(2) | 1167(2) | 46(1) |
| C(11) | 3617(4) | -915(2) | 1758(2) | 54(1) |
| C(12) | 3734(5) | -1630(3) | 2020(2) | 64(1) |
| C(13) | 3075(6) | -2190(3) | 1696(3) | 76(1) |
| C(14) | 2337(7) | -2049(3) | 1107(3) | 89(2) |
| C(15) | 2230(5) | -1335(2) | 838(3) | 70(1) |
| C(16) | 3977(4) | 656(2) | 1149(2) | 42(1) |
| C(17) | 5148(4) | 516(2) | 841(3) | 60(1) |
| C(18) | 6250(4) | 856(3) | 1089(3) | 67(1) |
| C(19) | 6178(4) | 1363(3) | 1625(3) | 61(1) |
| C(20) | 5023(4) | 1521(3) | 1925(2) | 63(1) |
| C(21) | 3927(4) | 1167(2) | 1689(2) | 53(1) |
| C(22) | 1992(4) | 481(2) | -1113(2) | 41(1) |
| C(23) | 2111(4) | 1688(2) | -1009(2) | 49(1) |
| C(24) | 3461(5) | 1371(2) | -1063(3) | 67(1) |
| C(25) | 1568(3) | -299(2) | -1143(2) | 39(1) |
| C(26) | 2456(4) | -815(2) | -1384(2) | 51(1) |
| C(27) | 2127(4) | -1559(2) | -1431(2) | 60(1) |
| C(28) | 935(4) | -1776(2) | -1234(2) | 59(1) |
| C(29) | 48(4) | -1272(2) | -996(2) | 48(1) |
| C(30) | 337(4) | -510(2) | -937(2) | 41(1) |
| C(31) | -1494(4) | 629(2) | -1281(2) | 42(1) |
| C(32) | -2159(5) | 1271(2) | -1132(2) | 62(1) |
| C(33) | -2753(6) | 1661(3) | -1672(3) | 81(2) |
| C(34) | -2695(5) | 1419(3) | -2362(3) | 77(1) |
| C(35) | -2033(5) | 782(3) | -2526(2) | 67(1) |
| C(36) | -1449(4) | 391(2) | -1988(2) | 50(1) |
| C(37) | -2121(4) | -490(2) | -291(2) | 45(1) |
| C(38) | -2060(5) | -867(2) | 359(2) | 64(1) |
| C(39) | -3029(6) | -1341(3) | 568(2) | 73(1) |
| C(40) | -4083(5) | -1436(2) | 149(2) | 65(1) |
| C(41) | -4174(5) | -1062(2) | -486(3) | 67(1) |
| C(42) | -3206(4) | -600(2) | -700(2) | 57(1) |

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**Table S1c.** Bond lengths [Å] and angles [°] for **4**

| | | | |
|---|---|---|---|
| P(1)-C(9) | 1.845(4) | P(1)-C(10) | 1.843(4) |
| P(1)-C(16) | 1.839(4) | P(2)-C(31) | 1.836(4) |
| P(2)-C(30) | 1.843(4) | P(2)-C(37) | 1.842(4) |
| O(1)-C(1) | 1.359(4) | O(1)-C(3) | 1.438(5) |
| O(2)-C(22) | 1.353(5) | O(2)-C(24) | 1.451(5) |
| N(1)-C(1) | 1.258(5) | N(1)-C(2) | 1.475(5) |
| N(2)-C(22) | 1.258(5) | N(2)-C(23) | 1.473(5) |
| C(1)-C(4) | 1.473(5) | C(2)-C(23) | 1.520(5) |
| C(2)-C(3) | 1.526(6) | C(4)-C(5) | 1.386(5) |
| C(4)-C(9) | 1.418(5) | C(5)-C(6) | 1.382(6) |
| C(6)-C(7) | 1.372(6) | C(7)-C(8) | 1.370(6) |
| C(8)-C(9) | 1.391(5) | C(10)-C(15) | 1.372(6) |
| C(10)-C(11) | 1.392(5) | C(11)-C(12) | 1.390(6) |
| C(12)-C(13) | 1.366(7) | C(13)-C(14) | 1.367(7) |
| C(14)-C(15) | 1.390(7) | C(16)-C(17) | 1.377(6) |
| C(16)-C(21) | 1.368(5) | C(17)-C(18) | 1.386(7) |
| C(18)-C(19) | 1.360(7) | C(19)-C(20) | 1.361(6) |
| C(20)-C(21) | 1.385(6) | C(22)-C(25) | 1.481(5) |
| C(23)-C(24) | 1.528(6) | C(25)-C(26) | 1.391(5) |
| C(25)-C(30) | 1.398(5) | C(26)-C(27) | 1.394(6) |
| C(27)-C(28) | 1.357(6) | C(28)-C(29) | 1.377(6) |
| C(29)-C(30) | 1.415(5) | C(31)-C(36) | 1.387(5) |
| C(31)-C(32) | 1.384(6) | C(32)-C(33) | 1.376(7) |
| C(33)-C(34) | 1.359(7) | C(34)-C(35) | 1.380(7) |
| C(35)-C(36) | 1.371(6) | C(37)-C(38) | 1.393(5) |
| C(37)-C(42) | 1.382(6) | C(38)-C(39) | 1.384(7) |
| C(39)-C(40) | 1.362(7) | C(40)-C(41) | 1.366(6) |
| C(41)-C(42) | 1.373(6) | C(9)-P(1)-C(10) | 99.72(17) |
| C(9)-P(1)-C(16) | 101.50(15) | C(10)-P(1)-C(16) | 100.15(17) |
| C(31)-P(2)-C(30) | 103.36(16) | C(31)-P(2)-C(37) | 99.92(16) |
| C(30)-P(2)-C(37) | 100.80(17) | C(1)-O(1)-C(3) | 105.8(3) |
| C(22)-O(2)-C(24) | 105.3(3) | C(1)-N(1)-C(2) | 107.0(3) |
| C(22)-N(2)-C(23) | 107.0(3) | N(1)-C(1)-O(1) | 118.3(3) |
| N(1)-C(1)-C(4) | 126.2(3) | O(1)-C(1)-C(4) | 115.5(3) |
| N(1)-C(2)-C(23) | 110.1(3) | N(1)-C(2)-C(3) | 104.0(3) |

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**Table S1c** continues

| | | | |
|---|---|---|---|
| C(23)-C(2)-C(3) | 114.4(3) | O(1)-C(3)-C(2) | 104.6(3) |
| C(5)-C(4)-C(9) | 120.1(3) | C(5)-C(4)-C(1) | 118.8(3) |
| C(9)-C(4)-C(1) | 121.0(3) | C(4)-C(5)-C(6) | 121.5(4) |
| C(7)-C(6)-C(5) | 118.5(4) | C(6)-C(7)-C(8) | 120.9(4) |
| C(7)-C(8)-C(9) | 122.4(4) | C(8)-C(9)-C(4) | 116.5(3) |
| C(8)-C(9)-P(1) | 122.5(3) | C(4)-C(9)-P(1) | 121.0(3) |
| C(15)-C(10)-C(11) | 118.3(4) | C(15)-C(10)-P(1) | 116.6(3) |
| C(11)-C(10)-P(1) | 125.1(3) | C(12)-C(11)-C(10) | 121.1(4) |
| C(13)-C(12)-C(11) | 119.4(4) | C(14)-C(13)-C(12) | 120.2(4) |
| C(13)-C(14)-C(15) | 120.6(5) | C(10)-C(15)-C(14) | 120.4(4) |
| C(17)-C(16)-C(21) | 117.7(4) | C(17)-C(16)-P(1) | 117.8(3) |
| C(21)-C(16)-P(1) | 124.4(3) | C(16)-C(17)-C(18) | 121.3(4) |
| C(17)-C(18)-C(19) | 119.9(4) | C(20)-C(19)-C(18) | 119.5(4) |
| C(19)-C(20)-C(21) | 120.6(4) | C(20)-C(21)-C(16) | 120.9(4) |
| N(2)-C(22)-O(2) | 119.0(3) | N(2)-C(22)-C(25) | 125.9(3) |
| O(2)-C(22)-C(25) | 115.1(3) | N(2)-C(23)-C(2) | 110.7(3) |
| N(2)-C(23)-C(24) | 104.1(3) | C(2)-C(23)-C(24) | 114.8(4) |
| O(2)-C(24)-C(23) | 104.5(3) | C(26)-C(25)-C(30) | 121.3(3) |
| C(26)-C(25)-C(22) | 116.9(3) | C(30)-C(25)-C(22) | 121.8(3) |
| C(25)-C(26)-C(27) | 120.3(4) | C(28)-C(27)-C(26) | 119.3(4) |
| C(27)-C(28)-C(29) | 120.9(4) | C(28)-C(29)-C(30) | 121.8(4) |
| C(25)-C(30)-C(29) | 116.3(4) | C(25)-C(30)-P(2) | 122.3(3) |
| C(29)-C(30)-P(2) | 121.1(3) | C(36)-C(31)-C(32) | 117.9(4) |
| C(36)-C(31)-P(2) | 125.1(3) | C(32)-C(31)-P(2) | 116.9(3) |
| C(33)-C(32)-C(31) | 120.8(4) | C(32)-C(33)-C(34) | 120.4(4) |
| C(35)-C(34)-C(33) | 120.1(4) | C(34)-C(35)-C(36) | 119.6(4) |
| C(31)-C(36)-C(35) | 121.3(4) | C(38)-C(37)-C(42) | 116.5(4) |
| C(38)-C(37)-P(2) | 117.6(3) | C(42)-C(37)-P(2) | 125.8(3) |
| C(37)-C(38)-C(39) | 121.0(4) | C(40)-C(39)-C(38) | 120.7(4) |
| C(39)-C(40)-C(41) | 119.4(4) | C(40)-C(41)-C(42) | 120.1(4) |
| C(41)-C(42)-C(37) | 122.3(4) | | |

Symmetry transformations used to generate equivalent atoms:

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**Table S1d.** Anisotropic displacement parameters ($Å^2 \times 10^3$) for **4**
The anisotropic displacement factor exponent takes the form:
$-2\ \phi^{\ 2}\ [\ h^2\ a^2\ U_{11} + ... + 2\ h\ k\ a^*\ b^*\ U_{12}\ ]$

| | U11 | U22 | U33 | U23 | U13 | U12 |
|---|---|---|---|---|---|---|
| P(1) | 55(1) | 33(1) | 39(1) | -1(1) | -3(1) | 2(1) |
| P(2) | 50(1) | 36(1) | 40(1) | -6(1) | -2(1) | -3(1) |
| O(1) | 51(2) | 44(2) | 69(2) | 19(1) | 7(1) | 10(1) |
| O(2) | 51(2) | 45(2) | 75(2) | -9(2) | 15(2) | -7(1) |
| N(1) | 49(2) | 38(2) | 46(2) | 4(1) | -1(2) | -5(2) |
| N(2) | 54(2) | 33(2) | 51(2) | -1(1) | -3(2) | -5(2) |
| C(1) | 38(2) | 30(2) | 50(2) | 2(2) | -4(2) | 1(2) |
| C(2) | 53(2) | 27(2) | 51(2) | 2(2) | 2(2) | -6(2) |
| C(3) | 76(3) | 40(2) | 58(2) | 14(2) | 10(2) | 9(2) |
| C(4) | 38(2) | 43(2) | 43(2) | 2(2) | -4(2) | -5(2) |
| C(5) | 47(2) | 66(3) | 58(2) | 11(2) | 6(2) | 18(2) |
| C(6) | 47(2) | 100(4) | 62(3) | 17(3) | 13(2) | 19(3) |
| C(7) | 45(2) | 86(3) | 57(2) | 28(2) | 4(2) | 1(2) |
| C(8) | 51(2) | 55(2) | 52(2) | 13(2) | -3(2) | 1(2) |
| C(9) | 41(2) | 37(2) | 40(2) | -1(2) | -8(2) | -3(2) |
| C(10) | 60(2) | 36(2) | 44(2) | -3(2) | -3(2) | 4(2) |
| C(11) | 65(2) | 41(2) | 57(2) | 4(2) | -5(2) | 3(2) |
| C(12) | 72(3) | 54(3) | 67(3) | 14(2) | -3(2) | 16(2) |
| C(13) | 96(4) | 42(2) | 89(3) | 15(2) | 3(3) | 8(3) |
| C(14) | 121(5) | 39(2) | 108(4) | -5(3) | -19(4) | -12(3) |
| C(15) | 98(4) | 35(2) | 76(3) | -5(2) | -28(3) | -3(2) |
| C(16) | 49(2) | 33(2) | 44(2) | 6(2) | 2(2) | 9(2) |
| C(17) | 60(3) | 36(2) | 85(3) | -3(2) | 18(2) | 8(2) |
| C(18) | 44(2) | 50(3) | 107(4) | 18(3) | 16(3) | 7(2) |
| C(19) | 46(2) | 56(3) | 81(3) | 19(3) | -11(2) | -7(2) |
| C(20) | 61(3) | 68(3) | 59(2) | -7(2) | -6(2) | -12(2) |
| C(21) | 43(2) | 60(3) | 55(2) | -9(2) | 1(2) | -4(2) |
| C(22) | 44(2) | 40(2) | 39(2) | -3(2) | 2(2) | -5(2) |
| C(23) | 62(2) | 33(2) | 52(2) | 5(2) | 6(2) | -14(2) |
| C(24) | 71(3) | 43(2) | 86(3) | -16(2) | 25(3) | -23(2) |
| C(25) | 44(2) | 31(2) | 42(2) | 0(2) | -5(2) | -1(2) |
| C(26) | 51(2) | 44(2) | 57(2) | -3(2) | 0(2) | 4(2) |
| C(27) | 66(3) | 40(2) | 73(3) | -8(2) | -4(2) | 13(2) |
| C(28) | 69(3) | 30(2) | 78(3) | -3(2) | -6(2) | 1(2) |
| C(29) | 56(2) | 31(2) | 57(2) | -1(2) | -3(2) | -7(2) |
| C(30) | 53(2) | 31(2) | 39(2) | 0(2) | -12(2) | -1(2) |
| C(31) | 47(2) | 33(2) | 45(2) | -4(2) | 3(2) | -4(2) |
| C(32) | 80(3) | 45(2) | 62(2) | -10(2) | 4(2) | 19(2) |
| C(33) | 99(4) | 52(3) | 92(4) | 2(3) | 1(3) | 35(3) |
| C(34) | 95(4) | 66(3) | 71(3) | 24(2) | -3(3) | 24(3) |
| C(35) | 85(3) | 67(3) | 49(2) | 9(2) | -1(2) | 11(3) |
| C(36) | 62(2) | 40(2) | 49(2) | 7(2) | 6(2) | 7(2) |
| C(37) | 56(2) | 41(2) | 40(2) | -2(2) | 1(2) | 1(2) |
| C(38) | 84(3) | 61(3) | 47(2) | 6(2) | -9(2) | -14(3) |
| C(39) | 113(4) | 57(3) | 51(2) | 11(2) | 10(3) | -19(3) |
| C(40) | 74(3) | 51(3) | 70(3) | -8(2) | 20(3) | -17(2) |
| C(41) | 59(2) | 59(3) | 84(3) | 8(2) | -6(2) | -10(2) |
| C(42) | 61(2) | 53(2) | 58(2) | 12(2) | -6(2) | -11(2) |

**Table S13e.** Hydrogen coordinates ( x $10^4$) and isotropic displacement parameters (Å$^2$ x $10^3$) for **4**.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| H(2) | 2435 | 2544 | -299 | 52 |
| H(3A) | 458 | 2937 | -197 | 69 |
| H(3B) | -19 | 2280 | -685 | 69 |
| H(5) | -759 | 1830 | 1607 | 68 |
| H(6) | -1316 | 1150 | 2609 | 83 |
| H(7) | -309 | 37 | 2815 | 75 |
| H(8) | 1283 | -363 | 2079 | 63 |
| H(11) | 4059 | -533 | 1982 | 65 |
| H(12) | 4257 | -1728 | 2413 | 77 |
| H(13) | 3128 | -2667 | 1877 | 91 |
| H(14) | 1902 | -2434 | 884 | 107 |
| H(15) | 1736 | -1248 | 432 | 84 |
| H(17) | 5201 | 187 | 459 | 72 |
| H(18) | 7037 | 738 | 888 | 80 |
| H(19) | 6912 | 1601 | 1786 | 73 |
| H(20) | 4970 | 1869 | 2290 | 76 |
| H(21) | 3146 | 1279 | 1902 | 63 |
| H(23) | 1951 | 2005 | -1426 | 59 |
| H(24A) | 3912 | 1580 | -1470 | 80 |
| H(24B) | 3943 | 1472 | -629 | 80 |
| H(26) | 3272 | -662 | -1514 | 61 |
| H(27) | 2717 | -1904 | -1596 | 71 |
| H(28) | 716 | -2273 | -1261 | 71 |
| H(29) | -763 | -1435 | -869 | 57 |
| H(32) | -2206 | 1442 | -662 | 75 |
| H(33) | -3197 | 2091 | -1564 | 97 |
| H(34) | -3101 | 1684 | -2724 | 93 |
| H(35) | -1982 | 619 | -2998 | 80 |
| H(36) | -1015 | -42 | -2099 | 60 |
| H(38) | -1358 | -800 | 658 | 77 |
| H(39) | -2960 | -1598 | 998 | 88 |
| H(40) | -4735 | -1752 | 293 | 78 |
| H(41) | -4894 | -1120 | -773 | 81 |
| H(42) | -3283 | -353 | -1136 | 69 |

**Supplementary Material**. $C_2$-Symmetric Bisphosphinobioxazoline as a Chiral Ligand. Highly Enantioselective.....
Sang-gi Lee, Chung Woo Lim, Choong Eui Song, Kwan Mook Kim, Chul Ho Jun

**Table S2a**. Crystal data and structure refinement for **19a**.

| | |
|---|---|
| Empirical formula | $C_{42}\ H_{34}\ Cl_2\ N_2\ O_2\ P_2\ Pd$ |
| Formula weight | 837.95 |
| Temperature, K | 293(2) |
| Wavelength, Å | 0.71073 |
| Crystal system, space group | orthorhombic, $P2_12_12_1$(No.19) |
| Unit cell dimensions | a = 11.228(5) Å alpha = 90 deg. |
| | b = 19.668(6) Å beta = 90 deg. |
| | c = 40.447(12) Å gamma = 90 deg. |
| Volume | 8932(6) $A^3$ |
| Z, Calculated density | 4, 1.246 $g/cm^3$ |
| Absorption coefficient | 0.640 $mm^{-1}$ |
| F(000) | 3408 |
| Crystal size | 0.10 x 0.10 x 0.25 mm |
| Theta range for data collection | 1.15 to 22.94 deg. |
| Index ranges | $0\leq h\leq 12, 0\leq k\leq 21, 0\leq l\leq 44$ |
| Reflections collected / unique | 2852 / 2852 [R(int) = 0.0000] |
| Completeness to 2theta = 22.94 | 41.6% |
| Refinement method | Full-matrix least-squares on $F^2$ |
| Data / restraints / parameters | 2852 / 3 / 469 |
| Goodness-of-fit on $F^2$ | 1.362 |
| Final R indices [$I>2\sigma$ (I)] | R1 = 0.1183, $wR_2$ = 0.3117 |
| R indices (all data) | R1 = 0.1265, $wR_2$ = 0.3188 |
| Absolute structure parameter | 0.1(2) |
| Largest diff. peak and hole | 1.138 and -0.693 $e.A^{-3}$ |

**Table S2b**. Atomic Coordinates ( x $10^4$) and Equivalent Isotropic Displacement parameters ($A^2$ x $10^3$) of **19a**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| Pd(1) | 1489(4) | 7238(2) | 2410(1) | 44(1) |
| Pd(2) | 5288(4) | 11218(2) | 766(1) | 41(1) |
| P(1) | 1410(15) | 7752(8) | 1918(3) | 47(4) |
| P(2) | 2067(13) | 6178(8) | 2267(3) | 43(4) |
| P(3) | 5974(13) | 10201(8) | 942(4) | 46(4) |
| P(4) | 5276(14) | 11082(8) | 211(3) | 48(4) |
| Cl(1) | 2799(14) | 954(8) | 1046(4) | 67(5) |
| Cl(2A) | 1296(18) | 1742(11) | 2314(5) | 64(7) |
| Cl(2B) | 4830(7) | 5160(4) | 974(18) | 110(2) |
| Cl(3A) | 5670(3) | 3344(14) | 2396(8) | 65(8) |
| Cl(3B) | 1650(6) | 3260(3) | 1340(14) | 83(17) |
| Cl(3C) | 1600(8) | 1960(4) | 1583(18) | 60(2) |
| Cl(4A) | 3210(4) | 3970(2) | 1728(11) | 83(14) |
| Cl(4B) | 7260(5) | 3650(2) | 1211(12) | 57(14) |
| Cl(4C) | 2770(5) | 3100(3) | 2334(14) | 81(18) |
| N(1) | 940(4) | 8140(2) | 2600(12) | 68(14) |
| N(2) | 1720(5) | 6940(3) | 2893(12) | 66(15) |
| N(3) | 5420(4) | 11550(2) | 1243(11) | 51(13) |
| N(4) | 4780(4) | 12187(19) | 704(9) | 41(11) |
| O(1) | 1090(4) | 9170(2) | 2795(10) | 77(13) |
| O(2) | 1480(4) | 6535(19) | 3387(10) | 68(12) |
| O(3) | 5030(4) | 11678(19) | 1766(9) | 66(12) |
| O(4) | 4660(4) | 13282(19) | 573(10) | 75(12) |
| C(1) | 2630(7) | 7420(3) | 1624(17) | 90(2) |
| C(2) | 2230(6) | 7080(3) | 1333(14) | 65(18) |
| C(3) | 3190(7) | 6890(4) | 1143(19) | 110(3) |
| C(4) | 4280(8) | 7170(4) | 1230(2) | 100(3) |
| C(5) | 4520(10) | 7390(5) | 1470(2) | 110(4) |
| C(6) | 3780(6) | 7620(3) | 1682(18) | 80(2) |
| C(7) | -40(5) | 7740(3) | 1722(13) | 50(14) |
| C(8) | -230(6) | 7900(3) | 1380(14) | 66(17) |
| C(9) | -1340(7) | 7890(3) | 1195(18) | 80(2) |
| C(10) | -2170(8) | 7680(4) | 1380(2) | 120(3) |
| C(11) | -2190(8) | 7530(4) | 1680(2) | 120(3) |
| C(12) | -910(7) | 7480(4) | 1872(19) | 90(3) |
| C(13) | 1750(5) | 8670(3) | 1959(13) | 43(15) |
| C(14) | 2030(5) | 9020(3) | 1695(15) | 59(17) |
| C(15) | 2140(6) | 9740(3) | 1661(17) | 70(2) |
| C(16) | 1930(6) | 9940(4) | 1993(18) | 90(2) |
| C(17) | 1680(4) | 9720(2) | 2233(12) | 29(13) |
| C(18) | 1560(5) | 9070(2) | 2218(11) | 32(12) |
| C(19) | 1210(5) | 8770(3) | 2529(13) | 57(16) |
| C(20) | 580(6) | 8820(3) | 3109(15) | 90(2) |
| C(21) | 720(6) | 8030(3) | 2971(14) | 80(2) |
| C(22) | 1530(5) | 7560(3) | 3120(13) | 60(17) |
| C(23) | 1340(6) | 7200(3) | 3443(13) | 60(16) |
| C(24) | 1560(5) | 6440(2) | 3066(11) | 25(12) |
| C(25) | 1620(6) | 5700(3) | 2859(14) | 70(18) |
| C(26) | 1380(6) | 5170(3) | 3153(16) | 73(19) |
| C(27) | 1340(5) | 4470(3) | 3059(12) | 47(14) |
| C(28) | 1420(4) | 4310(2) | 2716(10) | 35(12) |
| C(29) | 1670(4) | 4850(2) | 2471(11) | 32(12) |

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**Table S2b**. Continues

| | | | | |
|---|---|---|---|---|
| C(30) | 1650(4) | 5550(2) | 2567(11) | 28(11) |
| C(31) | 3690(5) | 6130(3) | 2238(12) | 50(14) |
| C(32) | 4450(5) | 6610(3) | 2335(14) | 62(18) |
| C(33) | 5590(5) | 6590(2) | 2340(12) | 43(14) |
| C(34) | 6080(6) | 6010(3) | 2203(14) | 72(19) |
| C(35) | 5570(6) | 5460(3) | 2114(14) | 71(19) |
| C(36) | 4230(5) | 5560(3) | 2130(14) | 61(18) |
| C(37) | 1290(5) | 5860(2) | 1924(11) | 32(13) |
| C(38) | 140(6) | 5790(3) | 1922(17) | 70(2) |
| C(39) | -520(8) | 5530(4) | 1652(19) | 130(3) |
| C(40) | 1160(6) | 5310(3) | 1354(17) | 80(2) |
| C(41) | -80(7) | 5290(4) | 1370(2) | 110(3) |
| C(42) | 1850(6) | 5600(3) | 1642(16) | 90(2) |
| C(43) | 7550(6) | 10200(3) | 912(15) | 63(18) |
| C(44) | 8260(6) | 10750(3) | 922(15) | 80(2) |
| C(45) | 9490(5) | 10710(3) | 939(12) | 49(15) |
| C(46) | 10070(6) | 10230(3) | 930(15) | 80(2) |
| C(47) | 9580(8) | 9600(5) | 960(2) | 130(3) |
| C(48) | 8090(7) | 9600(5) | 948(19) | 110(3) |
| C(49) | 5450(6) | 9450(3) | 733(16) | 69(18) |
| C(50) | 5880(8) | 9150(4) | 490(2) | 120(3) |
| C(51) | 5460(9) | 8520(5) | 360(2) | 140(3) |
| C(52) | 4390(10) | 8370(5) | 420(2) | 160(4) |
| C(53) | 3680(9) | 8730(4) | 720(2) | 130(3) |
| C(54) | 4300(6) | 9270(3) | 834(16) | 80(2) |
| C(55) | 5660(4) | 10040(2) | 1382(11) | 28(12) |
| C(56) | 5760(5) | 9410(3) | 1480(14) | 62(18) |
| C(57) | 5740(5) | 9180(3) | 1819(13) | 45(16) |
| C(58) | 5340(6) | 9680(3) | 1997(15) | 70(18) |
| C(59) | 5280(6) | 10380(3) | 1910(15) | 58(17) |
| C(60) | 5410(5) | 10530(2) | 1635(12) | 31(12) |
| C(61) | 5330(6) | 11230(3) | 1529(13) | 59(15) |
| C(62) | 4760(6) | 12310(3) | 1640(15) | 80(2) |
| C(63) | 5180(7) | 12320(4) | 1277(17) | 100(2) |
| C(64) | 4340(6) | 12560(3) | 990(15) | 67(18) |
| C(65) | 4340(6) | 13280(3) | 917(14) | 57(17) |
| C(66) | 4920(7) | 12580(4) | 491(19) | 80(2) |
| C(67) | 5390(5) | 12550(3) | 157(14) | 57(16) |
| C(68) | 5680(6) | 13170(3) | -36(14) | 69(19) |
| C(69) | 6160(7) | 13020(4) | -385(17) | 90(2) |
| C(70) | 6340(7) | 12450(3) | -528(19) | 90(2) |
| C(71) | 6040(7) | 11880(4) | -335(17) | 100(2) |
| C(72) | 5640(5) | 11890(3) | 12(13) | 52(16) |
| C(73) | 3820(6) | 10790(3) | 18(16) | 70(2) |
| C(74) | 3450(7) | 10910(4) | -267(18) | 90(2) |
| C(75) | 2400(6) | 10550(3) | -402(17) | 80(2) |
| C(76) | 1790(5) | 10210(3) | -223(13) | 58(17) |
| C(77) | 2300(7) | 10060(4) | 79(15) | 110(3) |
| C(78) | 3240(6) | 10320(3) | 256(15) | 71(19) |
| C(79) | 6290(7) | 10520(4) | 57(17) | 80(2) |
| C(80) | 6020(10) | 10000(5) | -150(3) | 160(4) |
| C(81) | 7010(11) | 9490(6) | -280(3) | 180(5) |
| C(82) | 8150(7) | 9610(4) | -195(18) | 110(3) |
| C(83) | 8590(8) | 10190(4) | -45(18) | 110(3) |
| C(84) | 7660(6) | 10700(4) | 139(17) | 90(2) |

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**Table S2c.** Bond lengths [Å] and angles [°] for **19a**

| | | | |
|---|---|---|---|
| Pd(1)-N(1) | 2.03(5) | Pd(1)-N(2) | 2.05(5) |
| Pd(1)-P(1) | 2.234(14) | Pd(1)-P(2) | 2.259(15) |
| Pd(2)-N(4) | 2.01(4) | Pd(2)-N(3) | 2.05(4) |
| Pd(2)-P(3) | 2.257(16) | Pd(2)-P(4) | 2.261(14) |
| P(1)-C(13) | 1.86(5) | P(1)-C(7) | 1.81(5) |
| P(1)-C(1) | 1.93(7) | P(2)-C(30) | 1.79(5) |
| P(2)-C(31) | 1.82(6) | P(2)-C(37) | 1.76(5) |
| P(3)-C(43) | 1.77(7) | P(3)-C(55) | 1.84(5) |
| P(3)-C(49) | 1.80(6) | P(4)-C(79) | 1.71(7) |
| P(4)-C(73) | 1.90(7) | P(4)-C(72) | 1.83(6) |
| N(1)-C(19) | 1.30(6) | N(1)-C(21) | 1.53(7) |
| N(2)-C(24) | 1.23(5) | N(2)-C(22) | 1.54(6) |
| N(3)-C(61) | 1.33(6) | N(3)-C(63) | 1.53(8) |
| N(4)-C(66) | 1.17(7) | N(4)-C(64) | 1.45(6) |
| O(1)-C(19) | 1.35(6) | O(1)-C(20) | 1.56(7) |
| O(2)-C(24) | 1.32(5) | O(2)-C(23) | 1.35(6) |
| O(3)-C(61) | 1.35(6) | O(3)-C(62) | 1.38(7) |
| O(4)-C(66) | 1.45(7) | O(4)-C(65) | 1.43(6) |
| C(1)-C(6) | 1.37(9) | C(1)-C(2) | 1.42(8) |
| C(2)-C(3) | 1.37(9) | C(3)-C(4) | 1.38(9) |
| C(4)-C(5) | 1.09(10) | C(5)-C(6) | 1.29(10) |
| C(7)-C(12) | 1.26(8) | C(7)-C(8) | 1.43(7) |
| C(8)-C(9) | 1.45(9) | C(9)-C(10) | 1.27(10) |
| C(10)-C(11) | 1.25(10) | C(11)-C(12) | 1.63(10) |
| C(13)-C(14) | 1.31(7) | C(13)-C(18) | 1.32(6) |
| C(14)-C(15) | 1.42(7) | C(15)-C(16) | 1.42(8) |
| C(16)-C(17) | 1.09(7) | C(17)-C(18) | 1.29(6) |
| C(18)-C(19) | 1.45(6) | C(20)-C(21) | 1.65(8) |
| C(21)-C(22) | 1.43(3) | C(22)-C(23) | 1.50(7) |
| C(24)-C(25) | 1.67(7) | C(25)-C(30) | 1.22(6) |
| C(25)-C(26) | 1.60(8) | C(26)-C(27) | 1.43(7) |
| C(27)-C(28) | 1.42(6) | C(28)-C(29) | 1.47(5) |
| C(29)-C(30) | 1.43(5) | C(31)-C(36) | 1.35(7) |
| C(31)-C(32) | 1.35(7) | C(32)-C(33) | 1.28(7) |
| C(33)-C(34) | 1.38(7) | C(34)-C(35) | 1.28(7) |
| C(35)-C(36) | 1.51(8) | C(37)-C(38) | 1.30(8) |
| C(37)-C(42) | 1.39(7) | C(38)-C(39) | 1.41(3) |
| C(39)-C(41) | 1.34(10) | C(40)-C(41) | 1.40(9) |
| C(40)-C(42) | 1.51(8) | C(43)-C(44) | 1.35(8) |
| C(43)-C(48) | 1.33(9) | C(44)-C(45) | 1.38(8) |
| C(45)-C(46) | 1.15(7) | C(46)-C(47) | 1.36(9) |
| C(47)-C(48) | 1.67(11) | C(49)-C(54) | 1.40(8) |
| C(49)-C(50) | 1.24(9) | C(50)-C(51) | 1.44(10) |
| C(51)-C(52) | 1.27(12) | C(52)-C(53) | 1.60(11) |
| C(53)-C(54) | 1.35(9) | C(55)-C(56) | 1.31(7) |
| C(55)-C(60) | 1.43(6) | C(56)-C(57) | 1.44(7) |
| C(57)-C(58) | 1.30(7) | C(58)-C(59) | 1.42(8) |
| C(59)-C(60) | 1.16(6) | C(60)-C(61) | 1.44(7) |
| C(62)-C(63) | 1.54(8) | C(63)-C(64) | 1.57(8) |
| C(64)-C(65) | 1.44(7) | C(64)-C(66) | 2.12(9) |
| C(66)-C(67) | 1.45(8) | C(67)-C(72) | 1.44(7) |
| C(67)-C(68) | 1.49(7) | C(68)-C(69) | 1.54(8) |
| C(69)-C(70) | 1.28(8) | C(70)-C(71) | 1.41(8) |
| C(71)-C(72) | 1.48(8) | C(73)-C(78) | 1.49(8) |

**Table S2c**. Continues

| | | | |
|---|---|---|---|
| C(73)-C(74) | 1.24(8) | C(74)-C(75) | 1.48(9) |
| C(75)-C(76) | 1.21(7) | C(76)-C(77) | 1.38(3) |
| C(77)-C(78) | 1.38(8) | C(79)-C(84) | 1.62(10) |
| C(79)-C(80) | 1.36(10) | C(80)-C(81) | 1.57(13) |
| C(81)-C(82) | 1.36(12) | C(82)-C(83) | 1.38(9) |
| C(83)-C(84) | 1.62(10) | N(1)-Pd(1)-N(2) | 86(2) |
| N(1)-Pd(1)-P(1) | 86.0(15) | N(2)-Pd(1)-P(1) | 168.6(15) |
| N(1)-Pd(1)-P(2) | 172.4(14) | N(2)-Pd(1)-P(2) | 86.9(14) |
| P(1)-Pd(1)-P(2) | 101.6(5) | N(4)-Pd(2)-N(3) | 80.3(16) |
| N(4)-Pd(2)-P(3) | 168.0(12) | N(3)-Pd(2)-P(3) | 88.0(13) |
| N(4)-Pd(2)-P(4) | 89.2(11) | N(3)-Pd(2)-P(4) | 167.3(13) |
| P(3)-Pd(2)-P(4) | 102.2(6) | C(13)-P(1)-C(7) | 104(3) |
| C(13)-P(1)-C(1) | 104(3) | C(7)-P(1)-C(1) | 111(3) |
| C(13)-P(1)-Pd(1) | 110.7(17) | C(7)-P(1)-Pd(1) | 114.7(18) |
| C(1)-P(1)-Pd(1) | 112(2) | C(30)-P(2)-C(31) | 106(2) |
| C(30)-P(2)-C(37) | 99(2) | C(31)-P(2)-C(37) | 115(2) |
| C(30)-P(2)-Pd(1) | 112.8(15) | C(31)-P(2)-Pd(1) | 110.7(19) |
| C(37)-P(2)-Pd(1) | 113.1(17) | C(43)-P(3)-C(55) | 105(3) |
| C(43)-P(3)-C(49) | 107(3) | C(55)-P(3)-C(49) | 104(3) |
| C(43)-P(3)-Pd(2) | 109(2) | C(55)-P(3)-Pd(2) | 113.1(16) |
| C(49)-P(3)-Pd(2) | 118(2) | C(79)-P(4)-C(73) | 103(3) |
| C(79)-P(4)-C(72) | 105(3) | C(73)-P(4)-C(72) | 106(3) |
| C(79)-P(4)-Pd(2) | 116(2) | C(73)-P(4)-Pd(2) | 117(2) |
| C(72)-P(4)-Pd(2) | 109.5(18) | C(19)-N(1)-C(21) | 112(5) |
| C(19)-N(1)-Pd(1) | 132(4) | C(21)-N(1)-Pd(1) | 107(3) |
| C(24)-N(2)-C(22) | 106(4) | C(24)-N(2)-Pd(1) | 139(4) |
| C(22)-N(2)-Pd(1) | 109(3) | C(61)-N(3)-C(63) | 113(5) |
| C(61)-N(3)-Pd(2) | 131(4) | C(63)-N(3)-Pd(2) | 113(4) |
| C(66)-N(4)-C(64) | 107(5) | C(66)-N(4)-Pd(2) | 133(5) |
| C(64)-N(4)-Pd(2) | 118(3) | C(19)-O(1)-C(20) | 115(4) |
| C(24)-O(2)-C(23) | 109(4) | C(61)-O(3)-C(62) | 113(4) |
| C(66)-O(4)-C(65) | 105(5) | C(6)-C(1)-C(2) | 125(7) |
| C(6)-C(1)-P(1) | 117(5) | C(2)-C(1)-P(1) | 116(5) |
| C(3)-C(2)-C(1) | 110(7) | C(2)-C(3)-C(4) | 117(7) |
| C(5)-C(4)-C(3) | 127(10) | C(4)-C(5)-C(6) | 125(10) |
| C(1)-C(6)-C(5) | 113(8) | C(12)-C(7)-C(8) | 116(6) |
| C(12)-C(7)-P(1) | 120(5) | C(8)-C(7)-P(1) | 124(4) |
| C(9)-C(8)-C(7) | 129(6) | C(10)-C(9)-C(8) | 110(7) |
| C(9)-C(10)-C(11) | 131(10) | C(12)-C(11)-C(10) | 118(9) |
| C(11)-C(12)-C(7) | 115(7) | C(14)-C(13)-C(18) | 112(5) |
| C(14)-C(13)-P(1) | 119(4) | C(18)-C(13)-P(1) | 128(4) |
| C(13)-C(14)-C(15) | 128(6) | C(14)-C(15)-C(16) | 100(6) |
| C(17)-C(16)-C(15) | 141(8) | C(18)-C(17)-C(16) | 111(6) |
| C(17)-C(18)-C(13) | 128(5) | C(17)-C(18)-C(19) | 113(5) |
| C(13)-C(18)-C(19) | 119(5) | N(1)-C(19)-O(1) | 111(5) |
| N(1)-C(19)-C(18) | 130(5) | O(1)-C(19)-C(18) | 118(5) |
| O(1)-C(20)-C(21) | 96(4) | C(22)-C(21)-N(1) | 114(5) |
| C(22)-C(21)-C(20) | 122(5) | N(1)-C(21)-C(20) | 103(4) |
| C(21)-C(22)-N(2) | 110(5) | C(21)-C(22)-C(23) | 126(5) |
| N(2)-C(22)-C(23) | 100(4) | O(2)-C(23)-C(22) | 107(4) |
| N(2)-C(24)-O(2) | 117(4) | N(2)-C(24)-C(25) | 114(4) |
| O(2)-C(24)-C(25) | 129(4) | C(30)-C(25)-C(24) | 134(5) |
| C(30)-C(25)-C(26) | 125(6) | C(24)-C(25)-C(26) | 100(4) |
| C(27)-C(26)-C(25) | 115(5) | C(26)-C(27)-C(28) | 118(5) |
| C(29)-C(28)-C(27) | 121(4) | C(30)-C(29)-C(28) | 120(4) |

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**Table S2c**. Continues

| | | | |
|---|---|---|---|
| C(25)-C(30)-C(29) | 120(5) | C(25)-C(30)-P(2) | 120(4) |
| C(29)-C(30)-P(2) | 118(3) | C(36)-C(31)-C(32) | 113(5) |
| C(36)-C(31)-P(2) | 121(5) | C(32)-C(31)-P(2) | 125(4) |
| C(33)-C(32)-C(31) | 128(6) | C(32)-C(33)-C(34) | 114(6) |
| C(35)-C(34)-C(33) | 130(7) | C(34)-C(35)-C(36) | 108(6) |
| C(31)-C(36)-C(35) | 125(6) | C(38)-C(37)-C(42) | 114(6) |
| C(38)-C(37)-P(2) | 122(5) | C(42)-C(37)-P(2) | 124(5) |
| C(39)-C(38)-C(37) | 124(8) | C(38)-C(39)-C(41) | 127(9) |
| C(41)-C(40)-C(42) | 120(7) | C(40)-C(41)-C(39) | 112(8) |
| C(40)-C(42)-C(37) | 123(6) | C(44)-C(43)-C(48) | 116(7) |
| C(44)-C(43)-P(3) | 126(5) | C(48)-C(43)-P(3) | 117(6) |
| C(43)-C(44)-C(45) | 123(6) | C(46)-C(45)-C(44) | 128(7) |
| C(45)-C(46)-C(47) | 121(8) | C(46)-C(47)-C(48) | 113(8) |
| C(43)-C(48)-C(47) | 118(8) | C(54)-C(49)-C(50) | 118(8) |
| C(54)-C(49)-P(3) | 112(5) | C(50)-C(49)-P(3) | 129(7) |
| C(49)-C(50)-C(51) | 125(9) | C(52)-C(51)-C(50) | 116(10) |
| C(51)-C(52)-C(53) | 121(10) | C(52)-C(53)-C(54) | 111(9) |
| C(49)-C(54)-C(53) | 125(8) | C(56)-C(55)-C(60) | 116(5) |
| C(56)-C(55)-P(3) | 116(4) | C(60)-C(55)-P(3) | 128(3) |
| C(55)-C(56)-C(57) | 125(5) | C(58)-C(57)-C(56) | 108(5) |
| C(59)-C(58)-C(57) | 127(6) | C(58)-C(59)-C(60) | 119(6) |
| C(61)-C(60)-C(55) | 116(4) | C(61)-C(60)-C(59) | 121(5) |
| C(55)-C(60)-C(59) | 123(5) | O(3)-C(61)-C(60) | 116(5) |
| O(3)-C(61)-N(3) | 108(5) | C(60)-C(61)-N(3) | 136(5) |
| O(3)-C(62)-C(63) | 107(5) | N(3)-C(63)-C(62) | 97(5) |
| N(3)-C(63)-C(64) | 110(5) | C(62)-C(63)-C(64) | 121(6) |
| N(4)-C(64)-C(65) | 109(5) | N(4)-C(64)-C(63) | 103(5) |
| C(65)-C(64)-C(63) | 117(5) | N(4)-C(64)-C(66) | 32(3) |
| C(65)-C(64)-C(66) | 78(4) | C(63)-C(64)-C(66) | 122(5) |
| O(4)-C(65)-C(64) | 102(5) | N(4)-C(66)-O(4) | 116(6) |
| N(4)-C(66)-C(67) | 134(7) | O(4)-C(66)-C(67) | 110(6) |
| N(4)-C(66)-C(64) | 41(3) | O(4)-C(66)-C(64) | 75(4) |
| C(67)-C(66)-C(64) | 175(6) | C(72)-C(67)-C(68) | 118(5) |
| C(72)-C(67)-C(66) | 120(5) | C(68)-C(67)-C(66) | 122(5) |
| C(69)-C(68)-C(67) | 114(5) | C(70)-C(69)-C(68) | 129(7) |
| C(69)-C(70)-C(71) | 115(8) | C(72)-C(71)-C(70) | 126(7) |
| C(67)-C(72)-C(71) | 117(5) | C(67)-C(72)-P(4) | 124(4) |
| C(71)-C(72)-P(4) | 118(5) | C(78)-C(73)-C(74) | 125(7) |
| C(78)-C(73)-P(4) | 107(5) | C(74)-C(73)-P(4) | 127(6) |
| C(75)-C(74)-C(73) | 121(7) | C(76)-C(75)-C(74) | 120(7) |
| C(75)-C(76)-C(77) | 115(7) | C(76)-C(77)-C(78) | 134(8) |
| C(73)-C(78)-C(77) | 104(6) | P(4)-C(79)-C(84) | 115(5) |
| P(4)-C(79)-C(80) | 125(7) | C(84)-C(79)-C(80) | 120(8) |
| C(81)-C(80)-C(79) | 122(10) | C(82)-C(81)-C(80) | 118(10) |
| C(83)-C(82)-C(81) | 126(10) | C(82)-C(83)-C(84) | 119(8) |
| C(83)-C(84)-C(79) | 113(6) | | |

Symmetry transformations used to generate equivalent atoms:

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**Table S2d**. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for **19a**.The anisotropic displacement factor exponent takes the form: $-2\ \phi^{\ 2}\ [\ h^2\ a^2\ U_{11} + ... + 2\ h\ k\ a^*\ b^*\ U_{12}\ ]$

| | U11 | U22 | U33 | U23 | U13 | U12 |
|---|---|---|---|---|---|---|
| Pd(1) | 50(3) | 38(2) | 45(2) | 6(2) | 0(3) | -5(2) |
| Pd(2) | 41(2) | 38(2) | 45(2) | 4(2) | -1(2) | -2(2) |
| P(1) | 45(9) | 52(9) | 44(8) | 2(8) | -8(8) | -15(9) |
| P(2) | 39(9) | 46(9) | 44(8) | 1(8) | 1(7) | 4(8) |
| P(3) | 26(8) | 45(9) | 67(10) | 1(8) | 1(8) | -3(7) |
| P(4) | 37(8) | 56(10) | 49(9) | 2(7) | -2(9) | -17(9) |
| Cl(1) | 54(10) | 66(10) | 82(11) | 19(8) | 9(9) | -15(8) |
| Cl(2A) | 50(14) | 81(15) | 61(14) | -17(11) | -12(12) | 42(12) |

**Table S2e**.Hydrogen coordinates ( $\times 10^4$) and isotropic displacement parameters ($Å^2 \times 10^3$) for **18a**

| | x | y | z | U(eq) |
|---|---|---|---|---|
| H(2) | 1439 | 6993 | 1280 | 78 |
| H(3) | 3114 | 6599 | 964 | 134 |
| H(4) | 4870 | 7159 | 1068 | 117 |
| H(5) | 5325 | 7413 | 1519 | 130 |
| H(6) | 3998 | 7900 | 1858 | 100 |
| H(8) | 441 | 8020 | 1261 | 79 |
| H(9) | -1419 | 8019 | 975 | 96 |
| H(10) | -2903 | 7627 | 1272 | 144 |
| H(11) | -2902 | 7445 | 1789 | 138 |
| H(12) | -837 | 7269 | 2077 | 106 |
| H(14) | 2188 | 8769 | 1506 | 71 |
| H(15) | 2302 | 10001 | 1475 | 78 |
| H(16) | 2053 | 10403 | 2014 | 103 |
| H(17) | 1557 | 9981 | 2423 | 35 |
| H(20A) | -242 | 8938 | 3152 | 112 |
| H(20B) | 1061 | 8900 | 3304 | 112 |
| H(21) | -71 | 7827 | 2989 | 97 |
| H(22) | 2298 | 7794 | 3136 | 72 |
| H(23A) | 1912 | 7361 | 3605 | 72 |
| H(23B) | 544 | 7296 | 3526 | 72 |
| H(26) | 1271 | 5312 | 3371 | 88 |
| H(27) | 1273 | 4133 | 3216 | 57 |
| H(28) | 1304 | 3869 | 2646 | 42 |
| H(29) | 1844 | 4731 | 2254 | 38 |
| H(32) | 4112 | 7017 | 2408 | 75 |
| H(33) | 6059 | 6940 | 2428 | 52 |
| H(34) | 6895 | 6026 | 2170 | 86 |
| H(35) | 5956 | 5060 | 2050 | 85 |
| H(36) | 3751 | 5198 | 2061 | 73 |
| H(38) | -280 | 5921 | 2110 | 89 |
| H(39) | -1339 | 5531 | 1675 | 161 |
| H(40) | 1564 | 5150 | 1169 | 97 |
| H(41) | -553 | 5118 | 1197 | 130 |
| H(42) | 2675 | 5614 | 1630 | 104 |
| H(44) | 7906 | 11180 | 916 | 91 |
| H(45) | 9888 | 11122 | 959 | 58 |

**Table S2e.** Continues

| | | | | |
|---|---|---|---|---|
| H(46) | 10889 | 10272 | 901 | 93 |
| H(47) | 10030 | 9206 | 993 | 162 |
| H(48) | 7661 | 9199 | 963 | 132 |
| H(50) | 6522 | 9360 | 386 | 139 |
| H(51) | 5947 | 8239 | 232 | 174 |
| H(52) | 4008 | 8039 | 296 | 189 |
| H(53) | 2943 | 8594 | 795 | 156 |
| H(54) | 3935 | 9533 | 995 | 94 |
| H(56) | 5861 | 9077 | 1318 | 74 |
| H(57) | 5966 | 8756 | 1896 | 54 |
| H(58) | 5051 | 9570 | 2206 | 84 |
| H(59) | 5148 | 10711 | 2069 | 70 |
| H(62A) | 5163 | 12663 | 1765 | 95 |
| H(62B) | 3908 | 12391 | 1651 | 95 |
| H(63) | 5940 | 12563 | 1263 | 120 |
| H(64) | 3526 | 12414 | 1038 | 80 |
| H(65A) | 3564 | 13476 | 953 | 68 |
| H(65B) | 4929 | 13517 | 1049 | 68 |
| H(68) | 5576 | 13603 | 47 | 83 |
| H(69) | 6340 | 13406 | -511 | 103 |
| H(70) | 6647 | 12416 | -741 | 112 |
| H(71) | 6108 | 11456 | -436 | 121 |
| H(74) | 3849 | 11232 | -397 | 107 |
| H(75) | 2213 | 10591 | -625 | 101 |
| H(76) | 1028 | 10064 | -282 | 70 |
| H(77) | 1926 | 9697 | 186 | 127 |
| H(78) | 3458 | 10228 | 472 | 85 |
| H(80) | 5239 | 9937 | -221 | 187 |
| H(81) | 6805 | 9123 | -415 | 220 |
| H(82) | 8702 | 9269 | -241 | 130 |
| H(83) | 9395 | 10291 | -50 | 134 |
| H(84) | 7898 | 11051 | 277 | 104 |