**Supplementary Material**

**Bis Phenylene Flattened 13-Membered Tetraamide Macrocyclic Ligand (TAML) For Square Planar Cobalt(III)**

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**Cif and checkcif files for 7b**

**1. Cif file**

data\_shelxl

\_audit\_creation\_method SHELXL-97

\_chemical\_name\_systematic

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?

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\_chemical\_name\_common ?

\_chemical\_melting\_point ?

\_chemical\_formula\_moiety ?

\_chemical\_formula\_sum

'C43 H43 Co N4 O4 P'

\_chemical\_formula\_weight 769.71

loop\_

\_atom\_type\_symbol

\_atom\_type\_description

\_atom\_type\_scat\_dispersion\_real

\_atom\_type\_scat\_dispersion\_imag

\_atom\_type\_scat\_source

'C' 'C' 0.0033 0.0016

'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

'H' 'H' 0.0000 0.0000

'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

'Co' 'Co' 0.3494 0.9721

'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

'N' 'N' 0.0061 0.0033

'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

'O' 'O' 0.0106 0.0060

'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

'P' 'P' 0.1023 0.0942

'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

\_symmetry\_cell\_setting monoclinic

\_symmetry\_space\_group\_name\_H-M P2(1)/c

loop\_

\_symmetry\_equiv\_pos\_as\_xyz

'x, y, z'

'-x, y+1/2, -z+1/2'

'-x, -y, -z'

'x, -y-1/2, z-1/2'

\_cell\_length\_a 11.1840(15)

\_cell\_length\_b 10.9650(3)

\_cell\_length\_c 28.742(3)

\_cell\_angle\_alpha 90.00

\_cell\_angle\_beta 96.469(10)

\_cell\_angle\_gamma 90.00

\_cell\_volume 3502.3(6)

\_cell\_formula\_units\_Z 4

\_cell\_measurement\_temperature 293(2)

\_cell\_measurement\_reflns\_used ?

\_cell\_measurement\_theta\_min ?

\_cell\_measurement\_theta\_max ?

\_exptl\_crystal\_description plate

\_exptl\_crystal\_colour purple

\_exptl\_crystal\_size\_max .4

\_exptl\_crystal\_size\_mid .4

\_exptl\_crystal\_size\_min .1

\_exptl\_crystal\_density\_meas ?

\_exptl\_crystal\_density\_diffrn 1.460

\_exptl\_crystal\_density\_method 'not measured'

\_exptl\_crystal\_F\_000 1612

\_exptl\_absorpt\_coefficient\_mu 0.588

\_exptl\_absorpt\_correction\_type ?

\_exptl\_absorpt\_correction\_T\_min ?

\_exptl\_absorpt\_correction\_T\_max ?

\_exptl\_absorpt\_process\_details ?

\_exptl\_special\_details

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?

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\_diffrn\_ambient\_temperature 293(2)

\_diffrn\_radiation\_wavelength 0.71073

\_diffrn\_radiation\_type MoK\a

\_diffrn\_radiation\_source 'fine-focus sealed tube'

\_diffrn\_radiation\_monochromator graphite

\_diffrn\_measurement\_device 'Bruyker-Nonius KappaCCD'

\_diffrn\_measurement\_method ?

\_diffrn\_detector\_area\_resol\_mean ?

\_diffrn\_standards\_number ?

\_diffrn\_standards\_interval\_count ?

\_diffrn\_standards\_interval\_time ?

\_diffrn\_standards\_decay\_% ?

\_diffrn\_reflns\_number 32212

\_diffrn\_reflns\_av\_R\_equivalents 0.0643

\_diffrn\_reflns\_av\_sigmaI/netI 0.0716

\_diffrn\_reflns\_limit\_h\_min -13

\_diffrn\_reflns\_limit\_h\_max 13

\_diffrn\_reflns\_limit\_k\_min -11

\_diffrn\_reflns\_limit\_k\_max 13

\_diffrn\_reflns\_limit\_l\_min -35

\_diffrn\_reflns\_limit\_l\_max 32

\_diffrn\_reflns\_theta\_min 4.57

\_diffrn\_reflns\_theta\_max 26.00

\_reflns\_number\_total 6842

\_reflns\_number\_gt 4409

\_reflns\_threshold\_expression >2sigma(I)

\_computing\_data\_collection 'Collect'

\_computing\_cell\_refinement ?

\_computing\_data\_reduction 'EvalCCD'

\_computing\_structure\_solution 'SHELXS-97 (Sheldrick, 1990)'

\_computing\_structure\_refinement 'SHELXL-97 (Sheldrick, 1997)'

\_computing\_molecular\_graphics ?

\_computing\_publication\_material ?

\_refine\_special\_details

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Refinement of F^2^ against ALL reflections. The weighted R-factor wR and

goodness of fit S are based on F^2^, conventional R-factors R are based

on F, with F set to zero for negative F^2^. The threshold expression of

F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is

not relevant to the choice of reflections for refinement. R-factors based

on F^2^ are statistically about twice as large as those based on F, and R-

factors based on ALL data will be even larger.

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\_refine\_ls\_structure\_factor\_coef Fsqd

\_refine\_ls\_matrix\_type full

\_refine\_ls\_weighting\_scheme calc

\_refine\_ls\_weighting\_details

'calc w=1/[\s^2^(Fo^2^)+(0.0433P)^2^+2.4503P] where P=(Fo^2^+2Fc^2^)/3'

\_atom\_sites\_solution\_primary direct

\_atom\_sites\_solution\_secondary difmap

\_atom\_sites\_solution\_hydrogens geom

\_refine\_ls\_hydrogen\_treatment noref

\_refine\_ls\_extinction\_method none

\_refine\_ls\_extinction\_coef ?

\_refine\_ls\_number\_reflns 6842

\_refine\_ls\_number\_parameters 478

\_refine\_ls\_number\_restraints 0

\_refine\_ls\_R\_factor\_all 0.1014

\_refine\_ls\_R\_factor\_gt 0.0484

\_refine\_ls\_wR\_factor\_ref 0.1097

\_refine\_ls\_wR\_factor\_gt 0.0913

\_refine\_ls\_goodness\_of\_fit\_ref 0.994

\_refine\_ls\_restrained\_S\_all 0.994

\_refine\_ls\_shift/su\_max 0.001

\_refine\_ls\_shift/su\_mean 0.000

loop\_

\_atom\_site\_label

\_atom\_site\_type\_symbol

\_atom\_site\_fract\_x

\_atom\_site\_fract\_y

\_atom\_site\_fract\_z

\_atom\_site\_U\_iso\_or\_equiv

\_atom\_site\_adp\_type

\_atom\_site\_occupancy

\_atom\_site\_symmetry\_multiplicity

\_atom\_site\_calc\_flag

\_atom\_site\_refinement\_flags

\_atom\_site\_disorder\_assembly

\_atom\_site\_disorder\_group

Co1 Co 0.90684(3) 0.15693(3) 0.686812(13) 0.03111(13) Uani 1 1 d . . .

P1 P 0.76466(7) 0.50004(7) 0.56098(3) 0.0350(2) Uani 1 1 d . . .

N1 N 0.8633(2) 0.0646(2) 0.63489(8) 0.0329(6) Uani 1 1 d . . .

O2 O 1.16975(18) 0.0541(2) 0.61768(7) 0.0466(6) Uani 1 1 d . . .

N3 N 0.74799(19) 0.1497(2) 0.69705(8) 0.0312(5) Uani 1 1 d . . .

N4 N 0.9711(2) 0.2431(2) 0.73879(8) 0.0318(6) Uani 1 1 d . . .

O4 O 0.62896(19) 0.1275(2) 0.75610(8) 0.0509(6) Uani 1 1 d . . .

C8 C 1.0759(3) 0.0769(3) 0.63333(10) 0.0346(7) Uani 1 1 d . . .

N2 N 1.0598(2) 0.1447(2) 0.67177(8) 0.0332(6) Uani 1 1 d . . .

O1 O 0.9470(2) -0.0323(2) 0.57489(8) 0.0609(7) Uani 1 1 d . . .

C1 C 0.6766(2) 0.0784(2) 0.66319(10) 0.0307(7) Uani 1 1 d . . .

C32 C 0.6411(3) 0.4904(3) 0.59537(10) 0.0358(7) Uani 1 1 d . . .

C14 C 1.0990(2) 0.2516(3) 0.74207(11) 0.0348(7) Uani 1 1 d . . .

C6 C 0.7411(2) 0.0331(2) 0.62773(10) 0.0314(7) Uani 1 1 d . . .

C9 C 1.1476(2) 0.1966(3) 0.70425(10) 0.0324(7) Uani 1 1 d . . .

C19 C 0.7102(2) 0.1792(3) 0.73953(10) 0.0338(7) Uani 1 1 d . . .

C2 C 0.5538(3) 0.0562(3) 0.66101(11) 0.0384(7) Uani 1 1 d . . .

H2 H 0.5101 0.0855 0.6843 0.046 Uiso 1 1 calc R . .

C7 C 0.9546(3) 0.0287(3) 0.61040(11) 0.0386(7) Uani 1 1 d . . .

C26 C 0.9028(3) 0.4908(3) 0.59864(11) 0.0380(7) Uani 1 1 d . . .

C20 C 0.7518(3) 0.6404(3) 0.52910(10) 0.0375(7) Uani 1 1 d . . .

O3 O 0.9536(2) 0.3532(4) 0.80397(13) 0.1392(18) Uani 1 1 d . . .

C15 C 0.9072(3) 0.2971(3) 0.77071(12) 0.0504(9) Uani 1 1 d . . .

C27 C 0.9081(3) 0.5288(3) 0.64464(12) 0.0490(9) Uani 1 1 d . . .

H27 H 0.8402 0.5621 0.6557 0.059 Uiso 1 1 calc R . .

C5 C 0.6834(3) -0.0348(3) 0.59124(11) 0.0440(8) Uani 1 1 d . . .

H5 H 0.7262 -0.0664 0.5680 0.053 Uiso 1 1 calc R . .

C4 C 0.5612(3) -0.0548(3) 0.58992(12) 0.0520(9) Uani 1 1 d . . .

H4 H 0.5215 -0.0998 0.5654 0.062 Uiso 1 1 calc R . .

C25 C 0.6392(3) 0.6800(3) 0.51009(11) 0.0485(9) Uani 1 1 d . . .

H25 H 0.5706 0.6387 0.5169 0.058 Uiso 1 1 calc R . .

C38 C 0.7626(3) 0.3781(3) 0.51930(11) 0.0379(7) Uani 1 1 d . . .

C33 C 0.6087(3) 0.5928(3) 0.61954(12) 0.0476(8) Uani 1 1 d . . .

H33 H 0.6472 0.6668 0.6160 0.057 Uiso 1 1 calc R . .

C3 C 0.4973(3) -0.0094(3) 0.62407(12) 0.0457(8) Uani 1 1 d . . .

H3 H 0.4148 -0.0231 0.6222 0.055 Uiso 1 1 calc R . .

C16 C 0.7698(3) 0.2919(3) 0.76417(10) 0.0360(7) Uani 1 1 d . . .

C21 C 0.8530(3) 0.7039(3) 0.51947(11) 0.0467(8) Uani 1 1 d . . .

H21 H 0.9288 0.6794 0.5328 0.056 Uiso 1 1 calc R . .

C43 C 0.7291(3) 0.3987(3) 0.47251(12) 0.0572(10) Uani 1 1 d . . .

H43 H 0.7012 0.4753 0.4625 0.069 Uiso 1 1 calc R . .

C12 C 1.2988(3) 0.3047(3) 0.77378(14) 0.0553(10) Uani 1 1 d . . .

H12 H 1.3506 0.3410 0.7974 0.066 Uiso 1 1 calc R . .

C39 C 0.8000(3) 0.2618(3) 0.53329(12) 0.0543(9) Uani 1 1 d . . .

H39 H 0.8201 0.2450 0.5649 0.065 Uiso 1 1 calc R . .

C29 C 1.1132(3) 0.4697(3) 0.65842(14) 0.0544(9) Uani 1 1 d . . .

H29 H 1.1839 0.4625 0.6786 0.065 Uiso 1 1 calc R . .

C10 C 1.2703(3) 0.1968(3) 0.70139(12) 0.0426(8) Uani 1 1 d . . .

H10 H 1.3014 0.1606 0.6761 0.051 Uiso 1 1 calc R . .

C37 C 0.5819(3) 0.3816(3) 0.60052(12) 0.0484(9) Uani 1 1 d . . .

H37 H 0.6028 0.3124 0.5846 0.058 Uiso 1 1 calc R . .

C18 C 0.7267(4) 0.4022(3) 0.73445(14) 0.0682(11) Uani 1 1 d . . .

H18A H 0.6403 0.4024 0.7295 0.102 Uiso 1 1 calc R . .

H18B H 0.7583 0.3980 0.7048 0.102 Uiso 1 1 calc R . .

H18C H 0.7543 0.4756 0.7504 0.102 Uiso 1 1 calc R . .

C41 C 0.7777(4) 0.1939(3) 0.45418(14) 0.0640(11) Uani 1 1 d . . .

H41 H 0.7852 0.1330 0.4322 0.077 Uiso 1 1 calc R . .

C31 C 1.0057(3) 0.4424(3) 0.58306(13) 0.0568(9) Uani 1 1 d . . .

H31 H 1.0044 0.4169 0.5522 0.068 Uiso 1 1 calc R . .

C22 C 0.8411(4) 0.8038(3) 0.49006(13) 0.0576(10) Uani 1 1 d . . .

H22 H 0.9089 0.8464 0.4833 0.069 Uiso 1 1 calc R . .

C13 C 1.1768(3) 0.3056(3) 0.77704(12) 0.0472(8) Uani 1 1 d . . .

H13 H 1.1468 0.3422 0.8025 0.057 Uiso 1 1 calc R . .

C24 C 0.6284(4) 0.7805(3) 0.48112(12) 0.0574(10) Uani 1 1 d . . .

H24 H 0.5527 0.8074 0.4686 0.069 Uiso 1 1 calc R . .

C35 C 0.4619(3) 0.4764(4) 0.65335(13) 0.0575(10) Uani 1 1 d . . .

H35 H 0.4015 0.4716 0.6731 0.069 Uiso 1 1 calc R . .

C30 C 1.1098(3) 0.4322(4) 0.61328(15) 0.0627(10) Uani 1 1 d . . .

H30 H 1.1784 0.3992 0.6027 0.075 Uiso 1 1 calc R . .

C11 C 1.3458(3) 0.2513(3) 0.73648(13) 0.0512(9) Uani 1 1 d . . .

H11 H 1.4285 0.2521 0.7350 0.061 Uiso 1 1 calc R . .

C23 C 0.7291(4) 0.8401(3) 0.47090(12) 0.0590(10) Uani 1 1 d . . .

H23 H 0.7216 0.9064 0.4506 0.071 Uiso 1 1 calc R . .

C40 C 0.8076(3) 0.1711(3) 0.50056(14) 0.0625(10) Uani 1 1 d . . .

H40 H 0.8334 0.0937 0.5103 0.075 Uiso 1 1 calc R . .

C17 C 0.7264(4) 0.3036(4) 0.81229(13) 0.0729(12) Uani 1 1 d . . .

H17A H 0.6401 0.3004 0.8092 0.109 Uiso 1 1 calc R . .

H17B H 0.7532 0.3799 0.8261 0.109 Uiso 1 1 calc R . .

H17C H 0.7586 0.2378 0.8319 0.109 Uiso 1 1 calc R . .

C34 C 0.5201(3) 0.5845(4) 0.64861(13) 0.0560(10) Uani 1 1 d . . .

H34 H 0.4994 0.6528 0.6652 0.067 Uiso 1 1 calc R . .

C36 C 0.4916(3) 0.3759(4) 0.62942(13) 0.0598(10) Uani 1 1 d . . .

H36 H 0.4509 0.3029 0.6326 0.072 Uiso 1 1 calc R . .

C42 C 0.7365(4) 0.3068(4) 0.44019(13) 0.0730(12) Uani 1 1 d . . .

H42 H 0.7133 0.3219 0.4086 0.088 Uiso 1 1 calc R . .

C28 C 1.0132(3) 0.5178(3) 0.67416(13) 0.0589(10) Uani 1 1 d . . .

H28 H 1.0159 0.5434 0.7051 0.071 Uiso 1 1 calc R . .

loop\_

\_atom\_site\_aniso\_label

\_atom\_site\_aniso\_U\_11

\_atom\_site\_aniso\_U\_22

\_atom\_site\_aniso\_U\_33

\_atom\_site\_aniso\_U\_23

\_atom\_site\_aniso\_U\_13

\_atom\_site\_aniso\_U\_12

Co1 0.0263(2) 0.0384(2) 0.0295(2) -0.00530(18) 0.00691(16) -0.00185(18)

P1 0.0398(5) 0.0348(4) 0.0312(5) -0.0003(4) 0.0075(3) 0.0000(4)

N1 0.0297(14) 0.0393(14) 0.0302(14) -0.0055(11) 0.0059(11) 0.0014(11)

O2 0.0371(13) 0.0612(14) 0.0450(14) -0.0043(11) 0.0194(10) 0.0060(11)

N3 0.0270(12) 0.0355(14) 0.0321(14) -0.0060(11) 0.0072(10) -0.0006(11)

N4 0.0285(13) 0.0350(14) 0.0327(14) -0.0057(11) 0.0074(10) -0.0014(10)

O4 0.0452(13) 0.0659(15) 0.0455(14) -0.0091(12) 0.0214(11) -0.0166(11)

C8 0.0332(17) 0.0379(18) 0.0343(18) 0.0039(14) 0.0109(14) 0.0016(14)

N2 0.0294(13) 0.0393(14) 0.0317(14) -0.0021(12) 0.0071(11) -0.0001(11)

O1 0.0526(15) 0.0876(18) 0.0437(15) -0.0307(14) 0.0102(11) 0.0043(13)

C1 0.0300(16) 0.0286(16) 0.0329(18) 0.0010(13) 0.0016(13) 0.0003(13)

C32 0.0348(17) 0.0424(19) 0.0301(17) 0.0015(14) 0.0030(13) 0.0019(14)

C14 0.0297(16) 0.0329(16) 0.0412(19) 0.0002(14) 0.0017(14) -0.0008(13)

C6 0.0310(16) 0.0309(16) 0.0319(17) -0.0018(13) 0.0024(13) -0.0004(13)

C9 0.0263(16) 0.0321(16) 0.0389(18) 0.0029(14) 0.0038(13) -0.0013(12)

C19 0.0254(16) 0.0441(19) 0.0327(17) -0.0011(14) 0.0069(13) 0.0040(13)

C2 0.0285(17) 0.0429(18) 0.044(2) -0.0037(15) 0.0033(14) 0.0001(14)

C7 0.0413(19) 0.0454(19) 0.0301(18) -0.0006(15) 0.0084(14) 0.0058(15)

C26 0.0401(18) 0.0365(18) 0.0383(19) 0.0000(14) 0.0084(14) -0.0019(14)

C20 0.0460(19) 0.0333(17) 0.0339(18) -0.0030(14) 0.0077(14) -0.0040(14)

O3 0.0428(17) 0.230(4) 0.145(3) -0.152(3) 0.0121(18) -0.013(2)

C15 0.0375(19) 0.059(2) 0.055(2) -0.0281(19) 0.0063(17) -0.0039(16)

C27 0.046(2) 0.058(2) 0.042(2) -0.0123(17) 0.0030(16) 0.0032(16)

C5 0.044(2) 0.051(2) 0.0365(19) -0.0132(16) 0.0057(15) -0.0024(16)

C4 0.047(2) 0.056(2) 0.051(2) -0.0158(18) -0.0080(17) -0.0084(17)

C25 0.057(2) 0.044(2) 0.044(2) 0.0037(16) 0.0013(17) -0.0063(16)

C38 0.0460(19) 0.0367(18) 0.0320(18) -0.0024(14) 0.0089(14) -0.0020(14)

C33 0.048(2) 0.046(2) 0.050(2) -0.0019(17) 0.0109(17) 0.0005(16)

C3 0.0318(18) 0.050(2) 0.053(2) -0.0024(17) -0.0026(16) -0.0038(15)

C16 0.0336(17) 0.0401(18) 0.0363(18) -0.0121(14) 0.0124(13) -0.0006(13)

C21 0.053(2) 0.044(2) 0.045(2) -0.0063(17) 0.0169(16) -0.0017(16)

C43 0.088(3) 0.042(2) 0.041(2) -0.0005(17) 0.0021(19) 0.0069(19)

C12 0.0332(19) 0.050(2) 0.078(3) -0.0150(19) -0.0128(18) -0.0048(16)

C39 0.080(3) 0.039(2) 0.042(2) -0.0004(17) 0.0006(18) 0.0046(18)

C29 0.043(2) 0.055(2) 0.063(3) 0.0072(19) -0.0039(18) -0.0066(17)

C10 0.0333(18) 0.0415(18) 0.054(2) -0.0002(16) 0.0102(15) 0.0000(14)

C37 0.051(2) 0.050(2) 0.046(2) -0.0026(17) 0.0122(17) -0.0035(16)

C18 0.076(3) 0.043(2) 0.081(3) -0.010(2) -0.011(2) 0.0055(19)

C41 0.088(3) 0.049(2) 0.056(3) -0.020(2) 0.008(2) -0.001(2)

C31 0.052(2) 0.075(3) 0.045(2) -0.0034(19) 0.0120(18) 0.0062(19)

C22 0.080(3) 0.043(2) 0.056(2) -0.0024(18) 0.032(2) -0.0129(19)

C13 0.0370(19) 0.050(2) 0.053(2) -0.0123(17) -0.0005(16) -0.0006(15)

C24 0.077(3) 0.044(2) 0.048(2) 0.0015(18) -0.0090(19) 0.0041(19)

C35 0.038(2) 0.088(3) 0.049(2) 0.007(2) 0.0141(16) 0.004(2)

C30 0.042(2) 0.078(3) 0.069(3) 0.006(2) 0.014(2) 0.0103(19)

C11 0.0271(17) 0.049(2) 0.077(3) -0.0045(19) 0.0040(17) -0.0033(15)

C23 0.099(3) 0.039(2) 0.040(2) 0.0033(17) 0.014(2) 0.001(2)

C40 0.084(3) 0.035(2) 0.066(3) -0.0038(19) -0.003(2) 0.0084(18)

C17 0.073(3) 0.097(3) 0.055(2) -0.037(2) 0.034(2) -0.029(2)

C34 0.047(2) 0.070(3) 0.052(2) -0.0090(19) 0.0115(18) 0.0124(19)

C36 0.053(2) 0.069(3) 0.060(3) 0.007(2) 0.0150(19) -0.0154(19)

C42 0.124(4) 0.058(3) 0.035(2) -0.0098(19) 0.001(2) 0.007(2)

C28 0.062(3) 0.063(2) 0.049(2) -0.0135(19) -0.0035(19) -0.0064(19)

\_geom\_special\_details

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All esds (except the esd in the dihedral angle between two l.s. planes)

are estimated using the full covariance matrix. The cell esds are taken

into account individually in the estimation of esds in distances, angles

and torsion angles; correlations between esds in cell parameters are only

used when they are defined by crystal symmetry. An approximate (isotropic)

treatment of cell esds is used for estimating esds involving l.s. planes.

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loop\_

\_geom\_bond\_atom\_site\_label\_1

\_geom\_bond\_atom\_site\_label\_2

\_geom\_bond\_distance

\_geom\_bond\_site\_symmetry\_2

\_geom\_bond\_publ\_flag

Co1 N2 1.816(2) . ?

Co1 N1 1.824(2) . ?

Co1 N3 1.835(2) . ?

Co1 N4 1.843(2) . ?

P1 C26 1.786(3) . ?

P1 C20 1.788(3) . ?

P1 C32 1.791(3) . ?

P1 C38 1.794(3) . ?

N1 C7 1.361(4) . ?

N1 C6 1.402(3) . ?

O2 C8 1.214(3) . ?

N3 C19 1.375(3) . ?

N3 C1 1.422(3) . ?

N4 C15 1.360(4) . ?

N4 C14 1.426(3) . ?

O4 C19 1.213(3) . ?

C8 N2 1.360(4) . ?

C8 C7 1.534(4) . ?

N2 C9 1.398(4) . ?

O1 C7 1.215(3) . ?

C1 C2 1.389(4) . ?

C1 C6 1.405(4) . ?

C32 C37 1.380(4) . ?

C32 C33 1.390(4) . ?

C14 C13 1.385(4) . ?

C14 C9 1.405(4) . ?

C6 C5 1.385(4) . ?

C9 C10 1.384(4) . ?

C19 C16 1.538(4) . ?

C2 C3 1.376(4) . ?

C2 H2 0.9300 . ?

C26 C27 1.381(4) . ?

C26 C31 1.387(4) . ?

C20 C21 1.383(4) . ?

C20 C25 1.385(4) . ?

O3 C15 1.204(4) . ?

C15 C16 1.529(4) . ?

C27 C28 1.376(5) . ?

C27 H27 0.9300 . ?

C5 C4 1.381(4) . ?

C5 H5 0.9300 . ?

C4 C3 1.371(5) . ?

C4 H4 0.9300 . ?

C25 C24 1.378(5) . ?

C25 H25 0.9300 . ?

C38 C43 1.373(4) . ?

C38 C39 1.387(4) . ?

C33 C34 1.370(4) . ?

C33 H33 0.9300 . ?

C3 H3 0.9300 . ?

C16 C17 1.522(4) . ?

C16 C18 1.527(5) . ?

C21 C22 1.381(5) . ?

C21 H21 0.9300 . ?

C43 C42 1.379(5) . ?

C43 H43 0.9300 . ?

C12 C13 1.378(4) . ?

C12 C11 1.377(5) . ?

C12 H12 0.9300 . ?

C39 C40 1.378(5) . ?

C39 H39 0.9300 . ?

C29 C30 1.357(5) . ?

C29 C28 1.359(5) . ?

C29 H29 0.9300 . ?

C10 C11 1.377(4) . ?

C10 H10 0.9300 . ?

C37 C36 1.379(5) . ?

C37 H37 0.9300 . ?

C18 H18A 0.9600 . ?

C18 H18B 0.9600 . ?

C18 H18C 0.9600 . ?

C41 C40 1.360(5) . ?

C41 C42 1.366(5) . ?

C41 H41 0.9300 . ?

C31 C30 1.376(5) . ?

C31 H31 0.9300 . ?

C22 C23 1.369(5) . ?

C22 H22 0.9300 . ?

C13 H13 0.9300 . ?

C24 C23 1.362(5) . ?

C24 H24 0.9300 . ?

C35 C36 1.361(5) . ?

C35 C34 1.366(5) . ?

C35 H35 0.9300 . ?

C30 H30 0.9300 . ?

C11 H11 0.9300 . ?

C23 H23 0.9300 . ?

C40 H40 0.9300 . ?

C17 H17A 0.9600 . ?

C17 H17B 0.9600 . ?

C17 H17C 0.9600 . ?

C34 H34 0.9300 . ?

C36 H36 0.9300 . ?

C42 H42 0.9300 . ?

C28 H28 0.9300 . ?

loop\_

\_geom\_angle\_atom\_site\_label\_1

\_geom\_angle\_atom\_site\_label\_2

\_geom\_angle\_atom\_site\_label\_3

\_geom\_angle

\_geom\_angle\_site\_symmetry\_1

\_geom\_angle\_site\_symmetry\_3

\_geom\_angle\_publ\_flag

N2 Co1 N1 86.32(10) . . ?

N2 Co1 N3 171.89(10) . . ?

N1 Co1 N3 86.17(10) . . ?

N2 Co1 N4 86.51(10) . . ?

N1 Co1 N4 172.47(10) . . ?

N3 Co1 N4 100.86(10) . . ?

C26 P1 C20 111.93(14) . . ?

C26 P1 C32 109.30(14) . . ?

C20 P1 C32 108.13(14) . . ?

C26 P1 C38 107.91(14) . . ?

C20 P1 C38 107.76(14) . . ?

C32 P1 C38 111.85(14) . . ?

C7 N1 C6 128.9(2) . . ?

C7 N1 Co1 115.93(19) . . ?

C6 N1 Co1 115.01(18) . . ?

C19 N3 C1 122.2(2) . . ?

C19 N3 Co1 122.14(18) . . ?

C1 N3 Co1 113.18(17) . . ?

C15 N4 C14 121.7(2) . . ?

C15 N4 Co1 125.7(2) . . ?

C14 N4 Co1 112.57(18) . . ?

O2 C8 N2 127.8(3) . . ?

O2 C8 C7 122.0(3) . . ?

N2 C8 C7 110.2(2) . . ?

C8 N2 C9 128.1(2) . . ?

C8 N2 Co1 116.63(19) . . ?

C9 N2 Co1 114.88(19) . . ?

C2 C1 C6 119.5(3) . . ?

C2 C1 N3 127.1(3) . . ?

C6 C1 N3 113.3(2) . . ?

C37 C32 C33 119.3(3) . . ?

C37 C32 P1 121.3(2) . . ?

C33 C32 P1 119.3(2) . . ?

C13 C14 C9 118.6(3) . . ?

C13 C14 N4 128.2(3) . . ?

C9 C14 N4 113.2(2) . . ?

C5 C6 N1 127.4(3) . . ?

C5 C6 C1 120.4(3) . . ?

N1 C6 C1 112.3(2) . . ?

C10 C9 N2 126.0(3) . . ?

C10 C9 C14 121.2(3) . . ?

N2 C9 C14 112.8(2) . . ?

O4 C19 N3 123.9(3) . . ?

O4 C19 C16 119.9(3) . . ?

N3 C19 C16 116.0(2) . . ?

C3 C2 C1 119.5(3) . . ?

C3 C2 H2 120.3 . . ?

C1 C2 H2 120.3 . . ?

O1 C7 N1 127.5(3) . . ?

O1 C7 C8 121.7(3) . . ?

N1 C7 C8 110.9(3) . . ?

C27 C26 C31 118.5(3) . . ?

C27 C26 P1 120.3(2) . . ?

C31 C26 P1 121.2(2) . . ?

C21 C20 C25 119.4(3) . . ?

C21 C20 P1 121.0(2) . . ?

C25 C20 P1 119.3(2) . . ?

O3 C15 N4 123.1(3) . . ?

O3 C15 C16 117.0(3) . . ?

N4 C15 C16 119.9(3) . . ?

C28 C27 C26 120.4(3) . . ?

C28 C27 H27 119.8 . . ?

C26 C27 H27 119.8 . . ?

C4 C5 C6 118.8(3) . . ?

C4 C5 H5 120.6 . . ?

C6 C5 H5 120.6 . . ?

C3 C4 C5 121.1(3) . . ?

C3 C4 H4 119.4 . . ?

C5 C4 H4 119.4 . . ?

C24 C25 C20 120.2(3) . . ?

C24 C25 H25 119.9 . . ?

C20 C25 H25 119.9 . . ?

C43 C38 C39 118.4(3) . . ?

C43 C38 P1 120.8(2) . . ?

C39 C38 P1 120.7(2) . . ?

C34 C33 C32 119.9(3) . . ?

C34 C33 H33 120.0 . . ?

C32 C33 H33 120.0 . . ?

C4 C3 C2 120.7(3) . . ?

C4 C3 H3 119.6 . . ?

C2 C3 H3 119.6 . . ?

C17 C16 C18 109.2(3) . . ?

C17 C16 C15 107.7(3) . . ?

C18 C16 C15 106.8(3) . . ?

C17 C16 C19 108.7(3) . . ?

C18 C16 C19 106.6(2) . . ?

C15 C16 C19 117.6(2) . . ?

C22 C21 C20 119.8(3) . . ?

C22 C21 H21 120.1 . . ?

C20 C21 H21 120.1 . . ?

C38 C43 C42 120.6(3) . . ?

C38 C43 H43 119.7 . . ?

C42 C43 H43 119.7 . . ?

C13 C12 C11 121.6(3) . . ?

C13 C12 H12 119.2 . . ?

C11 C12 H12 119.2 . . ?

C40 C39 C38 120.3(3) . . ?

C40 C39 H39 119.8 . . ?

C38 C39 H39 119.8 . . ?

C30 C29 C28 120.0(3) . . ?

C30 C29 H29 120.0 . . ?

C28 C29 H29 120.0 . . ?

C11 C10 C9 119.2(3) . . ?

C11 C10 H10 120.4 . . ?

C9 C10 H10 120.4 . . ?

C36 C37 C32 119.7(3) . . ?

C36 C37 H37 120.1 . . ?

C32 C37 H37 120.1 . . ?

C16 C18 H18A 109.5 . . ?

C16 C18 H18B 109.5 . . ?

H18A C18 H18B 109.5 . . ?

C16 C18 H18C 109.5 . . ?

H18A C18 H18C 109.5 . . ?

H18B C18 H18C 109.5 . . ?

C40 C41 C42 119.5(3) . . ?

C40 C41 H41 120.3 . . ?

C42 C41 H41 120.3 . . ?

C30 C31 C26 120.1(3) . . ?

C30 C31 H31 120.0 . . ?

C26 C31 H31 120.0 . . ?

C23 C22 C21 119.8(3) . . ?

C23 C22 H22 120.1 . . ?

C21 C22 H22 120.1 . . ?

C12 C13 C14 119.5(3) . . ?

C12 C13 H13 120.2 . . ?

C14 C13 H13 120.2 . . ?

C23 C24 C25 119.7(4) . . ?

C23 C24 H24 120.1 . . ?

C25 C24 H24 120.1 . . ?

C36 C35 C34 120.4(3) . . ?

C36 C35 H35 119.8 . . ?

C34 C35 H35 119.8 . . ?

C29 C30 C31 120.6(3) . . ?

C29 C30 H30 119.7 . . ?

C31 C30 H30 119.7 . . ?

C10 C11 C12 119.9(3) . . ?

C10 C11 H11 120.1 . . ?

C12 C11 H11 120.1 . . ?

C24 C23 C22 121.0(3) . . ?

C24 C23 H23 119.5 . . ?

C22 C23 H23 119.5 . . ?

C41 C40 C39 120.6(3) . . ?

C41 C40 H40 119.7 . . ?

C39 C40 H40 119.7 . . ?

C16 C17 H17A 109.5 . . ?

C16 C17 H17B 109.5 . . ?

H17A C17 H17B 109.5 . . ?

C16 C17 H17C 109.5 . . ?

H17A C17 H17C 109.5 . . ?

H17B C17 H17C 109.5 . . ?

C35 C34 C33 120.3(3) . . ?

C35 C34 H34 119.9 . . ?

C33 C34 H34 119.9 . . ?

C35 C36 C37 120.3(3) . . ?

C35 C36 H36 119.8 . . ?

C37 C36 H36 119.8 . . ?

C41 C42 C43 120.5(4) . . ?

C41 C42 H42 119.7 . . ?

C43 C42 H42 119.7 . . ?

C29 C28 C27 120.4(3) . . ?

C29 C28 H28 119.8 . . ?

C27 C28 H28 119.8 . . ?

\_diffrn\_measured\_fraction\_theta\_max 0.992

\_diffrn\_reflns\_theta\_full 26.00

\_diffrn\_measured\_fraction\_theta\_full 0.992

\_refine\_diff\_density\_max 0.432

\_refine\_diff\_density\_min -0.350

\_refine\_diff\_density\_rms 0.061

**2. CheckCIF/PLATON report**

You have not supplied any structure factors. As a result the full set of tests cannot be run.

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE

FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED

CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

**Datablock: shelxl**

Bond precision: C-C = 0.0050 A Wavelength=0.71073

Cell: a=11.1840(15) b=10.9650(3) c=28.742(3)

alpha=90 beta=96.469(10) gamma=90

Temperature: 293 K

Calculated Reported

Volume 3502.3(6) 3502.3(6)

Space group P 21/c P2(1)/c

Hall group -P 2ybc ?

Moiety formula

C19 H14 Co N4 O4, C24 H20

P

?

Sum formula C43 H34 Co N4 O4 P C43 H43 Co N4 O4 P

Mr 760.64 769.71

Dx,g cm-3 1.443 1.460

Z 4 4

Mu (mm-1) 0.588 0.588

F000 1576.0 1612.0

F000’ 1578.36

h,k,lmax 13,13,35 13,13,35

Nref 6899 6842

Tmin,Tmax 0.790,0.943

Tmin’ 0.790

Correction method= Not given

Data completeness= 0.992 Theta(max)= 26.000

R(reflections)= 0.0484( 4409) wR2(reflections)= 0.1097( 6842)

S = 0.994 Npar= 478

The following ALERTS were generated. Each ALERT has the format

**test-name\_ALERT\_alert-type\_alert-level**.

Click on the hyperlinks for more details of the test.

**Alert level A**

PLAT183\_ALERT\_1\_A Missing \_cell\_measurement\_reflns\_used Value .... Please Do !

PLAT184\_ALERT\_1\_A Missing \_cell\_measurement\_theta\_min Value ...... Please Do !

PLAT185\_ALERT\_1\_A Missing \_cell\_measurement\_theta\_max Value ...... Please Do !

**Alert level B**

PLAT043\_ALERT\_1\_B Calculated and Reported Mol. Weight Differ by .. 9.07 Check

**Alert level C**

CHEMW03\_ALERT\_2\_C The ratio of given/expected molecular weight as

calculated from the \_atom\_site\* data lies outside

the range 0.99 <> 1.01

From the CIF: \_cell\_formula\_units\_Z 4

From the CIF: \_chemical\_formula\_weight 769.71

TEST: Calculate formula weight from \_atom\_site\_\*

atom mass num sum

C 12.01 43.00 516.47

H 1.01 34.00 34.27

Co 58.93 1.00 58.93

N 14.01 4.00 56.03

O 16.00 4.00 64.00

P 30.97 1.00 30.97

Calculated formula weight 760.68

PLAT041\_ALERT\_1\_C Calc. and Reported SumFormula Strings Differ Please Check

PLAT052\_ALERT\_1\_C Info on Absorption Correction Method Not Given Please Do !

PLAT057\_ALERT\_3\_C Correction for Absorption Required RT(exp) ... 1.19 Do !

PLAT068\_ALERT\_1\_C Reported F000 Differs from Calcd (or Missing)... Please Check

PLAT213\_ALERT\_2\_C Atom O3 has ADP max/min Ratio ..... 3.4 prolate

PLAT242\_ALERT\_2\_C Low ’MainMol’ Ueq as Compared to Neighbors of C15 Check

PLAT242\_ALERT\_2\_C Low ’MainMol’ Ueq as Compared to Neighbors of C16 Check

PLAT369\_ALERT\_2\_C Long C(sp2)-C(sp2) Bond C7 - C8 . 1.53 Ang.

**Alert level G**

FORMU01\_ALERT\_2\_G There is a discrepancy between the atom counts in the

\_chemical\_formula\_sum and the formula from the \_atom\_site\* data.

Atom count from \_chemical\_formula\_sum:C43 H43 Co1 N4 O4 P1

Atom count from the \_atom\_site data: C43 H34 Co1 N4 O4 P1

CELLZ01\_ALERT\_1\_G Difference between formula and atom\_site contents detected.

CELLZ01\_ALERT\_1\_G WARNING: H atoms missing from atom site list. Is this intentional?

From the CIF: \_cell\_formula\_units\_Z 4

From the CIF: \_chemical\_formula\_sum C43 H43 Co N4 O4 P

TEST: Compare cell contents of formula and atom\_site data

atom Z\*formula cif sites diff

C 172.00 172.00 0.00

H 172.00 136.00 36.00

Co 4.00 4.00 0.00

N 16.00 16.00 0.00

O 16.00 16.00 0.00

P 4.00 4.00 0.00

PLAT005\_ALERT\_5\_G No Embedded Refinement Details Found in the CIF Please Do !

PLAT199\_ALERT\_1\_G Reported \_cell\_measurement\_temperature ..... (K) 293 Check

PLAT200\_ALERT\_1\_G Reported \_diffrn\_ambient\_temperature ..... (K) 293 Check

PLAT899\_ALERT\_4\_G SHELXL97 is Deprecated and Succeeded by SHELXL 2016 Note

3 **ALERT level A** = Most likely a serious problem - resolve or explain

1 **ALERT level B** = A potentially serious problem, consider carefully

9 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

7 **ALERT level G** = General information/check it is not something unexpected

11 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

6 ALERT type 2 Indicator that the structure model may be wrong or deficient

1 ALERT type 3 Indicator that the structure quality may be low

1 ALERT type 4 Improvement, methodology, query or suggestion

1 ALERT type 5 Informative message, check

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the

minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement

strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more

serious problems it may be necessary to carry out additional measurements or structure

refinements. However, the purpose of your study may justify the reported deviations and the more

serious of these should normally be commented upon in the discussion or experimental section of a

paper or in the "special\_details" fields of the CIF. checkCIF was carefully designed to identify

outliers and unusual parameters, but every test has its limitations and alerts that are not important

in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no

aspects of the results needing attention. It is up to the individual to critically assess their own

results and, if necessary, seek expert advice.

**Publication of your CIF in IUCr journals**

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs

submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied*

*Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta*

*Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks

are run on the final version of your CIF prior to submission.

**Publication of your CIF in other journals**

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to

CIF submission.

**PLATON version of 13/08/2017; check.def file version of 12/12/2017**

**Datablock shelxl** - ellipsoid plot



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