C30 H36 Co O P WART_KAKO23 - 9-NOV-99 : 19:26:38

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SUPPLEMENTARY MATERIAL
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BELONGING TO THE PAPER

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Reactions of Cyclopropenone Derivatives with a Cyclopentadienylcobalt(I) Chelate: Formation of a Cobaltacyclobutenone and a Transformation of 2,2-Dimethoxycyclopropenone to Methyl Acrylate at Cobalt

by
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Submitted to

Organometallics

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Table S1 - Crystal Data and Details of the Structure Determination
for: C30 H36 Co O P WART_KAKO23

Crystal Data

Compound number in the paper 6

CCDC-No. 137406

Empirical Formula C 30 H 36 Co O P

Formula Weight 502.52

Crystal System Monoclinic

Space group P 21/c (No. 14)

a, b, c [Angstrom] 11.445(2) 13.275(2) 17.294(2)

alpha, beta, gamma [deg] 90 99.50(2) 90

V [Ang**3] 2591.5(7)

Z 4

D(obs), D(calc) [g/cm**3] 0.000, 1.288

F(000) [Electrons] 1064

Mu(MoKa) [/cm] 7.4

Crystal: color redbrown, size [mm] 1.04 x 0.78 x 1.85

Data Collection

Diffractometer (19.10.1999) Stoe IPDS (Imaging Plate)
(For technical details compare ref. 1 and 2)

Temperature (K) 300

Radiation [Angstrom] MoKa 0.71073
(fine-focus sealed tube, graphite monochromator)

2Theta min,max [Deg] 3.6, 48.1

Scan type 160 exposures, delta phi 1.4 degrees

Dataset hkl-limits -13: 13 ; -15: 15 ; -18: 19

Total Data (after omitting 14 overloaded reflections) 18647

Data Reduction

Program used Stoe IPDS software and SHELXL

Unique Data 3894

Averaging symmetry equivalents, internal R(I) 0.044

Completeness of unique data set 95.7 %

Absorption correction spherical, mue*R = 0.53
min., max. transmission factors 0.4618, 0.4687

Extinction correction none

Observed data [I > 2.0 sigma(I)] 3194

Structure Solution

Direct methods, Program used SHELXS-86

Refinement

Program used (last cycle 9.11.1999, 19:20) SHELXL-93

Nref, Npar 3894, 298

R1, wR2, S 0.0265, 0.0656, 1.22

w = 1/(sig^2(Fo^2)+(0.03*P)^2)
where P=(max(Fo^2,0)+2*Fc^2)/3

Min. and Max. resd. dens. [e/Ang^3] -0.19, 0.24

Remarks

R1 is based on F of 3194 reflections with Fo>4sig(Fo)

wR2 is based on F^2 of all 3894 unique reflections

Hydrogen atoms in geometrically calculated positions

Programs used for plots MOPLO, PLATON

Program used for checks and tables PLATON

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Table S2 - Final Coordinates and Equivalent Isotropic Thermal Parameters of the non-Hydrogen atoms
for: C30 H36 Co O P WART_KAKO23

Atom	x	y	z	U(eq) [Ang^2]
Co(1)	0.24018(2)	0.10130(2)	0.23257(2)	0.0348(1)
P(1)	0.21827(4)	0.23549(4)	0.30802(3)	0.0330(2)
O(1)	0.05937(12)	-0.02739(11)	0.28049(10)	0.0598(6)
C(1)	0.17440(19)	0.19751(16)	0.13810(12)	0.0470(8)
C(2)	0.1135(2)	0.10454(18)	0.13073(13)	0.0557(8)
C(3)	0.1956(2)	0.02755(19)	0.12507(13)	0.0603(9)
C(4)	0.3077(2)	0.07243(19)	0.12753(13)	0.0570(9)
C(5)	0.29568(19)	0.17682(17)	0.13460(12)	0.0502(8)
C(6)	0.1231(2)	0.29672(17)	0.15584(13)	0.0560(8)
C(7)	0.18206(18)	0.33722(15)	0.23498(12)	0.0450(7)
C(8)	0.08893(17)	0.23513(16)	0.36391(13)	0.0460(7)
C(9)	-0.02197(18)	0.21425(19)	0.30290(16)	0.0629(9)
C(10)	0.0706(2)	0.33499(18)	0.40494(16)	0.0672(10)
C(11)	0.1026(2)	0.15086(19)	0.42543(15)	0.0609(9)
C(12)	0.35508(16)	0.28837(14)	0.37176(12)	0.0395(7)
C(13)	0.45408(17)	0.28880(16)	0.32164(14)	0.0493(8)
C(14)	0.3430(2)	0.39702(16)	0.40049(16)	0.0602(9)
C(15)	0.3915(2)	0.21957(17)	0.44274(13)	0.0536(8)
C(16)	0.16213(17)	-0.00197(14)	0.28450(13)	0.0410(7)
C(17)	0.27133(15)	-0.04801(13)	0.32446(12)	0.0362(6)
C(18)	0.27765(16)	-0.14426(14)	0.36926(12)	0.0377(6)
C(19)	0.35557(19)	-0.22086(15)	0.35862(14)	0.0493(8)
C(20)	0.3563(2)	-0.31015(16)	0.39917(15)	0.0587(9)
C(21)	0.2793(2)	-0.32585(16)	0.45055(15)	0.0607(9)
C(22)	0.2010(2)	-0.25125(18)	0.46126(16)	0.0630(9)
C(23)	0.19944(18)	-0.16149(16)	0.42107(14)	0.0504(8)
C(24)	0.35251(16)	0.01626(13)	0.30211(11)	0.0339(6)

Table S2 - Final Coordinates and Equivalent Isotropic Thermal Parameters of the non-Hydrogen atoms (continued)
for: C30 H36 Co O P WART_KAKO23

Atom	x	y	z	U(eq) [Ang^2]
C(25)	0.48198(15)	0.01620(13)	0.32575(11)	0.0345(6)
C(26)	0.55673(16)	0.05812(14)	0.27838(13)	0.0415(7)
C(27)	0.67743(18)	0.06697(16)	0.30357(15)	0.0507(8)
C(28)	0.72601(18)	0.03577(16)	0.37726(15)	0.0545(9)
C(29)	0.65459(18)	-0.00690(16)	0.42518(14)	0.0548(8)
C(30)	0.53444(17)	-0.01744(14)	0.39992(12)	0.0430(7)

U(eq) = 1/3 of the trace of the orthogonalized U

Table S3 - Hydrogen Atom Positions and Isotropic Thermal Parameters
for: C30 H36 Co O P WART_KAKO23

Atom	x	y	z	U(iso) [Ang^2]
H(1)	0.0326(2)	0.09587(18)	0.12978(13)	0.0668
H(2)	0.1790(2)	-0.04098(19)	0.12050(13)	0.0724
H(3)	0.3780(2)	0.03839(19)	0.12490(13)	0.0684
H(4)	0.35598(19)	0.22419(17)	0.13665(12)	0.0603
H(5)	0.0388(2)	0.28899(17)	0.15583(13)	0.0672
H(6)	0.1334(2)	0.34469(17)	0.11520(13)	0.0672
H(7)	0.12951(18)	0.38520(15)	0.25400(12)	0.0539
H(8)	0.25416(18)	0.37246(15)	0.22873(12)	0.0539
H(9)	-0.03129(18)	0.26665(19)	0.26411(16)	0.0755
H(10)	-0.09039(18)	0.21249(19)	0.32837(16)	0.0755
H(11)	-0.01354(18)	0.15058(19)	0.27809(16)	0.0755
H(12)	0.0618(2)	0.38864(18)	0.36720(16)	0.0807
H(13)	0.1379(2)	0.34813(18)	0.44470(16)	0.0807
H(14)	0.0005(2)	0.33069(18)	0.42860(16)	0.0807
H(15)	0.1142(2)	0.08773(19)	0.40069(15)	0.0731
H(16)	0.0324(2)	0.14732(19)	0.44900(15)	0.0731
H(17)	0.1698(2)	0.16478(19)	0.46510(15)	0.0731
H(18)	0.43182(17)	0.33181(16)	0.27701(14)	0.0592
H(19)	0.46630(17)	0.22155(16)	0.30418(14)	0.0592
H(20)	0.52598(17)	0.31331(16)	0.35239(14)	0.0592
H(21)	0.3201(2)	0.44052(16)	0.35623(16)	0.0723
H(22)	0.4175(2)	0.41902(16)	0.42937(16)	0.0723
H(23)	0.2837(2)	0.39929(16)	0.43381(16)	0.0723
H(24)	0.3300(2)	0.21894(17)	0.47435(13)	0.0643
H(25)	0.4635(2)	0.24420(17)	0.47329(13)	0.0643
H(26)	0.4038(2)	0.15244(17)	0.42507(13)	0.0643
H(27)	0.40821(19)	-0.21185(15)	0.32358(14)	0.0591

Table S3 - Hydrogen Atom Positions and Isotropic Thermal Parameters (continued)
for: C30 H36 Co O P WART_KAKO23

Atom	x	y	z	U(iso) [Ang^2]
H(28)	0.4098(2)	-0.36042(16)	0.39150(15)	0.0705
H(29)	0.2801(2)	-0.38630(16)	0.47782(15)	0.0728
H(30)	0.1482(2)	-0.26124(18)	0.49607(16)	0.0755
H(31)	0.14521(18)	-0.11185(16)	0.42881(14)	0.0604
H(32)	0.52457(16)	0.08073(14)	0.22850(13)	0.0498
H(33)	0.72550(18)	0.09411(16)	0.27044(15)	0.0609
H(34)	0.80679(18)	0.04331(16)	0.39493(15)	0.0654
H(35)	0.68774(18)	-0.02882(16)	0.47507(14)	0.0657
H(36)	0.48774(17)	-0.04734(14)	0.43271(12)	0.0516

The Temperature Factor has the Form of Exp(-T) Where
T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms

Table S4 - Anisotropic Thermal Parameters
for: C30 H36 Co O P WART_KAKO23

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
Co(1)	0.0350(2)	0.0381(2)	0.0302(2)	0.0015(1)	0.0018(1)	-0.0052(1)
P(1)	0.0322(3)	0.0352(3)	0.0321(3)	0.0070(2)	0.0066(2)	0.0024(2)
O(1)	0.0390(8)	0.0588(9)	0.0781(12)	0.0124(8)	-0.0005(8)	-0.0163(7)
C(1)	0.0528(13)	0.0585(14)	0.0268(12)	0.0098(9)	-0.0016(10)	-0.0043(10)
C(2)	0.0506(13)	0.0737(16)	0.0374(14)	0.0035(11)	-0.0083(10)	-0.0118(12)
C(3)	0.0772(17)	0.0606(15)	0.0383(14)	-0.0085(11)	-0.0045(12)	-0.0151(13)
C(4)	0.0634(15)	0.0732(17)	0.0339(14)	-0.0053(11)	0.0063(11)	0.0030(12)
C(5)	0.0536(13)	0.0681(16)	0.0292(13)	0.0042(10)	0.0076(10)	-0.0117(11)
C(6)	0.0571(13)	0.0625(15)	0.0448(15)	0.0213(11)	-0.0022(11)	0.0045(11)
C(7)	0.0465(12)	0.0453(12)	0.0437(14)	0.0140(10)	0.0092(10)	0.0067(9)
C(8)	0.0412(11)	0.0533(13)	0.0468(14)	0.0119(10)	0.0169(10)	0.0074(9)
C(9)	0.0347(11)	0.0774(17)	0.0782(19)	0.0214(14)	0.0136(11)	0.0029(11)
C(10)	0.0664(15)	0.0678(16)	0.076(2)	0.0040(13)	0.0375(14)	0.0146(12)
C(11)	0.0603(14)	0.0697(16)	0.0586(17)	0.0199(13)	0.0271(12)	0.0085(11)
C(12)	0.0424(11)	0.0355(11)	0.0398(13)	-0.0031(9)	0.0047(9)	0.0009(8)
C(13)	0.0397(11)	0.0461(12)	0.0619(16)	-0.0029(10)	0.0076(10)	-0.0050(9)
C(14)	0.0676(15)	0.0439(13)	0.0693(18)	-0.0140(12)	0.0115(13)	-0.0038(11)
C(15)	0.0584(14)	0.0577(14)	0.0403(14)	0.0007(10)	-0.0049(11)	0.0000(10)
C(16)	0.0406(12)	0.0377(11)	0.0440(13)	-0.0025(9)	0.0046(9)	-0.0098(9)
C(17)	0.0398(10)	0.0345(10)	0.0352(12)	-0.0004(8)	0.0084(8)	-0.0050(8)
C(18)	0.0398(10)	0.0344(10)	0.0383(12)	-0.0009(9)	0.0044(9)	-0.0078(8)
C(19)	0.0601(13)	0.0414(12)	0.0510(15)	0.0007(10)	0.0230(11)	-0.0010(10)
C(20)	0.0756(16)	0.0368(12)	0.0663(18)	0.0000(11)	0.0194(13)	0.0055(11)
C(21)	0.0811(17)	0.0397(13)	0.0625(18)	0.0124(11)	0.0156(13)	-0.0063(11)
C(22)	0.0702(15)	0.0610(15)	0.0652(18)	0.0145(13)	0.0334(13)	-0.0073(12)
C(23)	0.0496(12)	0.0453(13)	0.0598(16)	0.0061(11)	0.0195(11)	-0.0004(9)
C(24)	0.0373(10)	0.0338(10)	0.0309(12)	-0.0041(8)	0.0068(8)	-0.0022(8)

Table S4 - Anisotropic Thermal Parameters (continued)
for: C30 H36 Co O P WART_KAKO23

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
C(25)	0.0367(10)	0.0289(10)	0.0382(12)	-0.0035(8)	0.0073(9)	0.0001(7)
C(26)	0.0402(11)	0.0420(11)	0.0435(13)	0.0007(9)	0.0103(9)	0.0007(9)
C(27)	0.0401(12)	0.0491(13)	0.0668(17)	-0.0023(11)	0.0201(11)	-0.0026(9)
C(28)	0.0348(11)	0.0482(13)	0.0773(19)	-0.0018(12)	-0.0003(11)	0.0011(9)
C(29)	0.0484(13)	0.0519(13)	0.0583(16)	0.0095(11)	-0.0079(11)	-0.0002(10)
C(30)	0.0434(11)	0.0403(11)	0.0442(14)	0.0049(9)	0.0040(10)	-0.0031(8)

The Temperature Factor has the Form of Exp(-T) Where
T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms
T = 2*(Pi**2)*Sumij(h(i)*h(j)*U(i,j)*Astar(i)*Astar(j)), for
Anisotropic Atoms. Astar(i) are Reciprocal Axial Lengths and
h(i) are the Reflection Indices.

Table S5 - Bond Distances (Angstrom)
for: C30 H36 Co O P WART_KAKO23

Co(1)	-P(1) 2.2465(7)	C(18)	-C(23) 1.386(3)
Co(1)	-C(1) 2.112(2)	C(19)	-C(20) 1.377(3)
Co(1)	-C(2) 2.089(2)	C(20)	-C(21) 1.367(3)
Co(1)	-C(3) 2.089(2)	C(21)	-C(22) 1.369(3)
Co(1)	-C(4) 2.123(2)	C(22)	-C(23) 1.378(3)
Co(1)	-C(5) 2.153(2)	C(24)	-C(25) 1.471(3)
Co(1)	-C(16) 1.936(2)	C(25)	-C(26) 1.394(3)
Co(1)	-C(24) 1.9655(19)	C(25)	-C(30) 1.397(3)
P(1)	-C(7) 1.849(2)	C(26)	-C(27) 1.383(3)
P(1)	-C(8) 1.897(2)	C(27)	-C(28) 1.368(4)
P(1)	-C(12) 1.895(2)	C(28)	-C(29) 1.378(3)
O(1)	-C(16) 1.214(2)	C(29)	-C(30) 1.380(3)
C(1)	-C(2) 1.413(3)	C(2)	-H(1) 0.930(3)
C(1)	-C(5) 1.426(3)	C(3)	-H(2) 0.930(4)
C(1)	-C(6) 1.494(3)	C(4)	-H(3) 0.930(3)
C(2)	-C(3) 1.403(3)	C(5)	-H(4) 0.930(3)
C(3)	-C(4) 1.409(3)	C(6)	-H(5) 0.970(3)
C(4)	-C(5) 1.400(3)	C(6)	-H(6) 0.970(3)
C(6)	-C(7) 1.521(3)	C(7)	-H(7) 0.970(3)
C(8)	-C(9) 1.536(3)	C(7)	-H(8) 0.970(3)
C(8)	-C(10) 1.534(3)	C(9)	-H(9) 0.960(4)
C(8)	-C(11) 1.534(3)	C(9)	-H(10) 0.960(3)
C(12)	-C(13) 1.536(3)	C(9)	-H(11) 0.960(4)
C(12)	-C(14) 1.539(3)	C(10)	-H(12) 0.960(4)
C(12)	-C(15) 1.532(3)	C(10)	-H(13) 0.960(4)
C(16)	-C(17) 1.459(3)	C(10)	-H(14) 0.961(3)
C(17)	-C(18) 1.490(3)	C(11)	-H(15) 0.960(4)
C(17)	-C(24) 1.363(3)	C(11)	-H(16) 0.960(3)
C(18)	-C(19) 1.385(3)	C(11)	-H(17) 0.960(3)

Table S5 - Bond Distances (Angstrom) (continued)
for: C30 H36 Co O P WART_KAKO23

C(13) -H(18) 0.960(3) C(20) -H(28) 0.930(3)

C(13) -H(19) 0.960(3) C(21) -H(29) 0.930(3)

C(13) -H(20) 0.960(3) C(22) -H(30) 0.930(4)

C(14) -H(21) 0.960(4) C(23) -H(31) 0.930(3)

C(14) -H(22) 0.960(3) C(26) -H(32) 0.930(3)

C(14) -H(23) 0.961(4) C(27) -H(33) 0.930(3)

C(15) -H(24) 0.960(3) C(28) -H(34) 0.930(3)

C(15) -H(25) 0.960(3) C(29) -H(35) 0.930(3)

C(15) -H(26) 0.960(3) C(30) -H(36) 0.930(3)

C(19) -H(27) 0.930(3)

Table S6 - Bond Angles (Degrees)
for: C30 H36 Co O P WART_KAKO23

P(1) -Co(1) -C(1) 84.84(6) Co(1) -P(1) -C(8) 117.73(7)

P(1) -Co(1) -C(2) 110.18(7) Co(1) -P(1) -C(12) 118.10(6)

P(1) -Co(1) -C(3) 148.70(7) C(7) -P(1) -C(8) 104.13(10)

P(1) -Co(1) -C(4) 137.00(7) C(7) -P(1) -C(12) 101.38(9)

P(1) -Co(1) -C(5) 99.41(6) C(8) -P(1) -C(12) 110.12(9)

P(1) -Co(1) -C(16) 100.82(7) Co(1) -C(1) -C(2) 69.46(13)

P(1) -Co(1) -C(24) 102.97(6) Co(1) -C(1) -C(5) 72.01(12)

C(1) -Co(1) -C(2) 39.30(9) Co(1) -C(1) -C(6) 118.43(15)

C(1) -Co(1) -C(3) 65.88(9) C(2) -C(1) -C(5) 107.28(19)

C(1) -Co(1) -C(4) 65.22(9) C(2) -C(1) -C(6) 125.7(2)

C(1) -Co(1) -C(5) 39.05(9) C(5) -C(1) -C(6) 126.6(2)

C(1) -Co(1) -C(16) 130.85(9) Co(1) -C(2) -C(1) 71.24(13)

C(1) -Co(1) -C(24) 159.11(8) Co(1) -C(2) -C(3) 70.37(13)

C(2) -Co(1) -C(3) 39.24(9) C(1) -C(2) -C(3) 108.5(2)

C(2) -Co(1) -C(4) 65.31(9) Co(1) -C(3) -C(2) 70.39(13)

C(2) -Co(1) -C(5) 65.21(9) Co(1) -C(3) -C(4) 71.79(13)

C(2) -Co(1) -C(16) 95.54(9) C(2) -C(3) -C(4) 107.9(2)

C(2) -Co(1) -C(24) 145.15(9) Co(1) -C(4) -C(3) 69.14(13)

C(3) -Co(1) -C(4) 39.08(9) Co(1) -C(4) -C(5) 72.04(13)

C(3) -Co(1) -C(5) 65.05(9) C(3) -C(4) -C(5) 108.6(2)

C(3) -Co(1) -C(16) 90.99(9) Co(1) -C(5) -C(1) 68.94(12)

C(3) -Co(1) -C(24) 108.33(9) Co(1) -C(5) -C(4) 69.74(13)

C(4) -Co(1) -C(5) 38.21(9) C(1) -C(5) -C(4) 107.74(19)

C(4) -Co(1) -C(16) 122.01(9) C(1) -C(6) -C(7) 111.43(18)

C(4) -Co(1) -C(24) 97.25(9) P(1) -C(7) -C(6) 111.89(14)

C(5) -Co(1) -C(16) 155.99(9) P(1) -C(8) -C(9) 106.04(15)

C(5) -Co(1) -C(24) 120.06(8) P(1) -C(8) -C(10) 114.28(15)

C(16) -Co(1) -C(24) 67.34(8) P(1) -C(8) -C(11) 110.88(15)

Co(1) -P(1) -C(7) 102.49(7) C(9) -C(8) -C(10) 108.24(18)

Table S6 - Bond Angles (Degrees) (continued)
for: C30 H36 Co O P WART_KAKO23

C(9) -C(8) -C(11) 108.84(18) C(26) -C(27) -C(28) 119.9(2)

C(10) -C(8) -C(11) 108.39(19) C(27) -C(28) -C(29) 119.6(2)

P(1) -C(12) -C(13) 106.79(14) C(28) -C(29) -C(30) 120.7(2)

P(1) -C(12) -C(14) 115.17(14) C(25) -C(30) -C(29) 120.88(19)

P(1) -C(12) -C(15) 109.56(14) Co(1) -C(2) -H(1) 124.2(2)

C(13) -C(12) -C(14) 107.01(17) C(1) -C(2) -H(1) 125.8(3)

C(13) -C(12) -C(15) 109.02(17) C(3) -C(2) -H(1) 125.8(3)

C(14) -C(12) -C(15) 109.10(18) Co(1) -C(3) -H(2) 123.4(2)

Co(1) -C(16) -O(1) 133.38(16) C(2) -C(3) -H(2) 126.1(3)

Co(1) -C(16) -C(17) 95.26(13) C(4) -C(3) -H(2) 126.0(3)

O(1) -C(16) -C(17) 131.03(19) Co(1) -C(4) -H(3) 124.7(2)

C(16) -C(17) -C(18) 124.75(16) C(3) -C(4) -H(3) 125.7(3)

C(16) -C(17) -C(24) 100.03(16) C(5) -C(4) -H(3) 125.7(3)

C(18) -C(17) -C(24) 135.01(17) Co(1) -C(5) -H(4) 126.8(2)

C(17) -C(18) -C(19) 122.53(18) C(1) -C(5) -H(4) 126.1(3)

C(17) -C(18) -C(23) 119.78(17) C(4) -C(5) -H(4) 126.1(3)

C(19) -C(18) -C(23) 117.61(19) C(1) -C(6) -H(5) 109.3(2)

C(18) -C(19) -C(20) 121.0(2) C(1) -C(6) -H(6) 109.3(2)

C(19) -C(20) -C(21) 120.8(2) C(7) -C(6) -H(5) 109.3(2)

C(20) -C(21) -C(22) 119.0(2) C(7) -C(6) -H(6) 109.3(2)

C(21) -C(22) -C(23) 120.8(2) H(5) -C(6) -H(6) 108.0(3)

C(18) -C(23) -C(22) 120.8(2) P(1) -C(7) -H(7) 109.2(2)

Co(1) -C(24) -C(17) 97.20(13) P(1) -C(7) -H(8) 109.2(2)

Co(1) -C(24) -C(25) 134.24(13) C(6) -C(7) -H(7) 109.2(2)

C(17) -C(24) -C(25) 128.56(17) C(6) -C(7) -H(8) 109.2(2)

C(24) -C(25) -C(26) 121.62(17) H(7) -C(7) -H(8) 107.9(3)

C(24) -C(25) -C(30) 121.07(17) C(8) -C(9) -H(9) 109.5(2)

C(26) -C(25) -C(30) 117.05(17) C(8) -C(9) -H(10) 109.5(3)

C(25) -C(26) -C(27) 121.8(2) C(8) -C(9) -H(11) 109.5(2)

Table S6 - Bond Angles (Degrees) (continued)
for: C30 H36 Co O P WART_KAKO23

H(9) -C(9) -H(10) 109.5(3) C(12) -C(15) -H(24) 109.5(2)

H(9) -C(9) -H(11) 109.5(3) C(12) -C(15) -H(25) 109.5(2)

H(10) -C(9) -H(11) 109.5(3) C(12) -C(15) -H(26) 109.5(2)

C(8) -C(10) -H(12) 109.5(3) H(24) -C(15) -H(25) 109.5(3)

C(8) -C(10) -H(13) 109.5(3) H(24) -C(15) -H(26) 109.5(3)

C(8) -C(10) -H(14) 109.5(3) H(25) -C(15) -H(26) 109.5(3)

H(12) -C(10) -H(13) 109.5(3) C(18) -C(19) -H(27) 119.5(2)

H(12) -C(10) -H(14) 109.4(3) C(20) -C(19) -H(27) 119.5(2)

H(13) -C(10) -H(14) 109.5(3) C(19) -C(20) -H(28) 119.6(3)

C(8) -C(11) -H(15) 109.5(3) C(21) -C(20) -H(28) 119.6(3)

C(8) -C(11) -H(16) 109.5(3) C(20) -C(21) -H(29) 120.5(3)

C(8) -C(11) -H(17) 109.5(3) C(22) -C(21) -H(29) 120.5(3)

H(15) -C(11) -H(16) 109.5(3) C(21) -C(22) -H(30) 119.6(3)

H(15) -C(11) -H(17) 109.5(3) C(23) -C(22) -H(30) 119.6(3)

H(16) -C(11) -H(17) 109.5(3) C(18) -C(23) -H(31) 119.6(3)

C(12) -C(13) -H(18) 109.5(2) C(22) -C(23) -H(31) 119.6(3)

C(12) -C(13) -H(19) 109.5(2) C(25) -C(26) -H(32) 119.1(2)

C(12) -C(13) -H(20) 109.5(2) C(27) -C(26) -H(32) 119.1(2)

H(18) -C(13) -H(19) 109.5(3) C(26) -C(27) -H(33) 120.0(3)

H(18) -C(13) -H(20) 109.5(3) C(28) -C(27) -H(33) 120.0(3)

H(19) -C(13) -H(20) 109.5(3) C(27) -C(28) -H(34) 120.2(3)

C(12) -C(14) -H(21) 109.5(3) C(29) -C(28) -H(34) 120.2(3)

C(12) -C(14) -H(22) 109.5(2) C(28) -C(29) -H(35) 119.7(3)

C(12) -C(14) -H(23) 109.5(2) C(30) -C(29) -H(35) 119.7(3)

H(21) -C(14) -H(22) 109.5(3) C(25) -C(30) -H(36) 119.6(2)

H(21) -C(14) -H(23) 109.4(3) C(29) -C(30) -H(36) 119.6(2)

H(22) -C(14) -H(23) 109.5(3)

Table S7 - Torsion Angles (Degrees)
for: C30 H36 Co O P WART_KAKO23

C(1) -Co(1) -P(1) -C(7) -8.46(9)

C(2) -Co(1) -P(1) -C(7) -39.03(10)

C(3) -Co(1) -P(1) -C(7) -28.72(15)

C(4) -Co(1) -P(1) -C(7) 35.99(12)

C(5) -Co(1) -P(1) -C(7) 27.90(9)

C(16) -Co(1) -P(1) -C(7) -139.11(9)

C(24) -Co(1) -P(1) -C(7) 151.90(9)

C(1) -Co(1) -P(1) -C(8) 105.06(10)

C(2) -Co(1) -P(1) -C(8) 74.48(11)

C(3) -Co(1) -P(1) -C(8) 84.80(15)

C(4) -Co(1) -P(1) -C(8) 149.51(12)

C(5) -Co(1) -P(1) -C(8) 141.41(10)

C(16) -Co(1) -P(1) -C(8) -25.59(10)

C(24) -Co(1) -P(1) -C(8) -94.59(10)

C(1) -Co(1) -P(1) -C(12) -118.79(10)

C(2) -Co(1) -P(1) -C(12) -149.37(10)

C(3) -Co(1) -P(1) -C(12) -139.05(14)

C(4) -Co(1) -P(1) -C(12) -74.34(12)

C(5) -Co(1) -P(1) -C(12) -82.44(10)

C(16) -Co(1) -P(1) -C(12) 110.56(10)

C(24) -Co(1) -P(1) -C(12) 41.56(9)

P(1) -Co(1) -C(1) -C(2) -131.08(13)

C(3) -Co(1) -C(1) -C(2) 37.55(13)

C(4) -Co(1) -C(1) -C(2) 80.65(14)

C(5) -Co(1) -C(1) -C(2) 117.08(18)

C(16) -Co(1) -C(1) -C(2) -31.23(17)

C(24) -Co(1) -C(1) -C(2) 115.6(2)

P(1) -Co(1) -C(1) -C(5) 111.84(12)

C(2) -Co(1) -C(1) -C(5) -117.08(18)

Table S7 - Torsion Angles (Degrees) (continued)
for: C30 H36 Co O P WART_KAKO23

C(3) -Co(1) -C(1) -C(5) -79.53(14)

C(4) -Co(1) -C(1) -C(5) -36.43(13)

C(16) -Co(1) -C(1) -C(5) -148.31(13)

C(24) -Co(1) -C(1) -C(5) -1.5(3)

P(1) -Co(1) -C(1) -C(6) -10.68(16)

C(2) -Co(1) -C(1) -C(6) 120.4(2)

C(3) -Co(1) -C(1) -C(6) 158.0(2)

C(4) -Co(1) -C(1) -C(6) -158.9(2)

C(5) -Co(1) -C(1) -C(6) -122.5(2)

C(16) -Co(1) -C(1) -C(6) 89.17(19)

C(24) -Co(1) -C(1) -C(6) -124.0(2)

C(1) -Co(1) -C(24) -C(17) -150.5(2)

C(2) -Co(1) -C(24) -C(17) -62.5(2)

C(3) -Co(1) -C(24) -C(17) -80.33(14)

C(4) -Co(1) -C(24) -C(17) -118.86(13)

C(5) -Co(1) -C(24) -C(17) -151.56(12)

C(16) -Co(1) -C(24) -C(17) 2.87(13)

P(1) -Co(1) -C(24) -C(25) -80.62(19)

C(1) -Co(1) -C(24) -C(25) 29.5(3)

C(2) -Co(1) -C(24) -C(25) 117.5(2)

C(3) -Co(1) -C(24) -C(25) 99.71(19)

C(4) -Co(1) -C(24) -C(25) 61.2(2)

C(5) -Co(1) -C(24) -C(25) 28.5(2)

C(16) -Co(1) -C(24) -C(25) -177.1(2)

P(1) -Co(1) -C(2) -C(1) 53.11(13)

C(3) -Co(1) -C(2) -C(1) -118.43(19)

C(4) -Co(1) -C(2) -C(1) -80.42(14)

C(5) -Co(1) -C(2) -C(1) -38.16(13)

C(16) -Co(1) -C(2) -C(1) 156.80(13)

Table S7 - Torsion Angles (Degrees) (continued)
for: C30 H36 Co O P WART_KAKO23

C(24) -Co(1) -C(2) -C(1) -145.75(15)

P(1) -Co(1) -C(2) -C(3) 171.54(12)

C(1) -Co(1) -C(2) -C(3) 118.43(19)

C(4) -Co(1) -C(2) -C(3) 38.02(14)

C(5) -Co(1) -C(2) -C(3) 80.27(15)

C(16) -Co(1) -C(2) -C(3) -84.77(14)

C(24) -Co(1) -C(2) -C(3) -27.3(2)

C(4) -Co(1) -C(16) -C(17) 81.61(15)

C(5) -Co(1) -C(16) -C(17) 110.7(2)

P(1) -Co(1) -C(5) -C(1) -69.57(12)

P(1) -Co(1) -C(3) -C(2) -15.4(2)

C(1) -Co(1) -C(3) -C(2) -37.61(14)

C(4) -Co(1) -C(3) -C(2) -117.4(2)

C(5) -Co(1) -C(3) -C(2) -80.71(15)

C(16) -Co(1) -C(3) -C(2) 97.55(14)

C(24) -Co(1) -C(3) -C(2) 163.96(13)

P(1) -Co(1) -C(3) -C(4) 102.00(16)

C(1) -Co(1) -C(3) -C(4) 79.80(15)

C(2) -Co(1) -C(3) -C(4) 117.4(2)

C(5) -Co(1) -C(3) -C(4) 36.70(14)

C(16) -Co(1) -C(3) -C(4) -145.05(15)

C(24) -Co(1) -C(3) -C(4) -78.63(15)

C(2) -Co(1) -C(16) -C(17) 145.87(13)

C(3) -Co(1) -C(16) -C(17) 106.82(13)

C(24) -Co(1) -C(16) -C(17) -2.67(12)

P(1) -Co(1) -C(4) -C(3) -131.82(13)

C(1) -Co(1) -C(4) -C(3) -81.63(15)

C(2) -Co(1) -C(4) -C(3) -38.18(14)

C(5) -Co(1) -C(4) -C(3) -118.8(2)

Table S7 - Torsion Angles (Degrees) (continued)
for: C30 H36 Co O P WART_KAKO23

C(16) -Co(1) -C(4) -C(3) 42.50(17)

C(24) -Co(1) -C(4) -C(3) 110.26(14)

P(1) -Co(1) -C(4) -C(5) -12.97(17)

C(1) -Co(1) -C(4) -C(5) 37.21(13)

C(2) -Co(1) -C(4) -C(5) 80.67(14)

C(3) -Co(1) -C(4) -C(5) 118.8(2)

C(16) -Co(1) -C(4) -C(5) 161.34(13)

C(24) -Co(1) -C(4) -C(5) -130.89(13)

C(1) -Co(1) -C(16) -C(17) 165.13(12)

C(24) -Co(1) -C(5) -C(1) 179.40(12)

P(1) -Co(1) -C(5) -C(4) 171.07(12)

C(1) -Co(1) -C(5) -C(4) -119.36(18)

C(2) -Co(1) -C(5) -C(1) 38.40(13)

C(3) -Co(1) -C(5) -C(1) 81.84(14)

C(4) -Co(1) -C(5) -C(1) 119.36(18)

C(16) -Co(1) -C(5) -C(1) 77.6(2)

P(1) -Co(1) -C(16) -O(1) 83.9(2)

C(1) -Co(1) -C(16) -O(1) -8.6(3)

C(2) -Co(1) -C(16) -O(1) -27.9(2)

C(2) -Co(1) -C(5) -C(4) -80.96(14)

C(3) -Co(1) -C(5) -C(4) -37.51(14)

C(16) -Co(1) -C(5) -C(4) -41.8(3)

C(24) -Co(1) -C(5) -C(4) 60.04(15)

P(1) -Co(1) -C(16) -C(17) -102.33(12)

C(4) -Co(1) -C(16) -O(1) -92.1(2)

C(5) -Co(1) -C(16) -O(1) -63.0(3)

C(3) -Co(1) -C(16) -O(1) -66.9(2)

C(24) -Co(1) -C(16) -O(1) -176.4(2)

P(1) -Co(1) -C(24) -C(17) 99.33(12)

Table S7 - Torsion Angles (Degrees) (continued)
for: C30 H36 Co O P WART_KAKO23

C(8) -P(1) -C(7) -C(6) -96.32(16)

C(7) -P(1) -C(12) -C(15) 173.45(14)

Co(1) -P(1) -C(12) -C(15) -75.60(15)

C(7) -P(1) -C(12) -C(14) 50.04(17)

C(12) -P(1) -C(7) -C(6) 149.32(15)

Co(1) -P(1) -C(8) -C(9) -53.01(16)

Co(1) -P(1) -C(7) -C(6) 26.86(16)

C(12) -P(1) -C(8) -C(9) 167.60(14)

C(8) -P(1) -C(12) -C(14) -59.78(18)

Co(1) -P(1) -C(12) -C(14) 160.99(14)

C(7) -P(1) -C(8) -C(10) -59.55(18)

C(12) -P(1) -C(8) -C(10) 48.45(19)

Co(1) -P(1) -C(8) -C(11) 64.99(17)

C(7) -P(1) -C(8) -C(9) 59.60(16)

C(12) -P(1) -C(8) -C(11) -74.41(17)

C(8) -P(1) -C(12) -C(15) 63.63(16)

Co(1) -P(1) -C(8) -C(10) -172.16(14)

C(8) -P(1) -C(12) -C(13) -178.44(13)

C(7) -P(1) -C(8) -C(11) 177.59(16)

Co(1) -P(1) -C(12) -C(13) 42.34(15)

C(7) -P(1) -C(12) -C(13) -68.62(14)

Co(1) -C(1) -C(5) -C(4) 59.15(15)

C(2) -C(1) -C(5) -C(4) -1.7(2)

C(6) -C(1) -C(5) -Co(1) 112.5(2)

C(2) -C(1) -C(5) -Co(1) -60.83(15)

C(6) -C(1) -C(2) -C(3) -171.7(2)

Co(1) -C(1) -C(2) -C(3) -60.83(16)

Co(1) -C(1) -C(6) -C(7) 30.6(2)

C(6) -C(1) -C(5) -C(4) 171.6(2)

Table S7 - Torsion Angles (Degrees) (continued)
for: C30 H36 Co O P WART_KAKO23

C(5) -C(1) -C(6) -C(7) -57.4(3)

C(6) -C(1) -C(2) -Co(1) -110.9(2)

C(2) -C(1) -C(6) -C(7) 114.7(2)

C(5) -C(1) -C(2) -C(3) 1.7(2)

C(5) -C(1) -C(2) -Co(1) 62.49(15)

C(1) -C(2) -C(3) -C(4) -1.0(3)

Co(1) -C(2) -C(3) -C(4) -62.38(16)

C(1) -C(2) -C(3) -Co(1) 61.38(16)

C(2) -C(3) -C(4) -C(5) -0.1(3)

Co(1) -C(3) -C(4) -C(5) -61.55(16)

C(2) -C(3) -C(4) -Co(1) 61.48(16)

C(3) -C(4) -C(5) -C(1) 1.1(2)

C(3) -C(4) -C(5) -Co(1) 59.73(16)

Co(1) -C(4) -C(5) -C(1) -58.65(15)

C(1) -C(6) -C(7) -P(1) -36.9(2)

O(1) -C(16) -C(17) -C(24) 177.6(2)

O(1) -C(16) -C(17) -C(18) 2.2(4)

Co(1) -C(16) -C(17) -C(18) -171.74(17)

Co(1) -C(16) -C(17) -C(24) 3.61(16)

C(16) -C(17) -C(18) -C(19) 131.4(2)

C(18) -C(17) -C(24) -C(25) -9.0(4)

C(16) -C(17) -C(18) -C(23) -45.3(3)

C(24) -C(17) -C(18) -C(19) -42.1(3)

C(24) -C(17) -C(18) -C(23) 141.2(2)

C(16) -C(17) -C(24) -Co(1) -3.56(15)

C(16) -C(17) -C(24) -C(25) 176.40(19)

C(18) -C(17) -C(24) -Co(1) 171.0(2)

C(17) -C(18) -C(23) -C(22) 177.9(2)

C(17) -C(18) -C(19) -C(20) -177.8(2)

Table S7 - Torsion Angles (Degrees) (continued)
for: C30 H36 Co O P WART_KAKO23

C(23) -C(18) -C(19) -C(20) -1.1(3)

C(19) -C(18) -C(23) -C(22) 1.0(3)

C(18) -C(19) -C(20) -C(21) 0.6(4)

C(19) -C(20) -C(21) -C(22) 0.0(13)

C(20) -C(21) -C(22) -C(23) 0.0(4)

C(21) -C(22) -C(23) -C(18) -0.5(4)

Co(1) -C(24) -C(25) -C(26) -25.3(3)

Co(1) -C(24) -C(25) -C(30) 148.65(16)

C(17) -C(24) -C(25) -C(26) 154.8(2)

C(17) -C(24) -C(25) -C(30) -31.3(3)

C(24) -C(25) -C(26) -C(27) 173.66(18)

C(30) -C(25) -C(26) -C(27) -0.5(3)

C(24) -C(25) -C(30) -C(29) -172.63(18)

C(26) -C(25) -C(30) -C(29) 1.6(3)

C(25) -C(26) -C(27) -C(28) -1.2(3)

C(26) -C(27) -C(28) -C(29) 1.8(3)

C(27) -C(28) -C(29) -C(30) -0.7(3)

C(28) -C(29) -C(30) -C(25) -1.0(3)

C19 H32 Co O2 P WART_KAKO15 - 12-NOV-99 : 17:46:21

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SUPPLEMENTARY MATERIAL
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BELONGING TO THE PAPER

Reactions of Cyclopropenone Derivatives with a Cyclopentadienylcobalt(I) Chelate: Formation of a Cobaltacyclobutenone and a Transformation of 2,2-Dimethoxycyclopropenone to Methyl Acrylate at Cobalt

by
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Submitted to

Organometallics

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for: C19 H32 Co O2 P WART_KAKO15

Table S1 - Crystal Data and Details of the Structure Determination
for: C19 H32 Co O2 P WART_KAKO15

Crystal Data

Compound number in the paper 13

CCDC-No. 137405

Empirical Formula C 19 H 32 Co O 2 P

Formula Weight 382.35

Crystal System Monoclinic

Space group P 21/a (No. 14)

a, b, c [Angstrom] 17.748(2) 13.011(2) 17.979(2)

alpha, beta, gamma [deg] 90 108.66(1) 90

V [Ang**3] 3933.5(9)

Z 8

D(obs), D(calc) [g/cm**3] 0.000, 1.291

F(000) [Electrons] 1632

Mu(MoKa) [/cm] 9.6

Crystal: plate || (001), redbrown, size [mm] 0.44 x 0.31 x 0.03

Data Collection

Diffractometer (2.8.1999) Stoe IPDS (Imaging Plate)
(For technical details compare ref. 1 and 2)

Temperature (K) 300

Radiation [Angstrom] MoKa 0.71073
(fine-focus sealed tube, graphite monochromator)

2Theta min,max [Deg] 3.9, 48.3

Scan type 140 exposures, delta phi 1.4 degrees

Dataset hkl-limits -18: 18 ; -14: 14 ; -20: 20

Total Data 24680

Data Reduction

Program used Stoe IPDS software and SHELXL

Unique Data 5871

Averaging symmetry equivalents, internal R(I) 0.100

Completeness of data set 94.3 %

Absorption correction numerical
Min.,max. transmission factors 0.7081, 0.9714

Extinction correction none

Observed data [I > 2.0 sigma(I)] 2520

Structure Solution

Direct methods, Program used SHELXS-86

Refinement

Program used (last cycle 12.11.1999, 17:39) SHELXL-93

Nref, Npar 5871, 439

R1, wR2, S 0.0331, 0.0529, 0.63

w = 1/(sig^2(Fo^2))

Min. and Max. resd. dens. [e/Ang^3] -0.29, 0.26

Remarks

R1 is based on F of 2520 reflections with Fo>4sig(Fo)

wR2 is based on F^2 of all 5871 unique reflections

Hydrogen atoms in geometrically calculated positions, but
H27, H28, H29, H27', H28' and H29' free

Programs used for plots PLATON

Program used for checks and tables PLATON

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Table S2 - Final Coordinates and Equivalent Isotropic Thermal Parameters of the non-Hydrogen atoms
for: C19 H32 Co O2 P WART_KAKO15

Atom	x	y	z	U(eq) [Ang^2]
Co(1)	0.11508(3)	0.38002(4)	0.28443(3)	0.0435(2)
P(1)	0.18901(7)	0.24840(8)	0.34458(6)	0.0419(4)
O(1)	0.0516(2)	0.6251(3)	0.31689(19)	0.0982(16)
O(2)	0.0512(2)	0.5436(2)	0.42564(19)	0.0823(14)
C(1)	0.0646(3)	0.2785(3)	0.1967(3)	0.0542(19)
C(2)	0.0087(3)	0.2985(4)	0.2353(3)	0.063(2)
C(3)	-0.0073(3)	0.4041(4)	0.2304(3)	0.0649(19)
C(4)	0.0368(3)	0.4514(4)	0.1880(3)	0.072(2)
C(5)	0.0788(3)	0.3721(5)	0.1635(2)	0.073(2)
C(6)	0.1024(3)	0.1775(3)	0.1962(2)	0.076(2)
C(7)	0.1407(2)	0.1388(3)	0.2813(2)	0.0578(17)
C(8)	0.1805(3)	0.2047(3)	0.4419(3)	0.0582(19)
C(9)	0.2371(3)	0.2652(4)	0.5114(2)	0.106(3)
C(10)	0.0960(3)	0.2279(3)	0.4393(2)	0.084(2)
C(11)	0.1953(3)	0.0900(3)	0.4583(3)	0.088(3)
C(12)	0.2953(3)	0.2407(3)	0.3464(3)	0.0628(17)
C(13)	0.2958(3)	0.2619(4)	0.2630(3)	0.101(3)
C(14)	0.3472(3)	0.3247(4)	0.3994(3)	0.100(3)
C(15)	0.3366(3)	0.1367(4)	0.3710(3)	0.095(2)
C(16)	0.1868(4)	0.4986(4)	0.3159(4)	0.076(3)
C(17)	0.1433(3)	0.4886(3)	0.3676(3)	0.058(2)
C(18)	0.0799(3)	0.5598(4)	0.3648(3)	0.061(2)
C(19)	-0.0131(3)	0.6079(4)	0.4288(3)	0.109(3)
Co(1')	0.36636(3)	0.63395(4)	0.12853(3)	0.0423(2)
P(1')	0.26529(7)	0.74394(8)	0.09509(6)	0.0417(4)
O(1')	0.46220(19)	0.4621(2)	0.28150(16)	0.0671(14)

Table S2 - Final Coordinates and Equivalent Isotropic Thermal Parameters of the non-Hydrogen atoms (continued)
for: C19 H32 Co O2 P WART_KAKO15

Atom	x	y	z	U(eq) [Ang^2]
O(2')	0.4261(2)	0.5943(2)	0.34216(18)	0.0831(16)
C(1')	0.4201(3)	0.7370(4)	0.0758(3)	0.068(2)
C(2')	0.4695(3)	0.7211(4)	0.1522(3)	0.068(2)
C(3')	0.4885(3)	0.6174(6)	0.1597(3)	0.086(3)
C(4')	0.4518(4)	0.5701(4)	0.0882(5)	0.095(3)
C(5')	0.4124(3)	0.6431(6)	0.0376(3)	0.082(3)
C(6')	0.3790(4)	0.8341(4)	0.0422(4)	0.152(4)
C(7')	0.2951(3)	0.8369(3)	0.0327(3)	0.074(2)
C(8')	0.1652(3)	0.7005(3)	0.0265(2)	0.0522(17)
C(9')	0.1253(3)	0.6239(4)	0.0666(3)	0.094(2)
C(10')	0.1825(3)	0.6418(4)	-0.0398(3)	0.106(2)
C(11')	0.1064(3)	0.7867(3)	-0.0092(3)	0.084(2)
C(12')	0.2494(3)	0.8297(3)	0.1746(2)	0.0545(19)
C(13')	0.2043(4)	0.7746(4)	0.2208(3)	0.114(3)
C(14')	0.3306(3)	0.8524(4)	0.2322(3)	0.132(3)
C(15')	0.2058(3)	0.9290(3)	0.1457(3)	0.114(3)
C(16')	0.3207(4)	0.5003(4)	0.1469(3)	0.062(2)
C(17')	0.3436(3)	0.5574(4)	0.2151(3)	0.051(2)
C(18')	0.4162(3)	0.5295(3)	0.2805(3)	0.0562(19)
C(19')	0.5002(3)	0.5812(4)	0.4042(3)	0.130(3)

U(eq) = 1/3 of the trace of the orthogonalized U

Table S3 - Hydrogen Atom Positions and Isotropic Thermal Parameters
for: C19 H32 Co O2 P WART_KAKO15

Atom	x	y	z	U(iso) [Ang^2]
H(1)	-0.0137(3)	0.2500(4)	0.2598(3)	0.0754
H(2)	-0.0418(3)	0.4374(4)	0.2520(3)	0.0779
H(3)	0.0384(3)	0.5213(4)	0.1778(3)	0.0864
H(4)	0.1101(3)	0.3804(5)	0.1311(2)	0.0882
H(5)	0.1428(3)	0.1834(3)	0.1707(2)	0.0918
H(6)	0.0628(3)	0.1285(3)	0.1669(2)	0.0918
H(7)	0.1799(2)	0.0862(3)	0.2826(2)	0.0694
H(8)	0.1004(2)	0.1089(3)	0.3004(2)	0.0694
H(9)	0.2912(3)	0.2519(4)	0.5145(2)	0.1268
H(10)	0.2288(3)	0.2439(4)	0.5594(2)	0.1268
H(11)	0.2263(3)	0.3374(4)	0.5036(2)	0.1268
H(12)	0.0852(3)	0.2998(3)	0.4290(2)	0.1006
H(13)	0.0896(3)	0.2105(3)	0.4888(2)	0.1006
H(14)	0.0595(3)	0.1882(3)	0.3984(2)	0.1006
H(15)	0.2486(3)	0.0733(3)	0.4602(3)	0.1056
H(16)	0.1582(3)	0.0511(3)	0.4173(3)	0.1056
H(17)	0.1883(3)	0.0734(3)	0.5077(3)	0.1056
H(18)	0.2704(3)	0.3266(4)	0.2454(3)	0.1207
H(19)	0.2675(3)	0.2082(4)	0.2288(3)	0.1207
H(20)	0.3497(3)	0.2641(4)	0.2625(3)	0.1207
H(21)	0.3485(3)	0.3141(4)	0.4527(3)	0.1204
H(22)	0.3251(3)	0.3911(4)	0.3819(3)	0.1204
H(23)	0.4003(3)	0.3210(4)	0.3966(3)	0.1204
H(24)	0.3376(3)	0.1204(4)	0.4234(3)	0.1134
H(25)	0.3901(3)	0.1403(4)	0.3693(3)	0.1134
H(26)	0.3080(3)	0.0843(4)	0.3356(3)	0.1134
H(27)	0.239(3)	0.478(3)	0.330(2)	0.066(17)

Table S3 - Hydrogen Atom Positions and Isotropic Thermal Parameters (continued)
for: C19 H32 Co O2 P WART_KAKO15

Atom	x	y	z	U(iso) [Ang^2]
H(28)	0.173(3)	0.548(3)	0.281(2)	0.082(18)
H(29)	0.1632(18)	0.465(2)	0.4121(17)	0.014(10)
H(30)	-0.0284(3)	0.5897(4)	0.4738(3)	0.1312
H(31)	-0.0576(3)	0.5986(4)	0.3820(3)	0.1312
H(32)	0.0035(3)	0.6784(4)	0.4329(3)	0.1312
H(1')	0.4867(3)	0.7708(4)	0.1911(3)	0.0816
H(2')	0.5205(3)	0.5851(6)	0.2049(3)	0.1033
H(3')	0.4540(4)	0.5005(4)	0.0772(5)	0.1139
H(4')	0.3842(3)	0.6321(6)	-0.0151(3)	0.0993
H(5')	0.4049(4)	0.8906(4)	0.0759(4)	0.1826
H(6')	0.3857(4)	0.8452(4)	-0.0087(4)	0.1826
H(7')	0.2653(3)	0.8231(3)	-0.0218(3)	0.0892
H(8')	0.2813(3)	0.9056(3)	0.0450(3)	0.0892
H(9')	0.1617(3)	0.5692(4)	0.0892(3)	0.1133
H(10')	0.0787(3)	0.5962(4)	0.0285(3)	0.1133
H(11')	0.1106(3)	0.6583(4)	0.1071(3)	0.1133
H(12')	0.2195(3)	0.5873(4)	-0.0180(3)	0.1276
H(13')	0.2051(3)	0.6879(4)	-0.0687(3)	0.1276
H(14')	0.1340(3)	0.6134(4)	-0.0743(3)	0.1276
H(15')	0.1308(3)	0.8353(3)	-0.0345(3)	0.1012
H(16')	0.0917(3)	0.8206(3)	0.0316(3)	0.1012
H(17')	0.0598(3)	0.7584(3)	-0.0470(3)	0.1012
H(18')	0.2303(4)	0.7108(4)	0.2403(3)	0.1366
H(19')	0.1510(4)	0.7612(4)	0.1875(3)	0.1366
H(20')	0.2028(4)	0.8168(4)	0.2642(3)	0.1366
H(21')	0.3621(3)	0.8878(4)	0.2056(3)	0.1583

Table S3 - Hydrogen Atom Positions and Isotropic Thermal Parameters (continued)
for: C19 H32 Co O2 P WART_KAKO15

Atom	x	y	z	U(iso) [Ang^2]
H(22')	0.3563(3)	0.7892(4)	0.2536(3)	0.1583
H(23')	0.3250(3)	0.8948(4)	0.2738(3)	0.1583
H(24')	0.2330(3)	0.9664(3)	0.1158(3)	0.1367
H(25')	0.2043(3)	0.9696(3)	0.1897(3)	0.1367
H(26')	0.1525(3)	0.9141(3)	0.1130(3)	0.1367
H(27')	0.272(2)	0.501(2)	0.118(2)	0.040(13)
H(28')	0.352(2)	0.439(3)	0.1429(19)	0.056(13)
H(29')	0.313(2)	0.591(3)	0.2329(19)	0.036(13)
H(30')	0.5030(3)	0.6292(4)	0.4456(3)	0.1556
H(31')	0.5435(3)	0.5932(4)	0.3843(3)	0.1556
H(32')	0.5034(3)	0.5124(4)	0.4243(3)	0.1556

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The Temperature Factor has the Form of Exp(-T) Where
T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms

Table S4 - Anisotropic Thermal Parameters
for: C19 H32 Co O2 P WART_KAKO15

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
Co(1)	0.0386(4)	0.0502(4)	0.0403(3)	0.0047(3)	0.0106(3)	-0.0019(3)
P(1)	0.0361(7)	0.0473(7)	0.0415(6)	-0.0012(6)	0.0112(5)	-0.0019(6)
O(1)	0.123(3)	0.067(2)	0.107(3)	0.037(2)	0.040(2)	0.038(2)
O(2)	0.101(3)	0.080(2)	0.068(2)	-0.0019(19)	0.030(2)	0.032(2)
C(1)	0.050(4)	0.060(3)	0.042(3)	-0.005(2)	0.000(2)	-0.003(3)
C(2)	0.037(4)	0.089(4)	0.056(3)	0.009(3)	0.005(3)	-0.011(3)
C(3)	0.032(3)	0.097(4)	0.057(3)	0.010(3)	0.002(2)	0.011(3)
C(4)	0.077(5)	0.072(4)	0.059(3)	0.022(3)	0.010(3)	0.018(3)
C(5)	0.081(4)	0.101(4)	0.032(2)	0.009(3)	0.010(2)	-0.002(4)
C(6)	0.080(4)	0.079(4)	0.063(3)	-0.026(3)	0.013(3)	-0.017(3)
C(7)	0.060(3)	0.046(3)	0.066(3)	-0.004(3)	0.018(2)	0.005(2)
C(8)	0.061(4)	0.064(3)	0.055(3)	0.018(2)	0.026(3)	0.007(3)
C(9)	0.124(5)	0.123(5)	0.053(3)	0.005(3)	0.004(3)	-0.003(4)
C(10)	0.113(5)	0.095(4)	0.069(3)	0.033(3)	0.064(3)	0.026(3)
C(11)	0.090(5)	0.094(4)	0.084(4)	0.037(3)	0.032(3)	0.015(3)
C(12)	0.037(3)	0.073(3)	0.082(3)	-0.006(3)	0.024(3)	0.004(3)
C(13)	0.057(4)	0.143(5)	0.122(5)	0.019(4)	0.057(3)	0.013(3)
C(14)	0.040(4)	0.116(5)	0.133(5)	-0.009(4)	0.011(3)	-0.012(3)
C(15)	0.059(4)	0.101(4)	0.121(4)	0.013(4)	0.025(3)	0.031(3)
C(16)	0.076(6)	0.044(4)	0.102(5)	0.012(3)	0.022(4)	-0.003(3)
C(17)	0.070(5)	0.046(3)	0.052(4)	0.003(3)	0.011(3)	0.004(3)
C(18)	0.061(4)	0.053(3)	0.067(4)	-0.007(3)	0.019(3)	0.004(3)
C(19)	0.110(5)	0.128(5)	0.093(4)	-0.011(4)	0.037(3)	0.046(4)
Co(1')	0.0359(4)	0.0438(3)	0.0474(3)	0.0008(3)	0.0134(3)	-0.0020(3)
P(1')	0.0395(8)	0.0384(6)	0.0442(6)	0.0024(6)	0.0091(5)	-0.0014(6)
O(1')	0.071(3)	0.061(2)	0.069(2)	0.0135(16)	0.0219(18)	0.0297(18)

Table S4 - Anisotropic Thermal Parameters (continued)
for: C19 H32 Co O2 P WART_KAKO15

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
O(2')	0.090(3)	0.092(3)	0.059(2)	-0.0090(19)	0.0124(19)	0.031(2)
C(1')	0.078(4)	0.066(4)	0.081(4)	0.019(3)	0.054(3)	0.015(3)
C(2')	0.060(4)	0.081(4)	0.073(4)	-0.022(3)	0.035(3)	-0.036(3)
C(3')	0.040(4)	0.117(5)	0.099(5)	0.043(4)	0.019(3)	0.007(4)
C(4')	0.067(5)	0.068(4)	0.169(7)	-0.029(5)	0.066(5)	-0.001(3)
C(5')	0.051(4)	0.150(6)	0.058(3)	-0.022(4)	0.034(3)	-0.009(4)
C(6')	0.108(6)	0.147(6)	0.234(8)	0.137(5)	0.101(6)	0.058(5)
C(7')	0.075(4)	0.061(3)	0.088(4)	0.027(3)	0.027(3)	-0.005(3)
C(8')	0.037(3)	0.054(3)	0.057(3)	-0.005(2)	0.003(2)	0.002(2)
C(9')	0.050(4)	0.091(4)	0.124(4)	0.011(4)	0.002(3)	-0.019(3)
C(10')	0.075(4)	0.138(5)	0.080(3)	-0.057(4)	-0.011(3)	0.014(4)
C(11')	0.061(4)	0.086(4)	0.085(4)	0.010(3)	-0.006(3)	0.010(3)
C(12')	0.058(4)	0.048(3)	0.056(3)	-0.010(2)	0.016(3)	0.008(2)
C(13')	0.154(6)	0.116(5)	0.099(4)	0.002(4)	0.079(4)	0.033(4)
C(14')	0.071(5)	0.173(6)	0.135(5)	-0.107(5)	0.009(4)	-0.005(4)
C(15')	0.189(7)	0.062(3)	0.090(4)	-0.001(3)	0.044(4)	0.052(4)
C(16')	0.054(4)	0.046(3)	0.074(4)	-0.004(3)	0.005(3)	0.005(3)
C(17')	0.043(4)	0.042(3)	0.070(4)	0.016(3)	0.022(3)	0.009(3)
C(18')	0.064(4)	0.047(3)	0.063(3)	0.008(3)	0.028(3)	0.007(3)
C(19')	0.130(6)	0.160(6)	0.063(4)	-0.019(3)	-0.020(4)	0.050(4)

==========

The Temperature Factor has the Form of Exp(-T) Where
T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms
T = 2*(Pi**2)*Sumij(h(i)*h(j)*U(i,j)*Astar(i)*Astar(j)), for
Anisotropic Atoms. Astar(i) are Reciprocal Axial Lengths and
h(i) are the Reflection Indices.

Table S5 - Bond Distances (Angstrom)
for: C19 H32 Co O2 P WART_KAKO15

Co(1) -P(1) 2.2172(13) C(2) -H(1) 0.929(8)

Co(1) -C(1) 2.032(5) C(3) -H(2) 0.930(8)

Co(1) -C(2) 2.098(5) C(4) -H(3) 0.930(7)

Co(1) -C(3) 2.100(6) C(5) -H(4) 0.931(7)

Co(1) -C(4) 2.063(5) C(6) -H(5) 0.970(7)

Co(1) -C(5) 2.063(3) C(6) -H(6) 0.970(6)

Co(1) -C(16) 1.965(6) C(7) -H(7) 0.971(5)

Co(1) -C(17) 2.001(5) C(7) -H(8) 0.969(5)

P(1) -C(7) 1.854(4) C(9) -H(9) 0.960(8)

P(1) -C(8) 1.891(5) C(9) -H(10) 0.962(6)

P(1) -C(12) 1.879(6) C(9) -H(11) 0.960(7)

O(1) -C(18) 1.200(6) C(10) -H(12) 0.961(6)

O(2) -C(18) 1.363(6) C(10) -H(13) 0.960(5)

O(2) -C(19) 1.431(6) C(10) -H(14) 0.960(6)

C(1) -C(2) 1.405(8) C(11) -H(15) 0.960(8)

C(1) -C(5) 1.414(7) C(11) -H(16) 0.960(7)

C(1) -C(6) 1.477(6) C(11) -H(17) 0.960(7)

C(2) -C(3) 1.400(7) C(13) -H(18) 0.960(7)

C(3) -C(4) 1.398(8) C(13) -H(19) 0.960(7)

C(4) -C(5) 1.423(8) C(13) -H(20) 0.960(8)

C(6) -C(7) 1.546(5) C(14) -H(21) 0.961(7)

C(8) -C(9) 1.545(7) C(14) -H(22) 0.959(7)

C(8) -C(10) 1.516(8) C(14) -H(23) 0.961(8)

C(8) -C(11) 1.528(6) C(15) -H(24) 0.960(7)

C(12) -C(13) 1.527(7) C(15) -H(25) 0.961(8)

C(12) -C(14) 1.546(7) C(15) -H(26) 0.960(7)

C(12) -C(15) 1.535(7) C(16) -H(27) 0.92(5)

C(16) -C(17) 1.391(9) C(16) -H(28) 0.88(4)

C(17) -C(18) 1.446(7) C(17) -H(29) 0.82(3)

Table S5 - Bond Distances (Angstrom) (continued)
for: C19 H32 Co O2 P WART_KAKO15

C(19) -H(30) 0.962(7) C(12') -C(15') 1.510(6)

C(19) -H(31) 0.960(7) C(16') -C(17') 1.379(7)

C(19) -H(32) 0.959(7) C(17') -C(18') 1.485(7)

Co(1') -P(1') 2.2219(13) C(2') -H(1') 0.929(7)

Co(1') -C(1') 2.046(5) C(3') -H(2') 0.930(8)

Co(1') -C(2') 2.078(6) C(4') -H(3') 0.930(8)

Co(1') -C(3') 2.069(6) C(5') -H(4') 0.930(7)

Co(1') -C(4') 2.054(7) C(6') -H(5') 0.970(8)

Co(1') -C(5') 2.052(5) C(6') -H(6') 0.971(10)

Co(1') -C(16') 1.990(6) C(7') -H(7') 0.970(7)

Co(1') -C(17') 1.995(5) C(7') -H(8') 0.971(6)

P(1') -C(7') 1.839(5) C(9') -H(9') 0.960(8)

P(1') -C(8') 1.896(5) C(9') -H(10') 0.959(8)

P(1') -C(12') 1.904(4) C(9') -H(11') 0.959(7)

O(1') -C(18') 1.194(6) C(10') -H(12') 0.961(8)

O(2') -C(18') 1.359(6) C(10') -H(13') 0.961(8)

O(2') -C(19') 1.437(6) C(10') -H(14') 0.959(8)

C(1') -C(2') 1.388(7) C(11') -H(15') 0.959(7)

C(1') -C(5') 1.387(9) C(11') -H(16') 0.961(7)

C(1') -C(6') 1.487(8) C(11') -H(17') 0.960(7)

C(2') -C(3') 1.387(9) C(13') -H(18') 0.960(8)

C(3') -C(4') 1.386(10) C(13') -H(19') 0.960(9)

C(4') -C(5') 1.346(10) C(13') -H(20') 0.961(8)

C(6') -C(7') 1.444(9) C(14') -H(21') 0.962(8)

C(8') -C(9') 1.530(7) C(14') -H(22') 0.959(7)

C(8') -C(10') 1.527(7) C(14') -H(23') 0.960(7)

C(8') -C(11') 1.527(6) C(15') -H(24') 0.962(7)

C(12') -C(13') 1.507(8) C(15') -H(25') 0.959(7)

C(12') -C(14') 1.510(7) C(15') -H(26') 0.960(8)

Table S5 - Bond Distances (Angstrom) (continued)
for: C19 H32 Co O2 P WART_KAKO15

C(16') -H(27') 0.85(4) C(19') -H(30') 0.961(7)

C(16') -H(28') 0.99(4) C(19') -H(31') 0.959(8)

C(17') -H(29') 0.84(4) C(19') -H(32') 0.960(7)

Table S6 - Bond Angles (Degrees)
for: C19 H32 Co O2 P WART_KAKO15

P(1) -Co(1) -C(1) 85.51(13) Co(1) -P(1) -C(8) 118.26(16)

P(1) -Co(1) -C(2) 97.31(15) Co(1) -P(1) -C(12) 118.94(14)

P(1) -Co(1) -C(3) 134.75(15) C(7) -P(1) -C(8) 100.27(18)

P(1) -Co(1) -C(4) 153.10(15) C(7) -P(1) -C(12) 103.55(19)

P(1) -Co(1) -C(5) 114.32(18) C(8) -P(1) -C(12) 110.2(2)

P(1) -Co(1) -C(16) 103.79(19) C(18) -O(2) -C(19) 116.7(4)

P(1) -Co(1) -C(17) 102.31(14) Co(1) -C(1) -C(2) 72.7(3)

C(1) -Co(1) -C(2) 39.7(2) Co(1) -C(1) -C(5) 71.0(2)

C(1) -Co(1) -C(3) 66.7(2) Co(1) -C(1) -C(6) 119.7(3)

C(1) -Co(1) -C(4) 68.24(19) C(2) -C(1) -C(5) 107.4(4)

C(1) -Co(1) -C(5) 40.4(2) C(2) -C(1) -C(6) 124.2(4)

C(1) -Co(1) -C(16) 144.9(3) C(5) -C(1) -C(6) 128.4(5)

C(1) -Co(1) -C(17) 169.0(2) Co(1) -C(2) -C(1) 67.6(3)

C(2) -Co(1) -C(3) 39.0(2) Co(1) -C(2) -C(3) 70.6(3)

C(2) -Co(1) -C(4) 66.5(2) C(1) -C(2) -C(3) 108.2(4)

C(2) -Co(1) -C(5) 66.2(2) Co(1) -C(3) -C(2) 70.5(3)

C(2) -Co(1) -C(16) 158.6(2) Co(1) -C(3) -C(4) 69.0(3)

C(2) -Co(1) -C(17) 130.4(2) C(2) -C(3) -C(4) 109.2(5)

C(3) -Co(1) -C(4) 39.2(2) Co(1) -C(4) -C(3) 71.8(3)

C(3) -Co(1) -C(5) 65.9(2) Co(1) -C(4) -C(5) 69.8(3)

C(3) -Co(1) -C(16) 119.7(2) C(3) -C(4) -C(5) 106.8(5)

C(3) -Co(1) -C(17) 102.4(2) Co(1) -C(5) -C(1) 68.6(3)

C(4) -Co(1) -C(5) 40.3(2) Co(1) -C(5) -C(4) 69.8(3)

C(4) -Co(1) -C(16) 95.1(2) C(1) -C(5) -C(4) 108.2(4)

C(4) -Co(1) -C(17) 104.5(2) C(1) -C(6) -C(7) 109.9(3)

C(5) -Co(1) -C(16) 107.3(3) P(1) -C(7) -C(6) 109.1(3)

C(5) -Co(1) -C(17) 137.9(2) P(1) -C(8) -C(9) 111.8(3)

C(16) -Co(1) -C(17) 41.1(3) P(1) -C(8) -C(10) 106.4(3)

Co(1) -P(1) -C(7) 102.09(13) P(1) -C(8) -C(11) 114.4(3)

Table S6 - Bond Angles (Degrees) (continued)
for: C19 H32 Co O2 P WART_KAKO15

C(9) -C(8) -C(10) 107.7(4) C(1) -C(6) -H(6) 109.7(5)

C(9) -C(8) -C(11) 108.3(4) C(7) -C(6) -H(5) 109.6(5)

C(10) -C(8) -C(11) 107.9(4) C(7) -C(6) -H(6) 109.6(4)

P(1) -C(12) -C(13) 107.1(4) H(5) -C(6) -H(6) 108.2(5)

P(1) -C(12) -C(14) 111.7(3) P(1) -C(7) -H(7) 109.9(4)

P(1) -C(12) -C(15) 115.9(3) P(1) -C(7) -H(8) 109.9(3)

C(13) -C(12) -C(14) 106.7(4) C(6) -C(7) -H(7) 109.8(4)

C(13) -C(12) -C(15) 106.8(4) C(6) -C(7) -H(8) 109.9(4)

C(14) -C(12) -C(15) 108.1(4) H(7) -C(7) -H(8) 108.2(5)

Co(1) -C(16) -C(17) 70.9(3) C(8) -C(9) -H(9) 109.6(5)

Co(1) -C(17) -C(16) 68.1(3) C(8) -C(9) -H(10) 109.4(5)

Co(1) -C(17) -C(18) 114.9(4) C(8) -C(9) -H(11) 109.4(4)

C(16) -C(17) -C(18) 120.6(5) H(9) -C(9) -H(10) 109.5(6)

O(1) -C(18) -O(2) 120.5(5) H(9) -C(9) -H(11) 109.5(7)

O(1) -C(18) -C(17) 128.4(5) H(10) -C(9) -H(11) 109.4(6)

O(2) -C(18) -C(17) 111.1(4) C(8) -C(10) -H(12) 109.5(5)

Co(1) -C(2) -H(1) 127.4(5) C(8) -C(10) -H(13) 109.5(5)

C(1) -C(2) -H(1) 125.8(6) C(8) -C(10) -H(14) 109.6(5)

C(3) -C(2) -H(1) 126.0(6) H(12) -C(10) -H(13) 109.4(5)

Co(1) -C(3) -H(2) 126.7(5) H(12) -C(10) -H(14) 109.4(5)

C(2) -C(3) -H(2) 125.3(6) H(13) -C(10) -H(14) 109.4(6)

C(4) -C(3) -H(2) 125.5(6) C(8) -C(11) -H(15) 109.5(5)

Co(1) -C(4) -H(3) 123.4(5) C(8) -C(11) -H(16) 109.5(5)

C(3) -C(4) -H(3) 126.6(6) C(8) -C(11) -H(17) 109.5(5)

C(5) -C(4) -H(3) 126.6(6) H(15) -C(11) -H(16) 109.5(6)

Co(1) -C(5) -H(4) 127.3(5) H(15) -C(11) -H(17) 109.5(7)

C(1) -C(5) -H(4) 125.9(7) H(16) -C(11) -H(17) 109.4(6)

C(4) -C(5) -H(4) 125.9(7) C(12) -C(13) -H(18) 109.4(6)

C(1) -C(6) -H(5) 109.8(4) C(12) -C(13) -H(19) 109.3(6)

Table S6 - Bond Angles (Degrees) (continued)
for: C19 H32 Co O2 P WART_KAKO15

C(12) -C(13) -H(20) 109.5(6) H(31) -C(19) -H(32) 109.5(7)

H(18) -C(13) -H(19) 109.5(7) P(1') -Co(1') -C(1') 84.73(16)

H(18) -C(13) -H(20) 109.6(7) P(1') -Co(1') -C(2') 106.61(15)

H(19) -C(13) -H(20) 109.5(7) P(1') -Co(1') -C(3') 145.6(2)

C(12) -C(14) -H(21) 109.4(6) P(1') -Co(1') -C(4') 142.0(2)

C(12) -C(14) -H(22) 109.5(6) P(1') -Co(1') -C(5') 103.88(19)

C(12) -C(14) -H(23) 109.5(6) P(1') -Co(1') -C(16') 105.7(2)

H(21) -C(14) -H(22) 109.5(7) P(1') -Co(1') -C(17') 100.67(16)

H(21) -C(14) -H(23) 109.5(7) C(1') -Co(1') -C(2') 39.3(2)

H(22) -C(14) -H(23) 109.4(7) C(1') -Co(1') -C(3') 65.8(2)

C(12) -C(15) -H(24) 109.5(6) C(1') -Co(1') -C(4') 66.1(2)

C(12) -C(15) -H(25) 109.5(6) C(1') -Co(1') -C(5') 39.6(3)

C(12) -C(15) -H(26) 109.4(6) C(1') -Co(1') -C(16') 157.6(2)

H(24) -C(15) -H(25) 109.5(7) C(1') -Co(1') -C(17') 158.4(2)

H(24) -C(15) -H(26) 109.5(7) C(2') -Co(1') -C(3') 39.1(3)

H(25) -C(15) -H(26) 109.4(7) C(2') -Co(1') -C(4') 65.9(2)

Co(1) -C(16) -H(27) 111(3) C(2') -Co(1') -C(5') 65.3(2)

Co(1) -C(16) -H(28) 111(3) C(2') -Co(1') -C(16') 145.2(2)

C(17) -C(16) -H(27) 121(2) C(2') -Co(1') -C(17') 119.8(2)

C(17) -C(16) -H(28) 117(3) C(3') -Co(1') -C(4') 39.3(3)

H(27) -C(16) -H(28) 116(4) C(3') -Co(1') -C(5') 64.7(2)

Co(1) -C(17) -H(29) 112.9(19) C(3') -Co(1') -C(16') 108.1(3)

C(16) -C(17) -H(29) 122(2) C(3') -Co(1') -C(17') 101.1(2)

C(18) -C(17) -H(29) 111(2) C(4') -Co(1') -C(5') 38.3(3)

O(2) -C(19) -H(30) 109.4(6) C(4') -Co(1') -C(16') 95.2(3)

O(2) -C(19) -H(31) 109.5(6) C(4') -Co(1') -C(17') 115.5(2)

O(2) -C(19) -H(32) 109.5(6) C(5') -Co(1') -C(16') 118.0(3)

H(30) -C(19) -H(31) 109.4(7) C(5') -Co(1') -C(17') 151.9(3)

H(30) -C(19) -H(32) 109.5(7) C(16') -Co(1') -C(17') 40.5(2)

Table S6 - Bond Angles (Degrees) (continued)
for: C19 H32 Co O2 P WART_KAKO15

Co(1') -P(1') -C(7') 102.93(17) P(1') -C(8') -C(11') 115.3(3)
Co(1') -P(1') -C(8') 119.43(14) C(9') -C(8') -C(10') 106.3(4)
Co(1') -P(1') -C(12') 118.35(14) C(9') -C(8') -C(11') 108.6(4)
C(7') -P(1') -C(8') 101.1(2) C(10') -C(8') -C(11') 108.7(3)
C(7') -P(1') -C(12') 102.31(19) P(1') -C(12') -C(13') 111.6(3)
C(8') -P(1') -C(12') 109.3(2) P(1') -C(12') -C(14') 106.9(4)
C(18') -O(2') -C(19') 114.0(4) P(1') -C(12') -C(15') 115.2(3)
Co(1') -C(1') -C(2') 71.6(3) C(13') -C(12') -C(14') 105.9(4)
Co(1') -C(1') -C(5') 70.5(3) C(13') -C(12') -C(15') 107.0(4)
Co(1') -C(1') -C(6') 120.3(4) C(14') -C(12') -C(15') 109.9(4)
C(2') -C(1') -C(5') 106.8(5) Co(1') -C(16') -C(17') 69.9(3)
C(2') -C(1') -C(6') 126.9(5) Co(1') -C(17') -C(16') 69.6(3)
C(5') -C(1') -C(6') 126.1(5) Co(1') -C(17') -C(18') 113.5(4)
Co(1') -C(2') -C(1') 69.1(3) C(16') -C(17') -C(18') 120.4(5)
Co(1') -C(2') -C(3') 70.1(3) O(1') -C(18') -O(2') 122.3(5)
C(1') -C(2') -C(3') 107.3(5) O(1') -C(18') -C(17') 127.4(4)
Co(1') -C(3') -C(2') 70.8(3) O(2') -C(18') -C(17') 110.3(4)
Co(1') -C(3') -C(4') 69.8(4) Co(1') -C(2') -H(1') 126.1(6)
C(2') -C(3') -C(4') 108.3(5) C(1') -C(2') -H(1') 126.3(6)
Co(1') -C(4') -C(3') 71.0(4) C(3') -C(2') -H(1') 126.3(6)
Co(1') -C(4') -C(5') 70.8(4) Co(1') -C(3') -H(2') 125.3(6)
C(3') -C(4') -C(5') 107.6(6) C(2') -C(3') -H(2') 125.9(8)
Co(1') -C(5') -C(1') 70.0(3) C(4') -C(3') -H(2') 125.8(9)
Co(1') -C(5') -C(4') 71.0(4) Co(1') -C(4') -H(3') 123.7(8)
C(1') -C(5') -C(4') 109.8(5) C(3') -C(4') -H(3') 126.2(9)
C(1') -C(6') -C(7') 115.0(5) C(5') -C(4') -H(3') 126.2(10)
P(1') -C(7') -C(6') 113.5(4) Co(1') -C(5') -H(4') 125.5(6)
P(1') -C(8') -C(9') 111.5(3) C(1') -C(5') -H(4') 125.1(8)
P(1') -C(8') -C(10') 106.0(4) C(4') -C(5') -H(4') 125.0(9)

Table S6 - Bond Angles (Degrees) (continued)
for: C19 H32 Co O2 P WART_KAKO15

C(1') -C(6') -H(5') 108.5(7) C(12') -C(13') -H(19') 109.5(6)
C(1') -C(6') -H(6') 108.5(7) C(12') -C(13') -H(20') 109.5(6)
C(7') -C(6') -H(5') 108.6(7) H(18') -C(13') -H(19') 109.5(7)
C(7') -C(6') -H(6') 108.5(7) H(18') -C(13') -H(20') 109.4(7)
H(5') -C(6') -H(6') 107.4(8) H(19') -C(13') -H(20') 109.4(9)
P(1') -C(7') -H(7') 108.9(4) C(12') -C(14') -H(21') 109.4(5)
P(1') -C(7') -H(8') 108.9(5) C(12') -C(14') -H(22') 109.5(6)
C(6') -C(7') -H(7') 108.9(6) C(12') -C(14') -H(23') 109.4(6)
C(6') -C(7') -H(8') 108.8(6) H(21') -C(14') -H(22') 109.4(7)
H(7') -C(7') -H(8') 107.7(6) H(21') -C(14') -H(23') 109.5(7)
C(8') -C(9') -H(9') 109.4(6) H(22') -C(14') -H(23') 109.6(7)
C(8') -C(9') -H(10') 109.4(5) C(12') -C(15') -H(24') 109.4(5)
C(8') -C(9') -H(11') 109.5(5) C(12') -C(15') -H(25') 109.5(5)
H(9') -C(9') -H(10') 109.5(7) C(12') -C(15') -H(26') 109.5(4)
H(9') -C(9') -H(11') 109.5(7) H(24') -C(15') -H(25') 109.5(6)
H(10') -C(9') -H(11') 109.6(7) H(24') -C(15') -H(26') 109.4(7)
C(8') -C(10') -H(12') 109.4(5) H(25') -C(15') -H(26') 109.5(7)
C(8') -C(10') -H(13') 109.4(5) Co(1') -C(16') -H(27') 106.0(19)
C(8') -C(10') -H(14') 109.5(6) Co(1') -C(16') -H(28') 115(2)
H(12') -C(10') -H(13') 109.4(7) C(17') -C(16') -H(27') 119(2)
H(12') -C(10') -H(14') 109.5(7) C(17') -C(16') -H(28') 119(2)
H(13') -C(10') -H(14') 109.5(7) H(27') -C(16') -H(28') 117(3)
C(8') -C(11') -H(15') 109.4(6) Co(1') -C(17') -H(29') 111(3)
C(8') -C(11') -H(16') 109.4(5) C(16') -C(17') -H(29') 125(2)
C(8') -C(11') -H(17') 109.5(4) C(18') -C(17') -H(29') 109(2)
H(15') -C(11') -H(16') 109.5(5) O(2') -C(19') -H(30') 109.4(6)
H(15') -C(11') -H(17') 109.5(7) O(2') -C(19') -H(31') 109.6(5)
H(16') -C(11') -H(17') 109.5(7) O(2') -C(19') -H(32') 109.4(6)
C(12') -C(13') -H(18') 109.6(7) H(30') -C(19') -H(31') 109.5(7)

Table S6 - Bond Angles (Degrees) (continued)
for: C19 H32 Co O2 P WART_KAKO15

H(30') -C(19') -H(32') 109.4(7) H(31') -C(19') -H(32') 109.5(7)

Table S7 - Torsion Angles (Degrees)
for: C19 H32 Co O2 P WART_KAKO15

C(1) -Co(1) -P(1) -C(7) -9.3(2)

C(2) -Co(1) -P(1) -C(7) 28.69(19)

C(3) -Co(1) -P(1) -C(7) 41.1(2)

C(4) -Co(1) -P(1) -C(7) -21.7(4)

C(5) -Co(1) -P(1) -C(7) -38.4(2)

C(16) -Co(1) -P(1) -C(7) -155.0(2)

C(17) -Co(1) -P(1) -C(7) 162.8(2)

C(1) -Co(1) -P(1) -C(8) -118.1(2)

C(2) -Co(1) -P(1) -C(8) -80.1(2)

C(3) -Co(1) -P(1) -C(8) -67.7(3)

C(4) -Co(1) -P(1) -C(8) -130.5(4)

C(5) -Co(1) -P(1) -C(8) -147.2(2)

C(16) -Co(1) -P(1) -C(8) 96.2(3)

C(17) -Co(1) -P(1) -C(8) 54.1(2)

C(1) -Co(1) -P(1) -C(12) 103.8(2)

C(2) -Co(1) -P(1) -C(12) 141.8(2)

C(3) -Co(1) -P(1) -C(12) 154.2(3)

C(4) -Co(1) -P(1) -C(12) 91.4(4)

C(5) -Co(1) -P(1) -C(12) 74.7(2)

C(16) -Co(1) -P(1) -C(12) -41.9(3)

C(17) -Co(1) -P(1) -C(12) -84.1(2)

P(1) -Co(1) -C(1) -C(2) 107.1(3)

C(3) -Co(1) -C(1) -C(2) -36.3(3)

C(4) -Co(1) -C(1) -C(2) -78.9(3)

C(5) -Co(1) -C(1) -C(2) -116.0(4)

C(16) -Co(1) -C(1) -C(2) -145.2(4)

P(1) -Co(1) -C(1) -C(5) -136.9(3)

C(2) -Co(1) -C(1) -C(5) 116.0(4)

C(3) -Co(1) -C(1) -C(5) 79.7(3)

Table S7 - Torsion Angles (Degrees) (continued)
for: C19 H32 Co O2 P WART_KAKO15

C(4) -Co(1) -C(1) -C(5) 37.1(3)

C(16) -Co(1) -C(1) -C(5) -29.2(6)

P(1) -Co(1) -C(1) -C(6) -12.8(4)

C(2) -Co(1) -C(1) -C(6) -120.0(5)

C(3) -Co(1) -C(1) -C(6) -156.3(5)

C(4) -Co(1) -C(1) -C(6) 161.2(5)

C(5) -Co(1) -C(1) -C(6) 124.0(6)

C(16) -Co(1) -C(1) -C(6) 94.8(5)

C(17) -Co(1) -C(5) -C(1) -163.5(3)

P(1) -Co(1) -C(5) -C(4) 168.4(3)

C(1) -Co(1) -C(5) -C(4) 120.0(5)

C(2) -Co(1) -C(5) -C(4) 81.1(3)

C(3) -Co(1) -C(5) -C(4) 38.3(3)

C(16) -Co(1) -C(5) -C(4) -77.1(4)

C(17) -Co(1) -C(5) -C(4) -43.4(5)

C(16) -Co(1) -C(3) -C(4) 57.5(4)

C(17) -Co(1) -C(3) -C(4) 97.8(3)

C(5) -Co(1) -C(17) -C(16) -53.6(5)

P(1) -Co(1) -C(17) -C(18) -148.4(3)

C(2) -Co(1) -C(17) -C(18) -37.5(5)

P(1) -Co(1) -C(4) -C(3) 92.6(4)

P(1) -Co(1) -C(2) -C(1) -73.9(3)

C(3) -Co(1) -C(2) -C(1) 120.2(4)

C(4) -Co(1) -C(2) -C(1) 83.8(3)

C(5) -Co(1) -C(2) -C(1) 39.5(3)

C(16) -Co(1) -C(2) -C(1) 115.9(7)

C(17) -Co(1) -C(2) -C(1) 173.1(3)

P(1) -Co(1) -C(2) -C(3) 166.0(3)

C(1) -Co(1) -C(2) -C(3) -120.2(4)

Table S7 - Torsion Angles (Degrees) (continued)
for: C19 H32 Co O2 P WART_KAKO15

C(4) -Co(1) -C(2) -C(3) -36.4(3)

C(5) -Co(1) -C(2) -C(3) -80.6(3)

C(16) -Co(1) -C(2) -C(3) -4.3(8)

C(17) -Co(1) -C(2) -C(3) 52.9(4)

C(4) -Co(1) -C(17) -C(16) -80.9(4)

C(17) -Co(1) -C(3) -C(2) -141.5(3)

P(1) -Co(1) -C(5) -C(1) 48.4(3)

P(1) -Co(1) -C(3) -C(2) -19.8(4)

C(1) -Co(1) -C(3) -C(2) 37.0(3)

C(4) -Co(1) -C(3) -C(2) 120.7(4)

C(5) -Co(1) -C(3) -C(2) 81.3(3)

C(16) -Co(1) -C(3) -C(2) 178.2(3)

C(16) -Co(1) -C(4) -C(3) -132.6(3)

P(1) -Co(1) -C(3) -C(4) -140.5(3)

C(1) -Co(1) -C(3) -C(4) -83.7(3)

C(2) -Co(1) -C(3) -C(4) -120.7(4)

C(5) -Co(1) -C(3) -C(4) -39.4(3)

C(2) -Co(1) -C(17) -C(16) -152.2(4)

C(3) -Co(1) -C(17) -C(16) -121.3(4)

C(17) -Co(1) -C(4) -C(5) 151.6(3)

C(17) -Co(1) -C(4) -C(3) -92.0(3)

P(1) -Co(1) -C(4) -C(5) -23.8(5)

C(1) -Co(1) -C(4) -C(5) -37.1(3)

C(1) -Co(1) -C(4) -C(3) 79.3(3)

C(2) -Co(1) -C(4) -C(3) 36.2(3)

C(5) -Co(1) -C(4) -C(3) 116.5(5)

C(4) -Co(1) -C(5) -C(1) -120.0(5)

C(16) -Co(1) -C(5) -C(1) 162.9(3)

C(2) -Co(1) -C(16) -C(17) 77.0(8)

Table S7 - Torsion Angles (Degrees) (continued)
for: C19 H32 Co O2 P WART_KAKO15

C(3) -Co(1) -C(16) -C(17) 73.9(4)

C(2) -Co(1) -C(4) -C(5) -80.3(3)

C(3) -Co(1) -C(4) -C(5) -116.5(5)

C(16) -Co(1) -C(4) -C(5) 110.9(4)

P(1) -Co(1) -C(17) -C(16) 96.9(3)

C(4) -Co(1) -C(17) -C(18) 33.8(4)

C(5) -Co(1) -C(17) -C(18) 61.1(5)

C(16) -Co(1) -C(17) -C(18) 114.7(5)

C(4) -Co(1) -C(16) -C(17) 106.3(3)

C(2) -Co(1) -C(5) -C(1) -38.9(3)

C(3) -Co(1) -C(5) -C(1) -81.7(3)

C(3) -Co(1) -C(17) -C(18) -6.6(4)

C(1) -Co(1) -C(16) -C(17) 164.9(3)

C(5) -Co(1) -C(16) -C(17) 145.6(3)

P(1) -Co(1) -C(16) -C(17) -93.0(3)

C(12) -P(1) -C(7) -C(6) -94.9(3)

Co(1) -P(1) -C(8) -C(9) -86.9(4)

C(12) -P(1) -C(8) -C(11) -68.9(4)

Co(1) -P(1) -C(12) -C(15) -165.9(3)

Co(1) -P(1) -C(12) -C(14) 69.7(4)

C(7) -P(1) -C(12) -C(14) -178.0(3)

C(7) -P(1) -C(8) -C(9) 163.3(3)

C(7) -P(1) -C(12) -C(15) -53.6(4)

Co(1) -P(1) -C(8) -C(11) 149.6(3)

C(7) -P(1) -C(8) -C(11) 39.7(4)

C(8) -P(1) -C(12) -C(14) -71.5(4)

C(7) -P(1) -C(12) -C(13) 65.5(3)

Co(1) -P(1) -C(7) -C(6) 29.2(3)

C(8) -P(1) -C(7) -C(6) 151.2(3)

Table S7 - Torsion Angles (Degrees) (continued)
for: C19 H32 Co O2 P WART_KAKO15

C(12) -P(1) -C(8) -C(10) 172.0(3)

C(7) -P(1) -C(8) -C(10) -79.3(3)

C(8) -P(1) -C(12) -C(15) 52.9(4)

C(8) -P(1) -C(12) -C(13) 172.0(3)

Co(1) -P(1) -C(12) -C(13) -46.8(3)

Co(1) -P(1) -C(8) -C(10) 30.5(3)

C(12) -P(1) -C(8) -C(9) 54.6(4)

C(19) -O(2) -C(18) -O(1) -0.1(8)

C(19) -O(2) -C(18) -C(17) -178.8(4)

C(6) -C(1) -C(2) -C(3) 173.6(5)

C(5) -C(1) -C(2) -C(3) -3.8(6)

C(2) -C(1) -C(6) -C(7) -53.4(6)

C(5) -C(1) -C(2) -Co(1) -62.9(3)

C(6) -C(1) -C(5) -C(4) -172.0(5)

C(6) -C(1) -C(2) -Co(1) 114.5(5)

Co(1) -C(1) -C(6) -C(7) 35.0(5)

Co(1) -C(1) -C(2) -C(3) 59.1(4)

C(2) -C(1) -C(5) -C(4) 5.2(6)

C(6) -C(1) -C(5) -Co(1) -113.2(5)

C(2) -C(1) -C(5) -Co(1) 64.0(4)

C(5) -C(1) -C(6) -C(7) 123.4(5)

Co(1) -C(1) -C(5) -C(4) -58.8(3)

C(1) -C(2) -C(3) -Co(1) -57.3(4)

Co(1) -C(2) -C(3) -C(4) 58.2(4)

C(1) -C(2) -C(3) -C(4) 1.0(6)

C(2) -C(3) -C(4) -C(5) 2.3(6)

Co(1) -C(3) -C(4) -C(5) 61.4(3)

C(2) -C(3) -C(4) -Co(1) -59.1(4)

C(3) -C(4) -C(5) -C(1) -4.6(6)

Table S7 - Torsion Angles (Degrees) (continued)
for: C19 H32 Co O2 P WART_KAKO15

Co(1) -C(4) -C(5) -C(1) 58.1(3)

C(3) -C(4) -C(5) -Co(1) -62.7(4)

C(1) -C(6) -C(7) -P(1) -40.3(5)

Co(1) -C(16) -C(17) -C(18) -106.8(5)

Co(1) -C(17) -C(18) -O(1) -69.9(7)

C(16) -C(17) -C(18) -O(2) -173.1(5)

Co(1) -C(17) -C(18) -O(2) 108.7(4)

C(16) -C(17) -C(18) -O(1) 8.4(9)

C(1') -Co(1') -P(1') -C(7') 8.0(2)

C(2') -Co(1') -P(1') -C(7') 41.0(2)

C(3') -Co(1') -P(1') -C(7') 38.3(3)

C(4') -Co(1') -P(1') -C(7') -30.9(3)

C(5') -Co(1') -P(1') -C(7') -26.9(3)

C(16') -Co(1') -P(1') -C(7') -151.9(2)

C(17') -Co(1') -P(1') -C(7') 166.8(2)

C(1') -Co(1') -P(1') -C(8') 118.8(2)

C(2') -Co(1') -P(1') -C(8') 151.9(2)

C(3') -Co(1') -P(1') -C(8') 149.1(3)

C(4') -Co(1') -P(1') -C(8') 79.9(3)

C(5') -Co(1') -P(1') -C(8') 83.9(3)

C(16') -Co(1') -P(1') -C(8') -41.0(2)

C(17') -Co(1') -P(1') -C(8') -82.4(2)

C(1') -Co(1') -P(1') -C(12') -103.9(2)

C(2') -Co(1') -P(1') -C(12') -70.8(2)

C(3') -Co(1') -P(1') -C(12') -73.6(3)

C(4') -Co(1') -P(1') -C(12') -142.7(3)

C(5') -Co(1') -P(1') -C(12') -138.8(3)

C(16') -Co(1') -P(1') -C(12') 96.3(2)

C(17') -Co(1') -P(1') -C(12') 54.9(2)

Table S7 - Torsion Angles (Degrees) (continued)
for: C19 H32 Co O2 P WART_KAKO15

P(1') -Co(1') -C(1') -C(2') 124.4(3)

C(3') -Co(1') -C(1') -C(2') -37.4(3)

C(4') -Co(1') -C(1') -C(2') -80.5(4)

C(5') -Co(1') -C(1') -C(2') -116.2(5)

C(16') -Co(1') -C(1') -C(2') -116.1(6)

C(17') -Co(1') -C(1') -C(2') 18.6(7)

P(1') -Co(1') -C(1') -C(5') -119.3(3)

C(2') -Co(1') -C(1') -C(5') 116.2(5)

C(3') -Co(1') -C(1') -C(5') 78.9(4)

C(4') -Co(1') -C(1') -C(5') 35.7(4)

C(16') -Co(1') -C(1') -C(5') 0.1(7)

C(17') -Co(1') -C(1') -C(5') 134.9(6)

P(1') -Co(1') -C(1') -C(6') 1.8(4)

C(2') -Co(1') -C(1') -C(6') -122.6(6)

C(3') -Co(1') -C(1') -C(6') -160.0(5)

C(4') -Co(1') -C(1') -C(6') 156.8(5)

C(5') -Co(1') -C(1') -C(6') 121.1(6)

C(16') -Co(1') -C(1') -C(6') 121.2(7)

C(17') -Co(1') -C(1') -C(6') -104.0(7)

C(17') -Co(1') -C(5') -C(1') -146.3(5)

P(1') -Co(1') -C(5') -C(4') -176.1(4)

C(1') -Co(1') -C(5') -C(4') 120.5(5)

C(2') -Co(1') -C(5') -C(4') 81.8(4)

C(3') -Co(1') -C(5') -C(4') 38.5(4)

C(16') -Co(1') -C(5') -C(4') -59.4(5)

C(17') -Co(1') -C(5') -C(4') -25.8(7)

C(16') -Co(1') -C(3') -C(4') 75.6(4)

C(17') -Co(1') -C(3') -C(4') 116.9(4)

C(4') -Co(1') -C(17') -C(16') -66.2(4)

Table S7 - Torsion Angles (Degrees) (continued)
for: C19 H32 Co O2 P WART_KAKO15

C(5') -Co(1') -C(17') -C(16') -48.9(6)

P(1') -Co(1') -C(17') -C(18') -142.9(3)

P(1') -Co(1') -C(4') -C(3') 123.5(4)

P(1') -Co(1') -C(2') -C(1') -59.0(3)

C(3') -Co(1') -C(2') -C(1') 118.5(4)

C(4') -Co(1') -C(2') -C(1') 81.2(4)

C(5') -Co(1') -C(2') -C(1') 39.0(3)

C(16') -Co(1') -C(2') -C(1') 143.1(4)

C(17') -Co(1') -C(2') -C(1') -172.2(3)

P(1') -Co(1') -C(2') -C(3') -177.5(3)

C(1') -Co(1') -C(2') -C(3') -118.5(4)

C(4') -Co(1') -C(2') -C(3') -37.4(4)

C(5') -Co(1') -C(2') -C(3') -79.6(4)

C(16') -Co(1') -C(2') -C(3') 24.6(5)

C(17') -Co(1') -C(2') -C(3') 69.3(4)

C(3') -Co(1') -C(17') -C(16') -105.0(4)

C(17') -Co(1') -C(3') -C(2') -124.2(3)

P(1') -Co(1') -C(5') -C(1') 63.4(3)

P(1') -Co(1') -C(3') -C(2') 4.2(4)

C(1') -Co(1') -C(3') -C(2') 37.6(3)

C(4') -Co(1') -C(3') -C(2') 118.9(5)

C(5') -Co(1') -C(3') -C(2') 81.4(4)

C(16') -Co(1') -C(3') -C(2') -165.5(3)

C(16') -Co(1') -C(4') -C(3') -112.4(4)

P(1') -Co(1') -C(3') -C(4') -114.7(4)

C(1') -Co(1') -C(3') -C(4') -81.3(4)

C(2') -Co(1') -C(3') -C(4') -118.9(5)

C(5') -Co(1') -C(3') -C(4') -37.5(4)

C(1') -Co(1') -C(17') -C(16') -155.4(6)

Table S7 - Torsion Angles (Degrees) (continued)
for: C19 H32 Co O2 P WART_KAKO15

C(2') -Co(1') -C(17') -C(16') -141.9(4)

C(17') -Co(1') -C(4') -C(5') 166.9(4)

C(17') -Co(1') -C(4') -C(3') -75.8(4)

P(1') -Co(1') -C(4') -C(5') 6.2(6)

C(1') -Co(1') -C(4') -C(5') -36.9(4)

C(1') -Co(1') -C(4') -C(3') 80.4(4)

C(2') -Co(1') -C(4') -C(3') 37.2(4)

C(5') -Co(1') -C(4') -C(3') 117.3(6)

C(4') -Co(1') -C(5') -C(1') -120.5(5)

C(16') -Co(1') -C(5') -C(1') -180.0(9)

C(2') -Co(1') -C(16') -C(17') 69.9(5)

C(3') -Co(1') -C(16') -C(17') 85.9(4)

C(2') -Co(1') -C(4') -C(5') -80.1(4)

C(3') -Co(1') -C(4') -C(5') -117.3(6)

C(16') -Co(1') -C(4') -C(5') 130.3(4)

P(1') -Co(1') -C(17') -C(16') 101.8(4)

C(2') -Co(1') -C(17') -C(18') -26.6(4)

C(3') -Co(1') -C(17') -C(18') 10.4(4)

C(4') -Co(1') -C(17') -C(18') 49.1(4)

C(4') -Co(1') -C(16') -C(17') 123.9(4)

C(2') -Co(1') -C(5') -C(1') -38.7(3)

C(3') -Co(1') -C(5') -C(1') -82.0(4)

C(1') -Co(1') -C(17') -C(18') -40.1(8)

C(5') -Co(1') -C(17') -C(18') 66.4(6)

C(5') -Co(1') -C(16') -C(17') 156.3(3)

P(1') -Co(1') -C(16') -C(17') -88.1(3)

C(1') -Co(1') -C(16') -C(17') 156.2(5)

C(16') -Co(1') -C(17') -C(18') 115.3(5)

C(12') -P(1') -C(7') -C(6') 105.3(4)

Table S7 - Torsion Angles (Degrees) (continued)
for: C19 H32 Co O2 P WART_KAKO15

Co(1') -P(1') -C(12') -C(15') 155.1(3)

Co(1') -P(1') -C(8') -C(9') 70.4(4)

C(12') -P(1') -C(8') -C(11') 54.0(4)

C(7') -P(1') -C(8') -C(9') -177.7(3)

Co(1') -P(1') -C(12') -C(14') 32.7(3)

C(7') -P(1') -C(12') -C(14') -79.5(3)

C(7') -P(1') -C(8') -C(11') -53.3(4)

C(8') -P(1') -C(12') -C(14') 174.0(3)

C(7') -P(1') -C(12') -C(13') 165.1(4)

Co(1') -P(1') -C(7') -C(6') -18.0(4)

C(8') -P(1') -C(7') -C(6') -142.0(4)

C(7') -P(1') -C(12') -C(15') 42.9(4)

C(7') -P(1') -C(8') -C(10') 67.0(3)

C(12') -P(1') -C(8') -C(10') 174.3(3)

Co(1') -P(1') -C(8') -C(11') -165.2(3)

Co(1') -P(1') -C(12') -C(13') -82.6(4)

C(8') -P(1') -C(12') -C(15') -63.6(4)

C(8') -P(1') -C(12') -C(13') 58.6(4)

C(12') -P(1') -C(8') -C(9') -70.4(4)

Co(1') -P(1') -C(8') -C(10') -44.9(3)

C(19') -O(2') -C(18') -O(1') 6.2(6)

C(19') -O(2') -C(18') -C(17') -172.5(4)

C(6') -C(1') -C(2') -C(3') 174.4(6)

C(2') -C(1') -C(6') -C(7') -103.4(7)

C(6') -C(1') -C(5') -C(4') -173.7(6)

C(6') -C(1') -C(2') -Co(1') 114.5(6)

C(2') -C(1') -C(5') -C(4') 2.8(7)

Co(1') -C(1') -C(2') -C(3') 59.9(4)

C(5') -C(1') -C(2') -Co(1') -62.0(4)

Table S7 - Torsion Angles (Degrees) (continued)
for: C19 H32 Co O2 P WART_KAKO15

C(5') -C(1') -C(2') -C(3') -2.1(6)

Co(1') -C(1') -C(6') -C(7') -14.4(7)

Co(1') -C(1') -C(5') -C(4') -60.0(5)

C(6') -C(1') -C(5') -Co(1') -113.8(6)

C(2') -C(1') -C(5') -Co(1') 62.8(4)

C(5') -C(1') -C(6') -C(7') 72.5(8)

Co(1') -C(2') -C(3') -C(4') 59.9(5)

C(1') -C(2') -C(3') -C(4') 0.7(7)

C(1') -C(2') -C(3') -Co(1') -59.3(4)

Co(1') -C(3') -C(4') -C(5') 61.7(5)

C(2') -C(3') -C(4') -C(5') 1.1(8)

C(2') -C(3') -C(4') -Co(1') -60.6(4)

C(3') -C(4') -C(5') -Co(1') -61.8(5)

C(3') -C(4') -C(5') -C(1') -2.4(8)

Co(1') -C(4') -C(5') -C(1') 59.4(4)

C(1') -C(6') -C(7') -P(1') 21.1(6)

Co(1') -C(16') -C(17') -C(18') -105.9(5)

Co(1') -C(17') -C(18') -O(1') -76.4(6)

C(16') -C(17') -C(18') -O(2') -178.5(5)

Co(1') -C(17') -C(18') -O(2') 102.3(4)

C(16') -C(17') -C(18') -O(1') 2.9(9)