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Dichloridobis(triphenylphosphine oxide)cobalt(II) methanol 0.125-solvate, a lamellar structure

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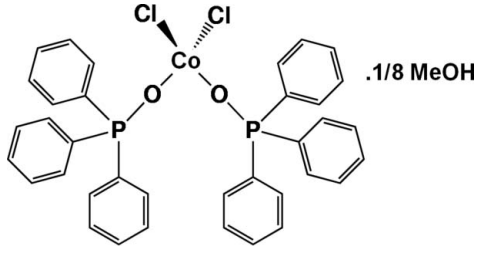
Key indicators: single-crystal X-ray study; T = 150 K; mean σ(C–C) = 0.017 Å; disorder in solvent or counterion; R factor = 0.059; wR factor = 0.133; data-to-parameter ratio = 8.4.

The title methanol solvate, $[CoCl_2(C_{18}H_{15}OP)_2]\cdot 0.125CH_3OH$, crystallized when a methanol solution of $CoCl_2(OPPh_3)_2$, contained in a 0.7 mm diameter tube, was subjected to vapour diffusion using Et_2O antisolvent but the more common unsolvated crystals formed when a 10 mm tube was used. The four crystallographically distinct $CoCl_2(OPPh_3)_2$ molecules in the asymmetric unit of the title structure have similar configurations. In each case, one O—P bond projects into the region between the two Cl atoms [P—O—Co—Cl = 21.2 (8)–42.1 (8)°], and the other is directed away [P—O—Co—Cl = 110.9 (8)–147.4 (6)°]. The Cl—Co—Cl angles range from 116.4 (1) to 125.6 (1)° and O—Co—O from 104.3 (3) to 107.2 (2)°. The crystal studied was an inversion twin.

Related literature

Unsolvated crystal structures of the title compound have been reported previously by Cotton *et al.* (2002) and Marsh (1997), who re-analysed a determination by Mangion *et al.* (1976). These structures are identical and isostructural with the analogous complexes of Mn(II) (Tomita, 1985), Ni(II) (Moreno-Fuquen *et al.*, 2004), Cu (II) (Bertrand & Kalyanaraman, 1971 and Weinberger *et al.*, 1997) and Zn(II) (Rose *et al.*, 1980 and Kosky *et al.*, 1982). A THF solvate of the latter complex has also been reported (Zeller *et al.*, 2001).



Experimental

Crystal data

$[CoCl_2(C_{18}H_{15}OP)_2]\cdot 0.125CH_4O$
M_r = 690.13
Monoclinic, *Cc*
a = 21.3691 (3) Å
b = 37.1989 (8) Å
c = 19.4382 (5) Å
β = 120.368 (1)°
V = 13331.4 (5) Å^3
Z = 16
Mo $K\alpha$ radiation
μ = 0.80 mm^{-1}
T = 150 (2) K
0.22 × 0.12 × 0.05 mm

Data collection

Bruker–Nonius KappaCCD diffractometer
Absorption correction: multi-scan (Blessing, 1995)
T_{min} = 0.843, T_{max} = 0.961
13944 measured reflections
13073 independent reflections
9468 reflections with $I > 2\sigma(I)$
R_{int} = 0.095

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.133
S = 1.07
13073 reflections
1559 parameters
2 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.63 e Å^{-3}
$\Delta\rho_{min}$ = −0.48 e Å^{-3}
Absolute structure: Flack (1983), no Friedel pairs
Flack parameter: 0.40 (4)

Table 1
Selected torsion angles (°).

Cl1—Co1—O1—P1	110.9 (8)	Cl5—Co3—O5—P5	−27.2 (6)
Cl2—Co1—O1—P1	−118.3 (8)	Cl6—Co3—O5—P5	102.9 (5)
Cl1—Co1—O2—P2	38.4 (9)	Cl5—Co3—O6—P6	−125.0 (6)
Cl2—Co1—O2—P2	−91.9 (9)	Cl6—Co3—O6—P6	106.2 (6)
Cl3—Co2—O3—P3	−21.2 (8)	Cl7—Co4—O7—P7	128.4 (6)
Cl4—Co2—O3—P3	109.5 (7)	Cl8—Co4—O7—P7	−97.6 (6)
Cl3—Co2—O4—P4	−147.4 (6)	Cl7—Co4—O8—P8	42.1 (8)
Cl4—Co2—O4—P4	87.5 (7)	Cl8—Co4—O8—P8	−91.9 (7)

Table 2
Table 1. Comparison of geometry (Å,°) in $CoCl_2(OPPh_3)_2$ molecules.

	(I)* range	(I) average	(II*a*)	(II*b*)
Co—Cl	2.221 (3)–2.260 (3)	2.242	2.227 (1)	2.203 (3)
Co—O	1.952 (6)–1.988 (6)	1.971	1.971 (2)	1.998 (7)
Cl—Co—Cl	116.4 (1)–123.6 (1)	119.7	112.76 (6)	114.1 (1)
O—Co—O	104.3 (3)–107.2 (2)	105.3	97.9 (2)	96.3 (3)
Co—O—P	138.4 (4)–154.3 (4)	145.8	153.6 (2)	152.6 (5)

*(I) refers to the title structure and (II) to the usolvated complex, (II*a*) Cotton *et al.* (2002) and (II*b*) Marsh (1997) with s.u.'s taken from Mangion *et al.* (1976)

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *SCALEPACK* and *DENZO* (Otwinowski & Minor 1997); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: KJ2068).

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supplementary materials

Acta Cryst. (2007). E**63**, m2783-m2784 [**doi:10.1107/S1600536807050726**]

Dichloridobis(triphenylphosphine oxide)cobalt(II) methanol 0.125-solvate, a lamellar structure

R. Lancaster and R. G. Pritchard

Comment

The title methanol solvate crystallized when a methanolic solution of $CoCl_2(OPPh_3)_2$, contained in a 0.7 mm tube, was subjected to vapour diffusion using Et_2O anti-solvent. The more common unsolvated crystals formed when a 10 mm diameter tube was used.

All unsolvated 1st row d-block $MCl_2(OPPh_3)_2$ crystal structures are isostructural, crystallizing in orthorhombic space group Fdd2 with each molecule having strict crystallographic C_2 symmetry In each case the O—P bonds project into the region between the two Cl ligands with a stagger angle ranging from 36.8 (2) to 42.3 (4)°, as measured by the P—O—M—Cl torsion angles. This contrasts with the situation in the only previously reported solvated structure, a Zn complex containing THF of crystallization, in which the two P atoms nearly eclipse the Zn—Cl bonds with P—O—Zn—Cl torsion angles of 8.3 (2) and 8.8 (2)°. In this case the O—P bonds project into a region just outside the range subtended by the two Cl atoms.

The four crystallographically distinct $CoCl_2(OPPh_3)_2$ molecules, which comprise the title structure (Figs. 1–5), have simmilar configurations to each other but differ from the above structures. In each case one O—P bond projects into the region between the two Cl atoms (P—O—Co—Cl 21.2 (8) to 42.1 (8)°), and the other is directed away (P—O—Co—Cl 110.9 (8) to 147.4 (6)°). Comparison of the pseudo-tetrahedral geometry in the title structure with that in the unsolvated Co structures shows that the above torsional changes are accompanied by other significant bond length and angle changes (Table 1).

The lamelar nature of the title structure can be seen in the packing digrams (Fig. 6). The methanol, which semi-populates its interlayer sites and displays high vibrational amplitudes, does not form well defined interactions with the host molecules. Furthermore residual voids (total 35 Å^3) in the interlayer region suggest that solvent molecules may have been lost after crystallization.

It is interesting to speculate what role the narrower crystallization container may have had in directing the formation of this lamelar solvate. As a greater depth of anti-solvent was attained in the narrower 0.7 mm crystallization tube, compared to what was achieved in the 10 mm bore tube, it would seem reasonable to suggest that the a mixed Et_2O/MeOH solvate may have been formed initially, with the reported structure resulting from partial solvent loss.

Experimental

Equal volumes of 0.1 *M* Ph_3P=O and $CoCl_2$ solutions in methanol (*ca* 5 drops) were mixed before being syringed into a 0.7 mm diameter special glass X-ray sample tube to a depth of 4 mm. This tube was sealed in a larger sample tube containing *ca* 2 ml Et_2O anti-solvent. The solvent level rose to the top of the 0.7 mm tube overnight (*ca* 30 mm), inducing the crystallization of blue plates. A suitable crystal was selected by immersing the 0.7 mm tube in fluorinated oil on a microscope slide before

crushing the glass to release the crystals. It is hoped that this method of working reduced solvent loss during crystal selection and transfer to the diffractometer.

Refinement

Hydrogen atoms were constrained to chemically reasonable positions. The methanol solvate molecule was treated isotropically with refined partial site occupancy, which was eventually fixed at 0.5 to allow the refinement to fully converge. Refinement of the Flack parameter indicated the prescence of a racemic twin with twin components ratio 0.60 (4):0.40 (4).

Figures

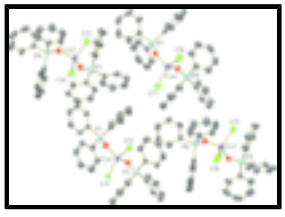


Fig. 1. View of the four Dichloro-bis(triphenylphosphine oxide)-cobalt(II) molecules that form the asymmetric unit of (I) (50% probability displacement ellipsoids). Hydrogen atoms and a methanol solvate molecule have been omitted for clarity.

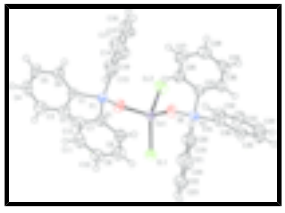


Fig. 2. View of the $CoCl_2(OPPh_3)_2$ molecule containing Co1 from (I) (50% probability displacement ellipsoids)

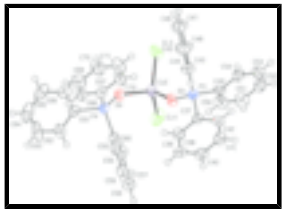


Fig. 3. View of the $CoCl_2(OPPh_3)_2$ molecule containing Co2 from (I) (50% probability displacement ellipsoids)

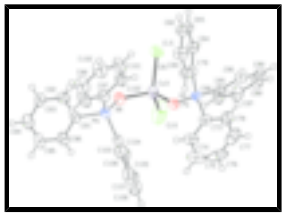


Fig. 4. View of the $CoCl_2(OPPh_3)_2$ molecule containing Co3 from (I) (50% probability displacement ellipsoids)

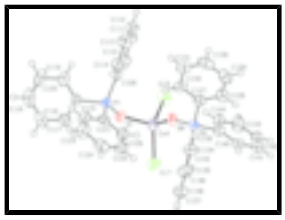


Fig. 5. View of the $CoCl_2(OPPh_3)_2$ molecule containing Co4 from (I) (50% probability displacement ellipsoids)

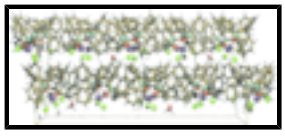


Fig. 6. Packing view of (I) viewed perpendicular to the *c* axis.

Dichloridobis(triphenylphosphine oxide)cobalt(II) methanol solvate

Crystal data

$[CoCl_2(C_{18}H_{15}O_1P_1)_2]\cdot 0.125CH_4O$	$F_{000} = 5683$
$M_r = 690.13$	$D_x = 1.375$ Mg m^{-3}
Monoclinic, *Cc*	Mo *K*α radiation λ = 0.71073 Å
a = 21.3691 (3) Å	Cell parameters from 12813 reflections
b = 37.1989 (8) Å	θ = 1.0–26.0º
c = 19.4382 (5) Å	μ = 0.80 mm^{-1}
β = 120.368 (1)º	*T* = 150 (2) K
V = 13331.4 (5) Å^3	Prism, blue
Z = 16	0.22 × 0.12 × 0.05 mm

Data collection

Bruker–Nonius KappaCCD diffractometer	$R_{int} = 0.095$
CCD rotation images, thick slices scans	$\theta_{max} = 26º$
Absorption correction: multi-scan (Blessing, 1995)	$\theta_{min} = 3.0º$
$T_{min} = 0.843$, $T_{max} = 0.961$	*h* = 0→26
13073 measured reflections	*k* = 0→45
13073 independent reflections	*l* = −23→20
9468 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	H-atom parameters constrained
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0321P)^2 + 57.6187P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.059$	$(\Delta/\sigma)_{max} = 0.021$
$wR(F^2) = 0.133$	$\Delta\rho_{max} = 0.63$ e Å^{-3}
S = 1.07	$\Delta\rho_{min} = -0.48$ e Å^{-3}
13073 reflections	Extinction correction: none
1559 parameters	Absolute structure: Flack (1983)
2 restraints	Flack parameter: 0.40 (4)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($Å^2$)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Co1	0.23624 (7)	0.03411 (3)	0.23354 (7)	0.0316 (3)	
Cl1	0.17186 (13)	−0.01712 (6)	0.20175 (15)	0.0449 (6)	
Cl2	0.25306 (14)	0.06209 (7)	0.14094 (15)	0.0504 (6)	
P1	0.19873 (12)	0.09329 (6)	0.33721 (14)	0.0340 (5)	
P2	0.39944 (12)	0.00193 (6)	0.37640 (14)	0.0340 (5)	
O1	0.1945 (3)	0.07046 (15)	0.2710 (4)	0.0415 (15)	
O2	0.3328 (3)	0.02443 (15)	0.3268 (3)	0.0383 (14)	
C1	0.1204 (4)	0.1213 (2)	0.2980 (5)	0.0321 (18)	
C2	0.0529 (5)	0.1060 (2)	0.2457 (5)	0.037 (2)	
H2	0.0504	0.0814	0.2314	0.045*	
C3	−0.0104 (5)	0.1260 (3)	0.2144 (6)	0.045 (2)	
H3	−0.056	0.1151	0.1802	0.054*	
C4	−0.0064 (5)	0.1618 (3)	0.2334 (6)	0.045 (2)	
H4	−0.0495	0.1758	0.21	0.054*	
C5	0.0590 (5)	0.1778 (2)	0.2860 (6)	0.045 (2)	
H5	0.0605	0.2024	0.2998	0.053*	
C6	0.1225 (5)	0.1579 (2)	0.3184 (6)	0.043 (2)	
H6	0.1675	0.1688	0.3545	0.052*	
C7	0.2000 (5)	0.0668 (2)	0.4141 (5)	0.036 (2)	
C8	0.2302 (5)	0.0319 (2)	0.4279 (6)	0.041 (2)	
H8	0.2495	0.023	0.3966	0.049*	
C9	0.2314 (6)	0.0107 (3)	0.4870 (6)	0.053 (3)	
H9	0.2526	−0.0125	0.4971	0.064*	
C10	0.2013 (5)	0.0236 (3)	0.5326 (6)	0.047 (2)	
H10	0.2	0.0089	0.5717	0.057*	
C11	0.1742 (5)	0.0579 (3)	0.5192 (6)	0.046 (2)	
H11	0.1561	0.067	0.5515	0.056*	
C12	0.1720 (5)	0.0794 (2)	0.4618 (5)	0.037 (2)	
H12	0.1518	0.1028	0.4537	0.044*	
C13	0.2771 (5)	0.1214 (2)	0.3823 (6)	0.043 (2)	
C14	0.2986 (6)	0.1380 (3)	0.3327 (8)	0.071 (4)	
H14	0.2741	0.1324	0.2774	0.085*	
C15	0.3552 (7)	0.1624 (4)	0.3639 (12)	0.091 (5)	
H15	0.3694	0.174	0.3303	0.109*	
C16	0.3907 (7)	0.1696 (3)	0.4444 (14)	0.102 (6)	
H16	0.4289	0.1868	0.4659	0.122*	
C17	0.3721 (7)	0.1524 (4)	0.4950 (10)	0.092 (5)	
H17	0.398	0.157	0.5507	0.11*	
C18	0.3154 (6)	0.1286 (3)	0.4627 (7)	0.062 (3)	
H18	0.3022	0.1167	0.4968	0.074*	
C19	0.3871 (5)	−0.0281 (2)	0.4407 (6)	0.038 (2)	
C20	0.4251 (5)	−0.0235 (3)	0.5235 (6)	0.047 (2)	
H20	0.4612	−0.0054	0.5473	0.057*	
C21	0.4098 (6)	−0.0458 (3)	0.5707 (6)	0.052 (3)	
H21	0.4359	−0.0429	0.627	0.063*	

C22	0.3572 (5)	−0.0717 (3)	0.5366 (6)	0.047 (2)
H22	0.3464	−0.0864	0.5693	0.057*
C23	0.3197 (5)	−0.0765 (2)	0.4549 (7)	0.051 (3)
H23	0.2837	−0.0947	0.4316	0.061*
C24	0.3347 (5)	−0.0547 (2)	0.4065 (6)	0.042 (2)
H24	0.3091	−0.0581	0.3503	0.051*
C25	0.4728 (4)	0.0318 (2)	0.4387 (5)	0.035 (2)
C26	0.4551 (5)	0.0652 (2)	0.4549 (6)	0.048 (2)
H26	0.4056	0.0721	0.4308	0.057*
C27	0.5091 (6)	0.0890 (3)	0.5063 (7)	0.055 (3)
H27	0.497	0.1118	0.5182	0.066*
C28	0.5816 (5)	0.0783 (3)	0.5400 (6)	0.052 (3)
H28	0.6194	0.0944	0.5737	0.062*
C29	0.5983 (5)	0.0451 (3)	0.5246 (6)	0.053 (3)
H29	0.6478	0.0382	0.5487	0.064*
C30	0.5458 (5)	0.0215 (2)	0.4755 (6)	0.043 (2)
H31	0.5586	−0.0017	0.4664	0.052*
C31	0.4219 (5)	−0.0249 (2)	0.3148 (6)	0.041 (2)
C32	0.3928 (5)	−0.0152 (2)	0.2352 (6)	0.044 (2)
H32	0.3622	0.0052	0.2136	0.053*
C33	0.4101 (6)	−0.0365 (3)	0.1888 (6)	0.050 (3)
H33	0.3899	−0.0304	0.1341	0.06*
C34	0.4545 (6)	−0.0655 (3)	0.2173 (7)	0.056 (3)
H34	0.4646	−0.0794	0.183	0.067*
C35	0.4845 (6)	−0.0746 (2)	0.2964 (6)	0.048 (2)
H35	0.5166	−0.0946	0.3173	0.058*
C36	0.4682 (5)	−0.0549 (2)	0.3454 (7)	0.048 (2)
H36	0.4882	−0.0615	0.3997	0.057*
Co2	0.01776 (7)	0.30892 (3)	0.23069 (7)	0.0365 (3)
Cl3	0.06155 (13)	0.35607 (8)	0.19555 (17)	0.0569 (7)
Cl4	−0.04817 (15)	0.26942 (8)	0.13493 (17)	0.0672 (8)
P3	0.17372 (12)	0.27415 (6)	0.37669 (14)	0.0351 (5)
P4	−0.07134 (12)	0.32353 (6)	0.32534 (14)	0.0345 (5)
O3	0.0947 (3)	0.28277 (16)	0.3247 (4)	0.0406 (14)
O4	−0.0449 (3)	0.32921 (16)	0.2674 (4)	0.0430 (15)
C37	0.1849 (4)	0.2401 (2)	0.4476 (5)	0.0331 (19)
C38	0.1271 (5)	0.2343 (2)	0.4603 (6)	0.048 (2)
H38	0.0823	0.2464	0.4285	0.057*
C39	0.1356 (5)	0.2102 (2)	0.5207 (6)	0.045 (2)
H39	0.0969	0.2065	0.5306	0.054*
C40	0.2018 (6)	0.1919 (2)	0.5662 (6)	0.049 (2)
H40	0.2077	0.1755	0.6065	0.059*
C41	0.2579 (5)	0.1979 (3)	0.5521 (6)	0.046 (2)
H41	0.3027	0.1856	0.583	0.055*
C42	0.2496 (5)	0.2215 (2)	0.4934 (6)	0.046 (2)
H42	0.2887	0.2251	0.484	0.055*
C43	0.2250 (5)	0.3121 (2)	0.4345 (6)	0.038 (2)
C44	0.2598 (5)	0.3127 (2)	0.5178 (6)	0.042 (2)
H44	0.2603	0.2918	0.5459	0.05*

C45	0.2929 (5)	0.3431 (3)	0.5586 (7)	0.053 (3)
H45	0.3159	0.3431	0.6151	0.063*
C46	0.2939 (5)	0.3742 (3)	0.5196 (7)	0.050 (3)
H46	0.3156	0.3955	0.5489	0.06*
C47	0.2625 (6)	0.3738 (2)	0.4366 (7)	0.052 (3)
H47	0.2645	0.3945	0.4091	0.063*
C48	0.2278 (5)	0.3421 (2)	0.3944 (6)	0.043 (2)
H48	0.2061	0.3415	0.3381	0.052*
C49	0.2130 (5)	0.2594 (2)	0.3191 (5)	0.035 (2)
C50	0.1683 (6)	0.2418 (3)	0.2482 (6)	0.051 (3)
H50	0.1184	0.2386	0.2308	0.061*
C51	0.1966 (6)	0.2289 (3)	0.2020 (6)	0.058 (3)
H51	0.1664	0.2161	0.1541	0.069*
C52	0.2690 (6)	0.2347 (3)	0.2264 (7)	0.055 (3)
H52	0.2881	0.2262	0.1947	0.066*
C53	0.3138 (6)	0.2529 (3)	0.2971 (7)	0.052 (3)
H53	0.3633	0.2569	0.3133	0.063*
C54	0.2863 (5)	0.2651 (2)	0.3438 (6)	0.047 (2)
H55	0.317	0.2773	0.3925	0.057*
C55	−0.0763 (5)	0.2771 (2)	0.3463 (6)	0.042 (2)
C56	−0.1099 (6)	0.2535 (3)	0.2799 (8)	0.067 (3)
H56	−0.1265	0.2622	0.2275	0.08*
C57	−0.1180 (8)	0.2177 (3)	0.2927 (11)	0.088 (5)
H57	−0.1397	0.2017	0.2486	0.106*
C58	−0.0958 (8)	0.2051 (3)	0.3663 (13)	0.093 (6)
H58	−0.103	0.1804	0.3735	0.112*
C59	−0.0631 (7)	0.2274 (4)	0.4309 (10)	0.079 (4)
H59	−0.0474	0.2181	0.4827	0.095*
C60	−0.0523 (6)	0.2640 (3)	0.4216 (8)	0.063 (3)
H60	−0.0289	0.2794	0.4667	0.076*
C61	−0.1606 (5)	0.3421 (2)	0.2862 (5)	0.039 (2)
C62	−0.2135 (5)	0.3264 (3)	0.2978 (6)	0.052 (3)
H62	−0.2043	0.3041	0.3251	0.062*
C63	−0.2791 (6)	0.3432 (4)	0.2699 (7)	0.072 (4)
H63	−0.3145	0.3326	0.2794	0.086*
C64	−0.2942 (7)	0.3742 (4)	0.2291 (7)	0.072 (4)
H64	−0.3402	0.3853	0.2098	0.086*
C65	−0.2426 (7)	0.3904 (3)	0.2151 (7)	0.067 (3)
H65	−0.2527	0.4125	0.1871	0.08*
C66	−0.1771 (6)	0.3736 (3)	0.2424 (6)	0.050 (2)
H66	−0.1425	0.3838	0.2311	0.06*
C67	−0.0137 (5)	0.3467 (2)	0.4187 (6)	0.040 (2)
C68	−0.0408 (5)	0.3602 (3)	0.4641 (6)	0.045 (2)
H68	−0.0907	0.3571	0.4469	0.054*
C69	0.0034 (6)	0.3782 (3)	0.5342 (7)	0.058 (3)
H69	−0.0154	0.3873	0.5658	0.069*
C70	0.0753 (6)	0.3828 (3)	0.5573 (7)	0.066 (3)
H70	0.1062	0.3956	0.605	0.079*
C71	0.1034 (6)	0.3690 (3)	0.5124 (8)	0.069 (3)

H71	0.1534	0.3719	0.5297	0.083*
C72	0.0586 (5)	0.3512 (3)	0.4426 (7)	0.056 (3)
H72	0.0772	0.3421	0.411	0.067*
Co3	0.76086 (7)	0.06559 (3)	0.23091 (7)	0.0396 (3)
Cl5	0.82120 (15)	0.11451 (7)	0.2284 (2)	0.0675 (9)
Cl6	0.69939 (19)	0.03291 (11)	0.1209 (2)	0.1013 (14)
P5	0.91512 (12)	0.02897 (6)	0.36261 (14)	0.0328 (5)
P6	0.67019 (12)	0.07520 (6)	0.32416 (14)	0.0355 (5)
O5	0.8341 (3)	0.03541 (15)	0.3196 (4)	0.0379 (14)
O6	0.6915 (3)	0.08228 (16)	0.2624 (4)	0.0420 (15)
C73	0.9351 (5)	−0.0082 (2)	0.4286 (5)	0.038 (2)
C74	0.8812 (6)	−0.0227 (3)	0.4394 (6)	0.052 (3)
H74	0.8335	−0.0132	0.4095	0.062*
C75	0.8941 (8)	−0.0505 (3)	0.4920 (8)	0.074 (4)
H75	0.8563	−0.0604	0.4985	0.089*
C76	0.9645 (9)	−0.0635 (3)	0.5350 (7)	0.075 (4)
H76	0.9746	−0.0825	0.5719	0.09*
C77	1.0200 (8)	−0.0503 (3)	0.5267 (7)	0.072 (4)
H77	1.0675	−0.0601	0.5567	0.086*
C78	1.0055 (6)	−0.0223 (3)	0.4735 (7)	0.056 (3)
H78	1.0435	−0.0125	0.4675	0.067*
C79	0.9670 (4)	0.0655 (2)	0.4244 (5)	0.0337 (19)
C80	0.9860 (5)	0.0675 (2)	0.5044 (5)	0.039 (2)
H80	0.9744	0.0482	0.528	0.047*
C81	1.0210 (6)	0.0969 (3)	0.5488 (6)	0.052 (3)
H81	1.0332	0.0978	0.603	0.062*
C82	1.0392 (5)	0.1256 (2)	0.5168 (6)	0.046 (2)
H82	1.0649	0.1456	0.5491	0.055*
C83	1.0194 (5)	0.1246 (2)	0.4374 (6)	0.040 (2)
H83	1.0304	0.1444	0.4145	0.048*
C84	0.9836 (5)	0.0949 (2)	0.3908 (5)	0.038 (2)
H84	0.9703	0.0945	0.3362	0.046*
C85	0.9460 (5)	0.0185 (2)	0.2945 (5)	0.0338 (19)
C86	0.8947 (5)	0.0094 (3)	0.2162 (6)	0.046 (2)
H86	0.8445	0.0096	0.1991	0.055*
C87	0.9178 (6)	0.0002 (3)	0.1632 (6)	0.055 (3)
H87	0.883	−0.0063	0.1101	0.067*
C88	0.9902 (6)	0.0004 (3)	0.1865 (6)	0.050 (3)
H88	1.0053	−0.0054	0.1495	0.061*
C89	1.0407 (6)	0.0091 (2)	0.2641 (6)	0.044 (2)
H89	1.0909	0.0082	0.2812	0.053*
C90	1.0187 (5)	0.0191 (2)	0.3171 (6)	0.040 (2)
H90	1.0538	0.0265	0.3695	0.048*
C91	0.5798 (4)	0.0913 (2)	0.2897 (5)	0.0346 (19)
C92	0.5616 (5)	0.1253 (2)	0.2527 (6)	0.049 (2)
H92	0.596	0.1385	0.2455	0.059*
C93	0.4935 (5)	0.1395 (2)	0.2269 (6)	0.045 (2)
H93	0.4812	0.1624	0.2021	0.054*
C94	0.4431 (5)	0.1204 (3)	0.2370 (6)	0.053 (3)

H94	0.3963	0.1303	0.2191	0.064*
C95	0.4602 (5)	0.0876 (3)	0.2725 (7)	0.057 (3)
H95	0.4252	0.0747	0.2791	0.069*
C96	0.5290 (5)	0.0725 (3)	0.2996 (6)	0.046 (2)
H96	0.5406	0.0496	0.3247	0.056*
C97	0.7287 (5)	0.0986 (3)	0.4149 (6)	0.043 (2)
C98	0.7045 (6)	0.1095 (3)	0.4662 (6)	0.059 (3)
H98	0.6567	0.1037	0.4542	0.071*
C99	0.7508 (6)	0.1289 (3)	0.5354 (7)	0.068 (3)
H99	0.7339	0.1365	0.5698	0.081*
C100	0.8202 (6)	0.1371 (3)	0.5540 (7)	0.066 (3)
H100	0.8518	0.1497	0.6018	0.079*
C101	0.8438 (6)	0.1268 (3)	0.5018 (8)	0.072 (4)
H101	0.891	0.1332	0.5131	0.086*
C102	0.7993 (5)	0.1073 (3)	0.4343 (6)	0.051 (3)
H102	0.8169	0.0996	0.4005	0.061*
C103	0.6704 (5)	0.0288 (3)	0.3438 (7)	0.054 (3)
C104	0.6970 (7)	0.0140 (3)	0.4187 (9)	0.073 (4)
H104	0.7208	0.029	0.4644	0.088*
C105	0.6894 (10)	−0.0224 (5)	0.4279 (15)	0.123 (8)
H105	0.707	−0.0318	0.4799	0.147*
C106	0.6571 (11)	−0.0450 (4)	0.3638 (17)	0.124 (9)
H106	0.6524	−0.07	0.3707	0.149*
C107	0.6317 (8)	−0.0307 (3)	0.2894 (13)	0.103 (6)
H107	0.6096	−0.0462	0.2444	0.123*
C108	0.6372 (6)	0.0056 (3)	0.2777 (9)	0.069 (4)
H208	0.6187	0.0147	0.2253	0.083*
Co4	0.48535 (7)	0.28576 (3)	0.22196 (7)	0.0389 (3)
Cl7	0.42672 (15)	0.23383 (7)	0.20164 (19)	0.0641 (8)
Cl8	0.50554 (17)	0.31232 (9)	0.13040 (18)	0.0708 (9)
P7	0.44717 (12)	0.35044 (6)	0.31112 (14)	0.0324 (5)
P8	0.64544 (12)	0.25569 (6)	0.36922 (14)	0.0354 (5)
O7	0.4355 (3)	0.32189 (15)	0.2500 (4)	0.0372 (14)
O8	0.5810 (3)	0.27918 (15)	0.3206 (4)	0.0392 (14)
C109	0.5199 (4)	0.3800 (2)	0.3309 (6)	0.037 (2)
C110	0.5265 (5)	0.3927 (2)	0.2679 (6)	0.044 (2)
H110	0.4948	0.384	0.2156	0.053*
C111	0.5782 (6)	0.4178 (2)	0.2796 (7)	0.052 (3)
H111	0.5812	0.4266	0.2355	0.062*
C112	0.6262 (5)	0.4304 (2)	0.3560 (6)	0.044 (2)
H112	0.6622	0.4477	0.3645	0.053*
C113	0.6207 (5)	0.4176 (3)	0.4186 (6)	0.051 (2)
H113	0.6539	0.4259	0.4709	0.061*
C114	0.5688 (5)	0.3932 (2)	0.4082 (6)	0.045 (2)
H114	0.5656	0.385	0.4526	0.054*
C115	0.3671 (5)	0.3770 (2)	0.2760 (5)	0.0341 (19)
C116	0.3018 (5)	0.3588 (3)	0.2486 (6)	0.051 (3)
H116	0.3011	0.3333	0.2458	0.061*
C117	0.2384 (5)	0.3771 (3)	0.2256 (6)	0.058 (3)

H117	0.1941	0.3646	0.2084	0.069*
C118	0.2408 (6)	0.4149 (4)	0.2282 (7)	0.068 (3)
H118	0.1973	0.428	0.2115	0.081*
C119	0.3041 (6)	0.4331 (3)	0.2540 (7)	0.071 (4)
H119	0.3046	0.4586	0.2557	0.086*
C120	0.3672 (5)	0.4142 (3)	0.2777 (6)	0.051 (3)
H120	0.4113	0.4269	0.2955	0.061*
C121	0.4630 (5)	0.3306 (2)	0.4026 (5)	0.037 (2)
C122	0.4421 (6)	0.3481 (3)	0.4511 (6)	0.051 (3)
H122	0.4188	0.3709	0.4355	0.062*
C123	0.4548 (6)	0.3328 (3)	0.5211 (6)	0.059 (3)
H123	0.441	0.3452	0.5542	0.07*
C124	0.4875 (6)	0.2994 (3)	0.5439 (6)	0.054 (3)
H124	0.4957	0.2888	0.5923	0.065*
C125	0.5077 (6)	0.2819 (3)	0.4973 (7)	0.055 (3)
H125	0.5291	0.2588	0.5124	0.066*
C126	0.4972 (5)	0.2978 (3)	0.4272 (6)	0.050 (2)
H126	0.5137	0.2858	0.3961	0.06*
C127	0.7198 (5)	0.2838 (2)	0.4323 (6)	0.041 (2)
C128	0.7929 (5)	0.2735 (3)	0.4630 (6)	0.049 (2)
H128	0.8041	0.251	0.4485	0.059*
C129	0.8482 (5)	0.2966 (3)	0.5148 (6)	0.056 (3)
H129	0.8975	0.29	0.5358	0.067*
C130	0.8314 (6)	0.3288 (3)	0.5354 (7)	0.061 (3)
H130	0.8697	0.3441	0.5712	0.074*
C131	0.7620 (6)	0.3398 (3)	0.5066 (7)	0.058 (3)
H131	0.752	0.3624	0.5214	0.07*
C132	0.7050 (6)	0.3170 (2)	0.4546 (6)	0.051 (3)
H132	0.6562	0.3242	0.4344	0.061*
C133	0.6312 (5)	0.2253 (2)	0.4311 (5)	0.036 (2)
C134	0.6720 (6)	0.2265 (3)	0.5137 (7)	0.057 (3)
H134	0.7114	0.2429	0.539	0.069*
C135	0.6555 (7)	0.2037 (3)	0.5608 (7)	0.059 (3)
H135	0.6831	0.2048	0.6173	0.071*
C136	0.5987 (6)	0.1799 (3)	0.5228 (7)	0.056 (3)
H136	0.5869	0.1646	0.5537	0.067*
C137	0.5591 (6)	0.1779 (3)	0.4420 (7)	0.052 (3)
H137	0.5208	0.1609	0.4171	0.063*
C138	0.5747 (5)	0.2006 (3)	0.3955 (6)	0.048 (2)
H138	0.5465	0.1992	0.339	0.057*
C139	0.6676 (5)	0.2291 (2)	0.3075 (6)	0.041 (2)
C140	0.7062 (5)	0.1967 (2)	0.3335 (6)	0.044 (2)
H140	0.7214	0.1878	0.3855	0.053*
C141	0.7218 (5)	0.1778 (3)	0.2829 (7)	0.051 (3)
H141	0.7489	0.1562	0.3013	0.061*
C142	0.6994 (6)	0.1893 (3)	0.2076 (7)	0.057 (3)
H142	0.7092	0.1754	0.1731	0.068*
C143	0.6619 (7)	0.2216 (3)	0.1815 (8)	0.071 (3)
H143	0.6481	0.2306	0.13	0.085*

C144	0.6445 (5)	0.2409 (3)	0.2310 (6)	0.052 (3)	
H144	0.6165	0.2623	0.212	0.062*	
O9	0.2083 (19)	0.1418 (9)	0.141 (2)	0.182 (13)*	0.5
H9B	0.2214	0.1258	0.1203	0.273*	0.5
C145	0.1384 (16)	0.1371 (8)	0.1174 (18)	0.092 (9)*	0.5
H145	0.1321	0.1375	0.164	0.137*	0.5
H146	0.1219	0.114	0.09	0.137*	0.5
H147	0.1099	0.1566	0.0809	0.137*	0.5

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0318 (6)	0.0354 (6)	0.0301 (7)	−0.0017 (5)	0.0175 (6)	−0.0032 (5)
Cl1	0.0483 (13)	0.0395 (12)	0.0559 (16)	−0.0099 (10)	0.0330 (13)	−0.0090 (11)
Cl2	0.0563 (15)	0.0641 (15)	0.0385 (14)	−0.0011 (12)	0.0296 (12)	0.0077 (12)
P1	0.0358 (12)	0.0332 (11)	0.0361 (14)	0.0030 (9)	0.0205 (11)	−0.0025 (10)
P2	0.0320 (12)	0.0363 (12)	0.0337 (13)	−0.0013 (9)	0.0167 (11)	−0.0003 (10)
O1	0.058 (4)	0.041 (3)	0.031 (4)	0.008 (3)	0.026 (3)	−0.003 (3)
O2	0.036 (3)	0.045 (3)	0.030 (4)	0.006 (3)	0.014 (3)	0.003 (3)
C1	0.034 (5)	0.026 (4)	0.036 (5)	−0.005 (3)	0.017 (4)	0.000 (4)
C2	0.044 (5)	0.028 (4)	0.036 (5)	−0.002 (4)	0.017 (5)	0.000 (4)
C3	0.041 (5)	0.052 (6)	0.036 (6)	0.001 (4)	0.014 (5)	0.008 (5)
C4	0.032 (5)	0.064 (6)	0.036 (6)	0.009 (4)	0.016 (5)	−0.004 (5)
C5	0.044 (5)	0.041 (5)	0.046 (6)	0.010 (4)	0.021 (5)	−0.009 (4)
C6	0.040 (5)	0.038 (5)	0.051 (6)	0.005 (4)	0.022 (5)	−0.001 (4)
C7	0.036 (5)	0.036 (5)	0.033 (5)	−0.003 (4)	0.016 (4)	−0.009 (4)
C8	0.040 (5)	0.044 (5)	0.037 (6)	0.007 (4)	0.019 (4)	0.003 (4)
C9	0.062 (7)	0.054 (6)	0.049 (7)	0.010 (5)	0.032 (6)	0.011 (5)
C10	0.044 (6)	0.057 (6)	0.038 (6)	0.005 (5)	0.019 (5)	0.014 (5)
C11	0.043 (5)	0.072 (7)	0.027 (5)	0.007 (5)	0.020 (5)	−0.007 (5)
C12	0.036 (5)	0.048 (5)	0.025 (5)	−0.001 (4)	0.015 (4)	0.000 (4)
C13	0.035 (5)	0.034 (5)	0.055 (7)	0.006 (4)	0.020 (5)	0.000 (4)
C14	0.051 (7)	0.056 (7)	0.090 (10)	0.002 (5)	0.025 (7)	0.029 (6)
C15	0.042 (7)	0.067 (8)	0.157 (16)	−0.002 (6)	0.046 (9)	0.038 (9)
C16	0.049 (8)	0.044 (7)	0.20 (2)	−0.012 (6)	0.058 (11)	−0.036 (10)
C17	0.047 (7)	0.093 (10)	0.131 (14)	−0.026 (7)	0.043 (8)	−0.063 (10)
C18	0.050 (6)	0.073 (7)	0.070 (8)	−0.011 (5)	0.036 (6)	−0.029 (6)
C19	0.033 (5)	0.042 (5)	0.038 (6)	0.001 (4)	0.018 (4)	−0.004 (4)
C20	0.055 (6)	0.044 (5)	0.043 (6)	−0.009 (4)	0.026 (5)	−0.005 (4)
C21	0.070 (7)	0.049 (6)	0.039 (6)	0.003 (5)	0.029 (6)	0.007 (5)
C22	0.059 (6)	0.048 (6)	0.045 (7)	0.002 (5)	0.035 (6)	0.002 (5)
C23	0.050 (6)	0.035 (5)	0.069 (8)	0.004 (4)	0.031 (6)	0.001 (5)
C24	0.034 (5)	0.045 (5)	0.047 (6)	0.001 (4)	0.020 (5)	0.001 (4)
C25	0.033 (5)	0.033 (4)	0.040 (5)	−0.004 (4)	0.019 (4)	0.002 (4)
C26	0.039 (5)	0.041 (5)	0.053 (7)	0.005 (4)	0.016 (5)	−0.002 (5)
C27	0.057 (7)	0.040 (5)	0.057 (7)	−0.002 (5)	0.021 (6)	−0.006 (5)
C28	0.041 (6)	0.052 (6)	0.052 (7)	−0.010 (5)	0.015 (5)	−0.011 (5)
C29	0.025 (5)	0.070 (7)	0.056 (7)	−0.001 (5)	0.015 (5)	0.008 (6)

C30	0.036 (5)	0.043 (5)	0.054 (7)	0.000 (4)	0.025 (5)	−0.007 (4)
C31	0.037 (5)	0.037 (5)	0.054 (6)	−0.004 (4)	0.027 (5)	0.003 (4)
C32	0.056 (6)	0.040 (5)	0.040 (6)	−0.002 (4)	0.027 (5)	−0.001 (4)
C33	0.069 (7)	0.051 (6)	0.038 (6)	0.009 (5)	0.032 (6)	−0.003 (5)
C34	0.069 (7)	0.045 (6)	0.077 (9)	−0.011 (5)	0.054 (7)	−0.021 (5)
C35	0.067 (7)	0.039 (5)	0.055 (7)	0.008 (5)	0.043 (6)	−0.005 (5)
C36	0.052 (6)	0.035 (5)	0.058 (7)	−0.005 (4)	0.029 (5)	0.008 (4)
Co2	0.0325 (6)	0.0449 (7)	0.0299 (7)	0.0057 (5)	0.0141 (6)	−0.0008 (6)
Cl3	0.0447 (14)	0.0758 (18)	0.0555 (17)	0.0080 (12)	0.0293 (13)	0.0252 (14)
Cl4	0.0619 (17)	0.0652 (17)	0.0473 (17)	0.0146 (14)	0.0075 (14)	−0.0203 (14)
P3	0.0319 (12)	0.0365 (12)	0.0332 (14)	−0.0005 (9)	0.0138 (11)	0.0022 (10)
P4	0.0347 (12)	0.0348 (12)	0.0385 (14)	0.0056 (9)	0.0217 (11)	0.0027 (10)
O3	0.026 (3)	0.052 (4)	0.034 (4)	0.006 (3)	0.008 (3)	0.007 (3)
O4	0.041 (4)	0.044 (4)	0.049 (4)	0.005 (3)	0.027 (3)	0.001 (3)
C37	0.035 (5)	0.028 (4)	0.032 (5)	−0.001 (3)	0.014 (4)	−0.003 (4)
C38	0.038 (5)	0.047 (5)	0.055 (7)	−0.002 (4)	0.020 (5)	0.001 (5)
C39	0.051 (6)	0.034 (5)	0.050 (6)	−0.007 (4)	0.026 (5)	0.004 (4)
C40	0.060 (6)	0.042 (5)	0.046 (6)	0.003 (5)	0.028 (5)	0.016 (5)
C41	0.042 (5)	0.049 (6)	0.039 (6)	0.007 (4)	0.013 (5)	0.006 (5)
C42	0.040 (5)	0.044 (5)	0.060 (7)	−0.005 (4)	0.031 (5)	0.002 (5)
C43	0.035 (5)	0.037 (5)	0.041 (6)	0.002 (4)	0.017 (4)	0.000 (4)
C44	0.045 (5)	0.036 (5)	0.041 (6)	−0.010 (4)	0.019 (5)	0.003 (4)
C45	0.050 (6)	0.055 (6)	0.046 (7)	−0.012 (5)	0.019 (5)	−0.001 (5)
C46	0.040 (5)	0.050 (6)	0.055 (7)	−0.009 (4)	0.020 (5)	−0.008 (5)
C47	0.059 (6)	0.032 (5)	0.055 (7)	−0.003 (4)	0.021 (6)	0.008 (5)
C48	0.048 (6)	0.036 (5)	0.036 (6)	−0.007 (4)	0.014 (5)	0.004 (4)
C49	0.034 (5)	0.033 (4)	0.037 (5)	−0.003 (4)	0.017 (4)	0.008 (4)
C50	0.046 (6)	0.069 (7)	0.033 (6)	−0.001 (5)	0.017 (5)	0.008 (5)
C51	0.063 (7)	0.070 (7)	0.035 (6)	−0.003 (6)	0.021 (6)	−0.005 (5)
C52	0.074 (8)	0.049 (6)	0.056 (7)	0.011 (5)	0.044 (6)	0.003 (5)
C53	0.050 (6)	0.059 (6)	0.060 (7)	−0.007 (5)	0.036 (6)	−0.006 (5)
C54	0.044 (5)	0.042 (5)	0.052 (7)	0.000 (4)	0.021 (5)	−0.010 (5)
C55	0.033 (5)	0.047 (5)	0.053 (7)	0.012 (4)	0.026 (5)	0.017 (5)
C56	0.068 (8)	0.055 (7)	0.096 (10)	−0.007 (6)	0.056 (8)	−0.011 (6)
C57	0.101 (11)	0.034 (6)	0.168 (17)	−0.010 (6)	0.097 (12)	0.000 (8)
C58	0.079 (10)	0.041 (7)	0.19 (2)	0.010 (7)	0.087 (12)	0.024 (10)
C59	0.061 (8)	0.068 (8)	0.131 (13)	0.031 (6)	0.066 (9)	0.063 (9)
C60	0.047 (6)	0.068 (7)	0.082 (9)	0.025 (5)	0.039 (6)	0.029 (6)
C61	0.044 (5)	0.036 (5)	0.036 (6)	0.002 (4)	0.019 (5)	−0.006 (4)
C62	0.043 (6)	0.066 (7)	0.055 (7)	0.008 (5)	0.031 (5)	0.002 (5)
C63	0.038 (6)	0.130 (11)	0.045 (7)	0.031 (7)	0.019 (5)	0.010 (7)
C64	0.061 (8)	0.090 (9)	0.038 (7)	0.039 (7)	0.005 (6)	−0.010 (6)
C65	0.069 (8)	0.050 (6)	0.049 (8)	0.020 (6)	0.006 (6)	−0.001 (5)
C66	0.059 (7)	0.044 (6)	0.036 (6)	−0.004 (5)	0.016 (5)	−0.004 (4)
C67	0.039 (5)	0.038 (5)	0.041 (6)	0.009 (4)	0.019 (5)	−0.002 (4)
C68	0.035 (5)	0.060 (6)	0.042 (6)	−0.002 (4)	0.021 (5)	−0.010 (5)
C69	0.055 (7)	0.068 (7)	0.050 (7)	0.002 (5)	0.027 (6)	−0.003 (5)
C70	0.040 (6)	0.093 (9)	0.053 (8)	−0.010 (6)	0.015 (6)	−0.021 (6)
C71	0.043 (6)	0.096 (9)	0.067 (9)	−0.005 (6)	0.027 (6)	−0.002 (7)

C72	0.037 (5)	0.078 (7)	0.060 (7)	−0.006 (5)	0.029 (5)	−0.012 (6)
Co3	0.0364 (7)	0.0501 (7)	0.0321 (7)	0.0050 (6)	0.0171 (6)	−0.0008 (6)
Cl5	0.0636 (17)	0.0620 (16)	0.099 (2)	0.0163 (13)	0.0573 (18)	0.0358 (16)
Cl6	0.073 (2)	0.132 (3)	0.056 (2)	0.029 (2)	0.0006 (17)	−0.048 (2)
P5	0.0353 (12)	0.0311 (11)	0.0351 (14)	0.0003 (9)	0.0200 (11)	0.0017 (10)
P6	0.0339 (12)	0.0391 (12)	0.0366 (14)	0.0018 (9)	0.0201 (11)	−0.0001 (10)
O5	0.035 (3)	0.039 (3)	0.041 (4)	0.001 (3)	0.020 (3)	0.002 (3)
O6	0.043 (4)	0.050 (4)	0.038 (4)	0.001 (3)	0.024 (3)	−0.001 (3)
C73	0.047 (5)	0.035 (5)	0.033 (5)	−0.006 (4)	0.021 (5)	−0.003 (4)
C74	0.063 (7)	0.045 (6)	0.048 (7)	−0.015 (5)	0.028 (6)	0.002 (5)
C75	0.089 (10)	0.071 (8)	0.056 (8)	−0.041 (7)	0.032 (8)	−0.002 (7)
C76	0.136 (13)	0.041 (6)	0.046 (7)	−0.018 (7)	0.045 (9)	0.005 (5)
C77	0.102 (10)	0.054 (7)	0.058 (8)	0.032 (7)	0.040 (8)	0.021 (6)
C78	0.060 (7)	0.053 (6)	0.062 (8)	0.019 (5)	0.036 (6)	0.023 (5)
C79	0.029 (4)	0.035 (4)	0.040 (5)	0.001 (3)	0.020 (4)	0.001 (4)
C80	0.048 (5)	0.040 (5)	0.035 (5)	0.001 (4)	0.025 (5)	0.010 (4)
C81	0.069 (7)	0.056 (6)	0.034 (6)	−0.008 (5)	0.029 (5)	−0.002 (5)
C82	0.055 (6)	0.041 (5)	0.049 (7)	−0.010 (4)	0.031 (5)	−0.006 (4)
C83	0.046 (5)	0.033 (5)	0.045 (6)	−0.001 (4)	0.027 (5)	0.001 (4)
C84	0.046 (5)	0.044 (5)	0.031 (5)	−0.001 (4)	0.025 (4)	−0.004 (4)
C85	0.042 (5)	0.032 (4)	0.031 (5)	−0.006 (4)	0.020 (4)	0.003 (4)
C86	0.045 (5)	0.055 (6)	0.039 (6)	0.002 (4)	0.023 (5)	−0.009 (5)
C87	0.065 (7)	0.066 (7)	0.039 (6)	0.008 (5)	0.030 (6)	−0.012 (5)
C88	0.068 (7)	0.053 (6)	0.046 (7)	0.011 (5)	0.041 (6)	0.001 (5)
C89	0.059 (6)	0.032 (5)	0.059 (7)	−0.002 (4)	0.043 (6)	−0.008 (4)
C90	0.040 (5)	0.043 (5)	0.037 (6)	−0.005 (4)	0.019 (4)	0.000 (4)
C91	0.031 (4)	0.043 (5)	0.030 (5)	−0.001 (4)	0.016 (4)	0.001 (4)
C92	0.040 (5)	0.046 (5)	0.055 (7)	−0.006 (4)	0.018 (5)	−0.001 (5)
C93	0.043 (5)	0.043 (5)	0.038 (6)	0.010 (4)	0.013 (5)	−0.004 (4)
C94	0.038 (5)	0.075 (7)	0.043 (6)	0.007 (5)	0.018 (5)	0.000 (5)
C95	0.036 (5)	0.089 (8)	0.053 (7)	0.009 (5)	0.027 (5)	0.006 (6)
C96	0.039 (5)	0.058 (6)	0.042 (6)	0.003 (4)	0.020 (5)	0.004 (5)
C97	0.040 (5)	0.053 (6)	0.037 (6)	−0.001 (4)	0.020 (5)	0.001 (4)
C98	0.047 (6)	0.101 (9)	0.038 (6)	−0.005 (6)	0.028 (5)	−0.010 (6)
C99	0.056 (7)	0.104 (9)	0.042 (7)	−0.003 (6)	0.023 (6)	−0.024 (6)
C100	0.046 (6)	0.098 (9)	0.037 (7)	−0.004 (6)	0.009 (5)	−0.014 (6)
C101	0.041 (6)	0.096 (9)	0.078 (9)	−0.009 (6)	0.030 (6)	−0.032 (7)
C102	0.036 (5)	0.062 (6)	0.051 (7)	−0.005 (4)	0.019 (5)	−0.017 (5)
C103	0.048 (6)	0.056 (6)	0.076 (8)	0.012 (5)	0.044 (6)	0.014 (6)
C104	0.071 (8)	0.069 (8)	0.104 (11)	0.022 (6)	0.062 (8)	0.032 (7)
C105	0.118 (14)	0.095 (12)	0.22 (2)	0.063 (11)	0.137 (17)	0.089 (14)
C106	0.137 (16)	0.054 (9)	0.26 (3)	0.039 (10)	0.16 (2)	0.058 (14)
C107	0.087 (10)	0.042 (7)	0.22 (2)	−0.015 (6)	0.110 (13)	−0.043 (10)
C108	0.064 (7)	0.046 (6)	0.119 (11)	−0.010 (5)	0.061 (8)	−0.026 (7)
Co4	0.0401 (7)	0.0434 (7)	0.0331 (7)	0.0064 (5)	0.0183 (6)	−0.0018 (6)
Cl7	0.0539 (16)	0.0477 (14)	0.077 (2)	−0.0043 (12)	0.0226 (15)	−0.0216 (13)
Cl8	0.079 (2)	0.096 (2)	0.0516 (18)	0.0331 (17)	0.0440 (17)	0.0305 (16)
P7	0.0341 (12)	0.0315 (11)	0.0331 (13)	0.0011 (9)	0.0180 (11)	−0.0017 (9)
P8	0.0328 (12)	0.0353 (12)	0.0384 (14)	−0.0009 (9)	0.0181 (11)	0.0002 (10)

O7	0.036 (3)	0.036 (3)	0.037 (4)	0.003 (2)	0.017 (3)	−0.002 (3)
O8	0.031 (3)	0.047 (3)	0.039 (4)	0.007 (3)	0.017 (3)	0.003 (3)
C109	0.030 (5)	0.038 (5)	0.042 (6)	0.004 (4)	0.017 (4)	−0.007 (4)
C110	0.055 (6)	0.047 (5)	0.044 (6)	0.000 (4)	0.035 (5)	0.008 (4)
C111	0.066 (7)	0.041 (5)	0.078 (9)	−0.002 (5)	0.058 (7)	−0.001 (5)
C112	0.039 (5)	0.043 (5)	0.053 (7)	0.000 (4)	0.025 (5)	−0.002 (5)
C113	0.040 (5)	0.064 (6)	0.035 (6)	−0.008 (5)	0.009 (5)	0.000 (5)
C114	0.039 (5)	0.051 (6)	0.041 (6)	−0.007 (4)	0.017 (5)	−0.004 (5)
C115	0.037 (5)	0.040 (5)	0.028 (5)	0.005 (4)	0.019 (4)	0.004 (4)
C116	0.039 (5)	0.060 (6)	0.053 (7)	0.003 (5)	0.023 (5)	0.009 (5)
C117	0.036 (6)	0.100 (9)	0.040 (7)	−0.001 (6)	0.021 (5)	−0.001 (6)
C118	0.046 (7)	0.103 (10)	0.045 (7)	0.022 (6)	0.016 (6)	−0.016 (7)
C119	0.065 (8)	0.058 (7)	0.064 (8)	0.022 (6)	0.012 (6)	−0.023 (6)
C120	0.043 (6)	0.052 (6)	0.042 (6)	0.011 (4)	0.010 (5)	−0.011 (5)
C121	0.036 (5)	0.041 (5)	0.037 (5)	−0.004 (4)	0.021 (4)	0.006 (4)
C122	0.074 (7)	0.041 (5)	0.051 (7)	0.014 (5)	0.040 (6)	0.008 (5)
C123	0.083 (8)	0.062 (7)	0.046 (7)	0.017 (6)	0.043 (6)	0.012 (5)
C124	0.061 (7)	0.074 (7)	0.034 (6)	−0.010 (5)	0.029 (5)	0.011 (5)
C125	0.067 (7)	0.039 (5)	0.061 (7)	0.003 (5)	0.033 (6)	0.011 (5)
C126	0.057 (6)	0.048 (6)	0.050 (7)	0.006 (5)	0.031 (5)	0.003 (5)
C127	0.042 (5)	0.041 (5)	0.037 (6)	0.000 (4)	0.018 (5)	0.006 (4)
C128	0.044 (6)	0.059 (6)	0.037 (6)	0.005 (5)	0.015 (5)	0.007 (5)
C129	0.038 (6)	0.081 (8)	0.042 (6)	−0.008 (5)	0.015 (5)	−0.008 (6)
C130	0.052 (7)	0.077 (8)	0.045 (7)	−0.028 (6)	0.017 (6)	−0.001 (6)
C131	0.067 (8)	0.044 (6)	0.056 (7)	−0.011 (5)	0.025 (6)	0.003 (5)
C132	0.057 (6)	0.036 (5)	0.052 (7)	−0.007 (4)	0.022 (6)	0.000 (5)
C133	0.038 (5)	0.039 (5)	0.033 (5)	0.003 (4)	0.019 (4)	0.001 (4)
C134	0.064 (7)	0.045 (6)	0.064 (8)	−0.015 (5)	0.034 (6)	−0.003 (5)
C135	0.096 (9)	0.037 (5)	0.044 (7)	−0.010 (5)	0.035 (6)	0.003 (5)
C136	0.064 (7)	0.047 (6)	0.064 (8)	0.000 (5)	0.038 (6)	0.010 (5)
C137	0.052 (6)	0.052 (6)	0.056 (7)	−0.009 (5)	0.029 (6)	0.000 (5)
C138	0.038 (5)	0.056 (6)	0.048 (6)	−0.008 (4)	0.020 (5)	0.002 (5)
C139	0.042 (5)	0.039 (5)	0.042 (6)	0.000 (4)	0.022 (5)	0.002 (4)
C140	0.047 (5)	0.037 (5)	0.055 (7)	0.000 (4)	0.030 (5)	−0.001 (4)
C141	0.052 (6)	0.040 (5)	0.073 (8)	0.002 (4)	0.041 (6)	0.000 (5)
C142	0.057 (6)	0.050 (6)	0.076 (9)	−0.003 (5)	0.042 (6)	−0.009 (6)
C143	0.082 (9)	0.082 (9)	0.069 (9)	0.012 (7)	0.053 (8)	0.000 (7)
C144	0.051 (6)	0.053 (6)	0.055 (7)	0.017 (5)	0.030 (6)	0.007 (5)

Geometric parameters (Å, °)

Co1—O1	1.952 (6)	Co3—Cl5	2.245 (3)
Co1—O2	1.972 (6)	P5—O5	1.513 (6)
Co1—Cl1	2.247 (2)	P5—C79	1.782 (9)
Co1—Cl2	2.260 (3)	P5—C73	1.787 (9)
P1—O1	1.506 (6)	P5—C85	1.795 (8)
P1—C7	1.780 (9)	P6—O6	1.507 (6)
P1—C1	1.784 (8)	P6—C103	1.766 (10)
P1—C13	1.784 (9)	P6—C97	1.789 (10)

P2—O2	1.507 (6)	P6—C91	1.796 (8)
P2—C19	1.792 (9)	C73—C74	1.379 (13)
P2—C31	1.800 (9)	C73—C78	1.404 (13)
P2—C25	1.799 (9)	C74—C75	1.381 (15)
C1—C2	1.398 (11)	C74—H74	0.95
C1—C6	1.410 (12)	C75—C76	1.387 (18)
C2—C3	1.387 (12)	C75—H75	0.95
C2—H2	0.95	C76—C77	1.366 (18)
C3—C4	1.372 (13)	C76—H76	0.95
C3—H3	0.95	C77—C78	1.389 (14)
C4—C5	1.381 (13)	C77—H77	0.95
C4—H4	0.95	C78—H78	0.95
C5—C6	1.386 (12)	C79—C80	1.398 (12)
C5—H5	0.95	C79—C84	1.409 (11)
C6—H6	0.95	C80—C81	1.357 (13)
C7—C12	1.413 (12)	C80—H80	0.95
C7—C8	1.414 (12)	C81—C82	1.385 (13)
C8—C9	1.381 (13)	C81—H81	0.95
C8—H8	0.95	C82—C83	1.380 (13)
C9—C10	1.416 (14)	C82—H82	0.95
C9—H9	0.95	C83—C84	1.386 (12)
C10—C11	1.370 (13)	C83—H83	0.95
C10—H10	0.95	C84—H84	0.95
C11—C12	1.352 (13)	C85—C90	1.385 (12)
C11—H11	0.95	C85—C86	1.394 (13)
C12—H12	0.95	C86—C87	1.390 (13)
C13—C18	1.375 (15)	C86—H86	0.95
C13—C14	1.402 (15)	C87—C88	1.375 (14)
C14—C15	1.385 (17)	C87—H87	0.95
C14—H14	0.95	C88—C89	1.376 (14)
C15—C16	1.38 (2)	C88—H88	0.95
C15—H15	0.95	C89—C90	1.382 (12)
C16—C17	1.39 (2)	C89—H89	0.95
C16—H16	0.95	C90—H90	0.95
C17—C18	1.370 (15)	C91—C96	1.384 (12)
C17—H17	0.95	C91—C92	1.412 (12)
C18—H18	0.95	C92—C93	1.380 (13)
C19—C24	1.387 (12)	C92—H92	0.95
C19—C20	1.398 (13)	C93—C94	1.386 (14)
C20—C21	1.393 (13)	C93—H93	0.95
C20—H20	0.95	C94—C95	1.357 (15)
C21—C22	1.372 (14)	C94—H94	0.95
C21—H21	0.95	C95—C96	1.404 (13)
C22—C23	1.383 (14)	C95—H95	0.95
C22—H22	0.95	C96—H96	0.95
C23—C24	1.397 (13)	C97—C98	1.396 (13)
C23—H23	0.95	C97—C102	1.396 (13)
C24—H24	0.95	C98—C99	1.402 (15)
C25—C26	1.382 (12)	C98—H98	0.95

C25—C30	1.400 (12)	C99—C100	1.372 (15)
C26—C27	1.394 (13)	C99—H99	0.95
C26—H26	0.95	C100—C101	1.395 (15)
C27—C28	1.401 (14)	C100—H100	0.95
C27—H27	0.95	C101—C102	1.375 (15)
C28—C29	1.358 (14)	C101—H101	0.95
C28—H28	0.95	C102—H102	0.95
C29—C30	1.364 (13)	C103—C104	1.382 (16)
C29—H29	0.95	C103—C108	1.407 (16)
C30—H31	0.95	C104—C105	1.39 (2)
C31—C32	1.393 (13)	C104—H104	0.95
C31—C36	1.407 (13)	C105—C106	1.37 (3)
C32—C33	1.384 (13)	C105—H105	0.95
C32—H32	0.95	C106—C107	1.37 (3)
C33—C34	1.358 (14)	C106—H106	0.95
C33—H33	0.95	C107—C108	1.385 (17)
C34—C35	1.375 (15)	C107—H107	0.95
C34—H34	0.95	C108—H208	0.95
C35—C36	1.381 (13)	Co4—O7	1.955 (6)
C35—H35	0.95	Co4—O8	1.988 (6)
C36—H36	0.95	Co4—Cl7	2.226 (3)
Co2—O4	1.959 (6)	Co4—Cl8	2.260 (3)
Co2—O3	1.988 (6)	P7—O7	1.518 (6)
Co2—Cl4	2.226 (3)	P7—C109	1.781 (9)
Co2—Cl3	2.251 (3)	P7—C115	1.786 (8)
P3—O3	1.500 (6)	P7—C121	1.791 (9)
P3—C49	1.791 (9)	P8—O8	1.495 (6)
P3—C43	1.793 (9)	P8—C127	1.777 (9)
P3—C37	1.797 (9)	P8—C133	1.785 (9)
P4—O4	1.508 (6)	P8—C139	1.792 (9)
P4—C55	1.790 (9)	C109—C110	1.384 (12)
P4—C61	1.796 (9)	C109—C114	1.415 (13)
P4—C67	1.815 (10)	C110—C111	1.374 (13)
C37—C38	1.391 (12)	C110—H110	0.95
C37—C42	1.394 (12)	C111—C112	1.391 (14)
C38—C39	1.413 (13)	C111—H111	0.95
C38—H38	0.95	C112—C113	1.367 (14)
C39—C40	1.407 (13)	C112—H112	0.95
C39—H39	0.95	C113—C114	1.367 (13)
C40—C41	1.377 (13)	C113—H113	0.95
C40—H40	0.95	C114—H114	0.95
C41—C42	1.378 (13)	C115—C120	1.385 (12)
C41—H41	0.95	C115—C116	1.392 (12)
C42—H42	0.95	C116—C117	1.375 (14)
C43—C48	1.379 (12)	C116—H116	0.95
C43—C44	1.399 (13)	C117—C118	1.405 (16)
C44—C45	1.356 (13)	C117—H117	0.95
C44—H44	0.95	C118—C119	1.361 (16)
C45—C46	1.389 (14)	C118—H118	0.95

C45—H45	0.95	C119—C120	1.377 (14)
C46—C47	1.399 (15)	C119—H119	0.95
C46—H46	0.95	C120—H120	0.95
C47—C48	1.413 (13)	C121—C126	1.381 (13)
C47—H47	0.95	C121—C122	1.392 (13)
C48—H48	0.95	C122—C123	1.370 (13)
C49—C50	1.381 (13)	C122—H122	0.95
C49—C54	1.404 (12)	C123—C124	1.385 (14)
C50—C51	1.398 (14)	C123—H123	0.95
C50—H50	0.95	C124—C125	1.350 (14)
C51—C52	1.386 (15)	C124—H124	0.95
C51—H51	0.95	C125—C126	1.396 (14)
C52—C53	1.389 (15)	C125—H125	0.95
C52—H52	0.95	C126—H126	0.95
C53—C54	1.384 (13)	C127—C132	1.394 (13)
C53—H53	0.95	C127—C128	1.414 (13)
C54—H55	0.95	C128—C129	1.397 (14)
C55—C60	1.372 (14)	C128—H128	0.95
C55—C56	1.418 (15)	C129—C130	1.368 (16)
C56—C57	1.384 (15)	C129—H129	0.95
C56—H56	0.95	C130—C131	1.355 (15)
C57—C58	1.34 (2)	C130—H130	0.95
C57—H57	0.95	C131—C132	1.407 (14)
C58—C59	1.37 (2)	C131—H131	0.95
C58—H58	0.95	C132—H132	0.95
C59—C60	1.410 (16)	C133—C134	1.387 (14)
C59—H59	0.95	C133—C138	1.391 (12)
C60—H60	0.95	C134—C135	1.416 (14)
C61—C66	1.388 (13)	C134—H134	0.95
C61—C62	1.389 (13)	C135—C136	1.378 (14)
C62—C63	1.369 (13)	C135—H135	0.95
C62—H62	0.95	C136—C137	1.357 (15)
C63—C64	1.345 (17)	C136—H136	0.95
C63—H63	0.95	C137—C138	1.396 (13)
C64—C65	1.399 (18)	C137—H137	0.95
C64—H64	0.95	C138—H138	0.95
C65—C66	1.369 (15)	C139—C144	1.381 (13)
C65—H65	0.95	C139—C140	1.403 (12)
C66—H66	0.95	C140—C141	1.380 (13)
C67—C68	1.372 (12)	C140—H140	0.95
C67—C72	1.379 (13)	C141—C142	1.360 (15)
C68—C69	1.377 (14)	C141—H141	0.95
C68—H68	0.95	C142—C143	1.391 (15)
C69—C70	1.377 (14)	C142—H142	0.95
C69—H69	0.95	C143—C144	1.392 (14)
C70—C71	1.383 (16)	C143—H143	0.95
C70—H70	0.95	C144—H144	0.95
C71—C72	1.371 (16)	O9—C145	1.33 (4)
C71—H71	0.95	O9—H9B	0.8402

C72—H72	0.95	C145—H145	0.98
Co3—O6	1.968 (6)	C145—H146	0.98
Co3—O5	1.988 (6)	C145—H147	0.98
Co3—Cl6	2.221 (3)		
O1—Co1—O2	104.3 (3)	O5—Co3—Cl5	105.51 (19)
O1—Co1—Cl1	111.0 (2)	Cl6—Co3—Cl5	119.28 (17)
O2—Co1—Cl1	107.96 (19)	O5—P5—C79	113.6 (4)
O1—Co1—Cl2	105.35 (19)	O5—P5—C73	108.1 (4)
O2—Co1—Cl2	107.60 (19)	C79—P5—C73	105.4 (4)
Cl1—Co1—Cl2	119.57 (11)	O5—P5—C85	111.7 (4)
O1—P1—C7	112.0 (4)	C79—P5—C85	109.1 (4)
O1—P1—C1	109.1 (4)	C73—P5—C85	108.6 (4)
C7—P1—C1	107.1 (4)	O6—P6—C103	111.9 (4)
O1—P1—C13	112.6 (4)	O6—P6—C97	111.0 (4)
C7—P1—C13	107.5 (4)	C103—P6—C97	109.8 (5)
C1—P1—C13	108.3 (4)	O6—P6—C91	110.2 (4)
O2—P2—C19	111.6 (4)	C103—P6—C91	106.9 (4)
O2—P2—C31	111.5 (4)	C97—P6—C91	106.9 (4)
C19—P2—C31	107.5 (4)	P5—O5—Co3	138.4 (4)
O2—P2—C25	107.9 (4)	P6—O6—Co3	140.5 (4)
C19—P2—C25	107.5 (4)	C74—C73—C78	118.3 (9)
C31—P2—C25	110.8 (4)	C74—C73—P5	119.9 (7)
P1—O1—Co1	150.3 (4)	C78—C73—P5	121.7 (7)
P2—O2—Co1	154.3 (4)	C75—C74—C73	122.5 (11)
C2—C1—C6	118.2 (8)	C75—C74—H74	118.8
C2—C1—P1	118.1 (6)	C73—C74—H74	118.8
C6—C1—P1	123.6 (7)	C74—C75—C76	117.1 (11)
C3—C2—C1	121.2 (8)	C74—C75—H75	121.5
C3—C2—H2	119.4	C76—C75—H75	121.5
C1—C2—H2	119.4	C77—C76—C75	123.2 (10)
C4—C3—C2	119.3 (9)	C77—C76—H76	118.4
C4—C3—H3	120.3	C75—C76—H76	118.4
C2—C3—H3	120.3	C76—C77—C78	118.4 (12)
C3—C4—C5	121.2 (9)	C76—C77—H77	120.8
C3—C4—H4	119.4	C78—C77—H77	120.8
C5—C4—H4	119.4	C77—C78—C73	120.6 (10)
C4—C5—C6	119.9 (8)	C77—C78—H78	119.7
C4—C5—H5	120.1	C73—C78—H78	119.7
C6—C5—H5	120.1	C80—C79—C84	118.4 (8)
C5—C6—C1	120.2 (9)	C80—C79—P5	121.5 (6)
C5—C6—H6	119.9	C84—C79—P5	119.8 (7)
C1—C6—H6	119.9	C81—C80—C79	120.5 (8)
C12—C7—C8	118.9 (8)	C81—C80—H80	119.8
C12—C7—P1	122.4 (7)	C79—C80—H80	119.8
C8—C7—P1	118.6 (6)	C80—C81—C82	121.6 (9)
C9—C8—C7	119.7 (9)	C80—C81—H81	119.2
C9—C8—H8	120.1	C82—C81—H81	119.2
C7—C8—H8	120.1	C83—C82—C81	119.0 (9)
C8—C9—C10	120.2 (9)	C83—C82—H82	120.5

C8—C9—H9	119.9	C81—C82—H82	120.5
C10—C9—H9	119.9	C82—C83—C84	120.5 (8)
C11—C10—C9	118.6 (9)	C82—C83—H83	119.7
C11—C10—H10	120.7	C84—C83—H83	119.7
C9—C10—H10	120.7	C83—C84—C79	120.0 (8)
C12—C11—C10	122.7 (9)	C83—C84—H84	120
C12—C11—H11	118.6	C79—C84—H84	120
C10—C11—H11	118.6	C90—C85—C86	119.1 (8)
C11—C12—C7	119.7 (8)	C90—C85—P5	122.2 (7)
C11—C12—H12	120.1	C86—C85—P5	118.7 (7)
C7—C12—H12	120.1	C87—C86—C85	119.4 (9)
C18—C13—C14	118.8 (10)	C87—C86—H86	120.3
C18—C13—P1	122.9 (8)	C85—C86—H86	120.3
C14—C13—P1	118.2 (9)	C88—C87—C86	121.1 (10)
C15—C14—C13	120.3 (14)	C88—C87—H87	119.5
C15—C14—H14	119.8	C86—C87—H87	119.5
C13—C14—H14	119.8	C89—C88—C87	119.4 (9)
C16—C15—C14	118.9 (14)	C89—C88—H88	120.3
C16—C15—H15	120.6	C87—C88—H88	120.3
C14—C15—H15	120.6	C88—C89—C90	120.4 (9)
C15—C16—C17	121.6 (12)	C88—C89—H89	119.8
C15—C16—H16	119.2	C90—C89—H89	119.8
C17—C16—H16	119.2	C89—C90—C85	120.6 (9)
C18—C17—C16	118.5 (15)	C89—C90—H90	119.7
C18—C17—H17	120.7	C85—C90—H90	119.7
C16—C17—H17	120.7	C96—C91—C92	119.3 (8)
C17—C18—C13	121.8 (13)	C96—C91—P6	123.5 (7)
C17—C18—H18	119.1	C92—C91—P6	117.2 (6)
C13—C18—H18	119.1	C93—C92—C91	119.8 (9)
C24—C19—C20	119.8 (9)	C93—C92—H92	120.1
C24—C19—P2	118.6 (7)	C91—C92—H92	120.1
C20—C19—P2	121.5 (7)	C92—C93—C94	120.4 (9)
C21—C20—C19	119.5 (9)	C92—C93—H93	119.8
C21—C20—H20	120.2	C94—C93—H93	119.8
C19—C20—H20	120.2	C95—C94—C93	120.2 (9)
C22—C21—C20	120.5 (10)	C95—C94—H94	119.9
C22—C21—H21	119.7	C93—C94—H94	119.9
C20—C21—H21	119.7	C94—C95—C96	120.9 (10)
C21—C22—C23	120.2 (9)	C94—C95—H95	119.6
C21—C22—H22	119.9	C96—C95—H95	119.6
C23—C22—H22	119.9	C91—C96—C95	119.5 (9)
C22—C23—C24	120.2 (9)	C91—C96—H96	120.3
C22—C23—H23	119.9	C95—C96—H96	120.3
C24—C23—H23	119.9	C98—C97—C102	118.7 (9)
C19—C24—C23	119.7 (10)	C98—C97—P6	121.2 (7)
C19—C24—H24	120.1	C102—C97—P6	120.0 (7)
C23—C24—H24	120.1	C97—C98—C99	119.9 (10)
C26—C25—C30	119.4 (8)	C97—C98—H98	120.1
C26—C25—P2	117.6 (7)	C99—C98—H98	120.1

C30—C25—P2	122.8 (7)	C100—C99—C98	120.8 (10)
C25—C26—C27	120.7 (9)	C100—C99—H99	119.6
C25—C26—H26	119.6	C98—C99—H99	119.6
C27—C26—H26	119.6	C99—C100—C101	119.1 (10)
C26—C27—C28	118.4 (9)	C99—C100—H100	120.4
C26—C27—H27	120.8	C101—C100—H100	120.4
C28—C27—H27	120.8	C102—C101—C100	120.7 (10)
C29—C28—C27	120.4 (9)	C102—C101—H101	119.7
C29—C28—H28	119.8	C100—C101—H101	119.7
C27—C28—H28	119.8	C101—C102—C97	120.7 (10)
C28—C29—C30	121.6 (9)	C101—C102—H102	119.6
C28—C29—H29	119.2	C97—C102—H102	119.6
C30—C29—H29	119.2	C104—C103—C108	117.7 (11)
C29—C30—C25	119.5 (9)	C104—C103—P6	124.9 (10)
C29—C30—H31	120.3	C108—C103—P6	117.3 (9)
C25—C30—H31	120.3	C103—C104—C105	120.9 (16)
C32—C31—C36	119.9 (9)	C103—C104—H104	119.6
C32—C31—P2	118.4 (7)	C105—C104—H104	119.6
C36—C31—P2	121.7 (8)	C106—C105—C104	121.5 (19)
C33—C32—C31	117.3 (9)	C106—C105—H105	119.3
C33—C32—H32	121.3	C104—C105—H105	119.3
C31—C32—H32	121.3	C105—C106—C107	118.1 (16)
C34—C33—C32	123.4 (10)	C105—C106—H106	120.9
C34—C33—H33	118.3	C107—C106—H106	120.9
C32—C33—H33	118.3	C106—C107—C108	122.1 (17)
C33—C34—C35	119.2 (9)	C106—C107—H107	119
C33—C34—H34	120.4	C108—C107—H107	119
C35—C34—H34	120.4	C107—C108—C103	119.7 (15)
C34—C35—C36	120.1 (9)	C107—C108—H208	120.2
C34—C35—H35	119.9	C103—C108—H208	120.2
C36—C35—H35	119.9	O7—Co4—O8	104.8 (2)
C35—C36—C31	120.0 (10)	O7—Co4—Cl7	108.01 (19)
C35—C36—H36	120	O8—Co4—Cl7	106.05 (19)
C31—C36—H36	120	O7—Co4—Cl8	105.44 (19)
O4—Co2—O3	104.7 (3)	O8—Co4—Cl8	107.5 (2)
O4—Co2—Cl4	107.4 (2)	Cl7—Co4—Cl8	123.64 (14)
O3—Co2—Cl4	109.0 (2)	O7—P7—C109	112.3 (4)
O4—Co2—Cl3	106.02 (19)	O7—P7—C115	110.0 (4)
O3—Co2—Cl3	112.52 (19)	C109—P7—C115	107.7 (4)
Cl4—Co2—Cl3	116.42 (13)	O7—P7—C121	111.3 (4)
O3—P3—C49	111.6 (4)	C109—P7—C121	109.5 (4)
O3—P3—C43	112.2 (4)	C115—P7—C121	105.7 (4)
C49—P3—C43	107.5 (4)	O8—P8—C127	108.0 (4)
O3—P3—C37	109.5 (4)	O8—P8—C133	112.4 (4)
C49—P3—C37	110.0 (4)	C127—P8—C133	107.8 (4)
C43—P3—C37	105.8 (4)	O8—P8—C139	111.7 (4)
O4—P4—C55	113.1 (4)	C127—P8—C139	109.9 (4)
O4—P4—C61	110.4 (4)	C133—P8—C139	107.1 (4)
C55—P4—C61	107.1 (4)	P7—O7—Co4	143.4 (4)

O4—P4—C67	111.0 (4)	P8—O8—Co4	148.3 (4)
C55—P4—C67	108.6 (5)	C110—C109—C114	118.1 (8)
C61—P4—C67	106.3 (4)	C110—C109—P7	119.3 (7)
P3—O3—Co2	148.2 (4)	C114—C109—P7	122.5 (7)
P4—O4—Co2	143.2 (4)	C111—C110—C109	121.2 (10)
C38—C37—C42	119.5 (8)	C111—C110—H110	119.4
C38—C37—P3	117.4 (7)	C109—C110—H110	119.4
C42—C37—P3	122.9 (7)	C110—C111—C112	120.2 (9)
C37—C38—C39	119.5 (9)	C110—C111—H111	119.9
C37—C38—H38	120.2	C112—C111—H111	119.9
C39—C38—H38	120.2	C113—C112—C111	118.9 (9)
C40—C39—C38	119.7 (9)	C113—C112—H112	120.5
C40—C39—H39	120.2	C111—C112—H112	120.5
C38—C39—H39	120.2	C112—C113—C114	121.9 (9)
C41—C40—C39	119.8 (9)	C112—C113—H113	119
C41—C40—H40	120.1	C114—C113—H113	119
C39—C40—H40	120.1	C113—C114—C109	119.7 (9)
C40—C41—C42	120.4 (9)	C113—C114—H114	120.2
C40—C41—H41	119.8	C109—C114—H114	120.2
C42—C41—H41	119.8	C120—C115—C116	119.0 (8)
C41—C42—C37	121.1 (8)	C120—C115—P7	123.7 (7)
C41—C42—H42	119.5	C116—C115—P7	117.3 (7)
C37—C42—H42	119.5	C117—C116—C115	121.0 (10)
C48—C43—C44	119.4 (8)	C117—C116—H116	119.5
C48—C43—P3	118.1 (7)	C115—C116—H116	119.5
C44—C43—P3	122.5 (7)	C116—C117—C118	118.1 (10)
C45—C44—C43	120.4 (9)	C116—C117—H117	120.9
C45—C44—H44	119.8	C118—C117—H117	120.9
C43—C44—H44	119.8	C119—C118—C117	121.6 (10)
C44—C45—C46	121.4 (10)	C119—C118—H118	119.2
C44—C45—H45	119.3	C117—C118—H118	119.2
C46—C45—H45	119.3	C118—C119—C120	119.4 (11)
C45—C46—C47	119.3 (9)	C118—C119—H119	120.3
C45—C46—H46	120.3	C120—C119—H119	120.3
C47—C46—H46	120.3	C119—C120—C115	120.8 (10)
C46—C47—C48	118.9 (9)	C119—C120—H120	119.6
C46—C47—H47	120.5	C115—C120—H120	119.6
C48—C47—H47	120.5	C126—C121—C122	118.3 (9)
C43—C48—C47	120.5 (9)	C126—C121—P7	120.6 (7)
C43—C48—H48	119.8	C122—C121—P7	121.1 (7)
C47—C48—H48	119.8	C123—C122—C121	120.6 (9)
C50—C49—C54	120.1 (9)	C123—C122—H122	119.7
C50—C49—P3	117.6 (7)	C121—C122—H122	119.7
C54—C49—P3	122.3 (7)	C122—C123—C124	120.4 (9)
C49—C50—C51	120.0 (9)	C122—C123—H123	119.8
C49—C50—H50	120	C124—C123—H123	119.8
C51—C50—H50	120	C125—C124—C123	119.8 (9)
C52—C51—C50	119.7 (10)	C125—C124—H124	120.1
C52—C51—H51	120.2	C123—C124—H124	120.1

C50—C51—H51	120.2	C124—C125—C126	120.3 (9)
C51—C52—C53	120.5 (10)	C124—C125—H125	119.8
C51—C52—H52	119.8	C126—C125—H125	119.8
C53—C52—H52	119.8	C121—C126—C125	120.5 (9)
C54—C53—C52	120.0 (9)	C121—C126—H126	119.8
C54—C53—H53	120	C125—C126—H126	119.8
C52—C53—H53	120	C132—C127—C128	119.1 (9)
C53—C54—C49	119.8 (9)	C132—C127—P8	118.1 (7)
C53—C54—H55	120.1	C128—C127—P8	122.8 (7)
C49—C54—H55	120.1	C129—C128—C127	119.1 (10)
C60—C55—C56	119.8 (10)	C129—C128—H128	120.4
C60—C55—P4	123.5 (9)	C127—C128—H128	120.4
C56—C55—P4	116.7 (8)	C130—C129—C128	119.9 (10)
C57—C56—C55	119.0 (13)	C130—C129—H129	120
C57—C56—H56	120.5	C128—C129—H129	120
C55—C56—H56	120.5	C131—C130—C129	122.4 (10)
C58—C57—C56	121.2 (15)	C131—C130—H130	118.8
C58—C57—H57	119.4	C129—C130—H130	118.8
C56—C57—H57	119.4	C130—C131—C132	119.0 (11)
C57—C58—C59	120.5 (13)	C130—C131—H131	120.5
C57—C58—H58	119.7	C132—C131—H131	120.5
C59—C58—H58	119.7	C127—C132—C131	120.4 (10)
C58—C59—C60	120.7 (13)	C127—C132—H132	119.8
C58—C59—H59	119.7	C131—C132—H132	119.8
C60—C59—H59	119.7	C134—C133—C138	118.4 (9)
C55—C60—C59	118.8 (13)	C134—C133—P8	122.5 (7)
C55—C60—H60	120.6	C138—C133—P8	118.9 (7)
C59—C60—H60	120.6	C133—C134—C135	120.8 (10)
C66—C61—C62	118.6 (9)	C133—C134—H134	119.6
C66—C61—P4	118.1 (7)	C135—C134—H134	119.6
C62—C61—P4	123.3 (7)	C136—C135—C134	118.6 (11)
C63—C62—C61	119.9 (10)	C136—C135—H135	120.7
C63—C62—H62	120	C134—C135—H135	120.7
C61—C62—H62	120	C137—C136—C135	121.3 (10)
C64—C63—C62	121.2 (12)	C137—C136—H136	119.3
C64—C63—H63	119.4	C135—C136—H136	119.3
C62—C63—H63	119.4	C136—C137—C138	120.2 (10)
C63—C64—C65	120.3 (10)	C136—C137—H137	119.9
C63—C64—H64	119.8	C138—C137—H137	119.9
C65—C64—H64	119.8	C133—C138—C137	120.6 (10)
C66—C65—C64	118.8 (11)	C133—C138—H138	119.7
C66—C65—H65	120.6	C137—C138—H138	119.7
C64—C65—H65	120.6	C144—C139—C140	119.1 (9)
C65—C66—C61	121.0 (10)	C144—C139—P8	118.3 (7)
C65—C66—H66	119.5	C140—C139—P8	122.5 (7)
C61—C66—H66	119.5	C141—C140—C139	119.3 (10)
C68—C67—C72	120.1 (9)	C141—C140—H140	120.3
C68—C67—P4	121.5 (7)	C139—C140—H140	120.3
C72—C67—P4	118.3 (7)	C142—C141—C140	121.9 (10)

C67—C68—C69	120.9 (9)	C142—C141—H141	119
C67—C68—H68	119.5	C140—C141—H141	119
C69—C68—H68	119.5	C141—C142—C143	119.2 (10)
C70—C69—C68	118.4 (10)	C141—C142—H142	120.4
C70—C69—H69	120.8	C143—C142—H142	120.4
C68—C69—H69	120.8	C142—C143—C144	120.0 (12)
C69—C70—C71	121.1 (11)	C142—C143—H143	120
C69—C70—H70	119.4	C144—C143—H143	120
C71—C70—H70	119.4	C139—C144—C143	120.4 (10)
C72—C71—C70	119.6 (10)	C139—C144—H144	119.8
C72—C71—H71	120.2	C143—C144—H144	119.8
C70—C71—H71	120.2	C145—O9—H9B	109.2
C71—C72—C67	119.7 (10)	O9—C145—H145	109.5
C71—C72—H72	120.1	O9—C145—H146	109.4
C67—C72—H72	120.1	H145—C145—H146	109.5
O6—Co3—O5	107.2 (2)	O9—C145—H147	109.5
O6—Co3—Cl6	107.5 (2)	H145—C145—H147	109.5
O5—Co3—Cl6	110.4 (2)	H146—C145—H147	109.5
O6—Co3—Cl5	106.4 (2)		
C7—P1—O1—Co1	−62.7 (9)	C79—P5—O5—Co3	71.1 (6)
C1—P1—O1—Co1	178.9 (7)	C73—P5—O5—Co3	−172.3 (5)
C13—P1—O1—Co1	58.7 (9)	C85—P5—O5—Co3	−52.9 (6)
O2—Co1—O1—P1	−5.1 (9)	O6—Co3—O5—P5	−140.3 (5)
Cl1—Co1—O1—P1	110.9 (8)	Cl5—Co3—O5—P5	−27.2 (6)
Cl2—Co1—O1—P1	−118.3 (8)	Cl6—Co3—O5—P5	102.9 (5)
C19—P2—O2—Co1	−85.6 (9)	C103—P6—O6—Co3	−40.4 (8)
C31—P2—O2—Co1	34.6 (10)	C97—P6—O6—Co3	82.6 (7)
C25—P2—O2—Co1	156.5 (8)	C91—P6—O6—Co3	−159.3 (6)
O1—Co1—O2—P2	156.5 (9)	O5—Co3—O6—P6	−12.5 (7)
Cl1—Co1—O2—P2	38.4 (9)	Cl5—Co3—O6—P6	−125.0 (6)
Cl2—Co1—O2—P2	−91.9 (9)	Cl6—Co3—O6—P6	106.2 (6)
O1—P1—C1—C2	43.9 (8)	O5—P5—C73—C74	−7.3 (9)
C7—P1—C1—C2	−77.5 (8)	C79—P5—C73—C74	114.5 (8)
C13—P1—C1—C2	166.8 (7)	C85—P5—C73—C74	−128.7 (8)
O1—P1—C1—C6	−137.7 (8)	O5—P5—C73—C78	175.9 (8)
C7—P1—C1—C6	100.8 (8)	C79—P5—C73—C78	−62.3 (9)
C13—P1—C1—C6	−14.8 (9)	C85—P5—C73—C78	54.5 (9)
C6—C1—C2—C3	0.1 (13)	C78—C73—C74—C75	−0.5 (15)
P1—C1—C2—C3	178.6 (7)	P5—C73—C74—C75	−177.4 (9)
C1—C2—C3—C4	1.8 (14)	C73—C74—C75—C76	0.5 (17)
C2—C3—C4—C5	−3.0 (14)	C74—C75—C76—C77	−0.7 (19)
C3—C4—C5—C6	2.1 (15)	C75—C76—C77—C78	0.9 (19)
C4—C5—C6—C1	−0.1 (14)	C76—C77—C78—C73	−0.9 (18)
C2—C1—C6—C5	−1.0 (13)	C74—C73—C78—C77	0.7 (16)
P1—C1—C6—C5	−179.4 (7)	P5—C73—C78—C77	177.5 (9)
O1—P1—C7—C12	−151.0 (7)	O5—P5—C79—C80	90.4 (8)
C1—P1—C7—C12	−31.4 (8)	C73—P5—C79—C80	−27.7 (8)
C13—P1—C7—C12	84.7 (8)	C85—P5—C79—C80	−144.2 (7)
O1—P1—C7—C8	29.1 (8)	O5—P5—C79—C84	−83.4 (7)

C1—P1—C7—C8	148.7 (7)	C73—P5—C79—C84	158.5 (7)
C13—P1—C7—C8	−95.2 (7)	C85—P5—C79—C84	42.0 (8)
C12—C7—C8—C9	0.4 (13)	C84—C79—C80—C81	−1.3 (13)
P1—C7—C8—C9	−179.7 (8)	P5—C79—C80—C81	−175.2 (7)
C7—C8—C9—C10	1.3 (15)	C79—C80—C81—C82	−0.3 (15)
C8—C9—C10—C11	−2.9 (15)	C80—C81—C82—C83	1.9 (16)
C9—C10—C11—C12	3.0 (15)	C81—C82—C83—C84	−1.8 (14)
C10—C11—C12—C7	−1.3 (14)	C82—C83—C84—C79	0.2 (13)
C8—C7—C12—C11	−0.4 (13)	C80—C79—C84—C83	1.4 (12)
P1—C7—C12—C11	179.7 (7)	P5—C79—C84—C83	175.4 (6)
O1—P1—C13—C18	−142.7 (8)	O5—P5—C85—C90	165.8 (7)
C7—P1—C13—C18	−18.8 (9)	C79—P5—C85—C90	39.4 (8)
C1—P1—C13—C18	96.6 (9)	C73—P5—C85—C90	−75.1 (8)
O1—P1—C13—C14	40.1 (9)	O5—P5—C85—C86	−14.1 (8)
C7—P1—C13—C14	164.0 (7)	C79—P5—C85—C86	−140.5 (7)
C1—P1—C13—C14	−80.6 (8)	C73—P5—C85—C86	105.0 (7)
C18—C13—C14—C15	−2.9 (15)	C90—C85—C86—C87	1.9 (14)
P1—C13—C14—C15	174.4 (9)	P5—C85—C86—C87	−178.1 (8)
C13—C14—C15—C16	1.0 (18)	C85—C86—C87—C88	−1.1 (16)
C14—C15—C16—C17	1(2)	C86—C87—C88—C89	1.5 (16)
C15—C16—C17—C18	−2(2)	C87—C88—C89—C90	−2.9 (15)
C16—C17—C18—C13	0.1 (18)	C88—C89—C90—C85	3.9 (13)
C14—C13—C18—C17	2.3 (16)	C86—C85—C90—C89	−3.3 (13)
P1—C13—C18—C17	−174.9 (9)	P5—C85—C90—C89	176.7 (7)
O2—P2—C19—C24	63.9 (8)	O6—P6—C91—C96	138.2 (8)
C31—P2—C19—C24	−58.6 (8)	C103—P6—C91—C96	16.3 (9)
C25—P2—C19—C24	−177.9 (7)	C97—P6—C91—C96	−101.1 (8)
O2—P2—C19—C20	−111.3 (8)	O6—P6—C91—C92	−43.7 (8)
C31—P2—C19—C20	126.2 (8)	C103—P6—C91—C92	−165.5 (8)
C25—P2—C19—C20	6.9 (9)	C97—P6—C91—C92	77.0 (8)
C24—C19—C20—C21	−0.2 (14)	C96—C91—C92—C93	0.0 (14)
P2—C19—C20—C21	175.0 (7)	P6—C91—C92—C93	−178.3 (8)
C19—C20—C21—C22	−0.8 (15)	C91—C92—C93—C94	−0.1 (15)
C20—C21—C22—C23	1.2 (15)	C92—C93—C94—C95	0.1 (16)
C21—C22—C23—C24	−0.7 (14)	C93—C94—C95—C96	0.1 (17)
C20—C19—C24—C23	0.7 (13)	C92—C91—C96—C95	0.3 (14)
P2—C19—C24—C23	−174.6 (7)	P6—C91—C96—C95	178.4 (8)
C22—C23—C24—C19	−0.2 (13)	C94—C95—C96—C91	−0.3 (16)
O2—P2—C25—C26	23.1 (8)	O6—P6—C97—C98	151.8 (8)
C19—P2—C25—C26	−97.4 (8)	C103—P6—C97—C98	−84.0 (9)
C31—P2—C25—C26	145.4 (7)	C91—P6—C97—C98	31.6 (10)
O2—P2—C25—C30	−161.8 (7)	O6—P6—C97—C102	−26.2 (10)
C19—P2—C25—C30	77.6 (8)	C103—P6—C97—C102	98.0 (9)
C31—P2—C25—C30	−39.5 (9)	C91—P6—C97—C102	−146.4 (8)
C30—C25—C26—C27	1.2 (15)	C102—C97—C98—C99	0.4 (17)
P2—C25—C26—C27	176.4 (8)	P6—C97—C98—C99	−177.6 (9)
C25—C26—C27—C28	1.0 (16)	C97—C98—C99—C100	−0.8 (19)
C26—C27—C28—C29	−2.1 (16)	C98—C99—C100—C101	2(2)
C27—C28—C29—C30	1.0 (17)	C99—C100—C101—C102	−3(2)

C28—C29—C30—C25	1.2 (16)	C100—C101—C102—C97	2.4 (19)
C26—C25—C30—C29	−2.3 (14)	C98—C97—C102—C101	−1.2 (16)
P2—C25—C30—C29	−177.3 (8)	P6—C97—C102—C101	176.8 (9)
O2—P2—C31—C32	18.6 (8)	O6—P6—C103—C104	138.1 (8)
C19—P2—C31—C32	141.1 (7)	C97—P6—C103—C104	14.4 (10)
C25—P2—C31—C32	−101.7 (8)	C91—P6—C103—C104	−101.1 (9)
O2—P2—C31—C36	−162.1 (7)	O6—P6—C103—C108	−45.8 (9)
C19—P2—C31—C36	−39.5 (8)	C97—P6—C103—C108	−169.4 (7)
C25—P2—C31—C36	77.7 (8)	C91—P6—C103—C108	75.0 (8)
C36—C31—C32—C33	1.3 (13)	C108—C103—C104—C105	−1.7 (15)
P2—C31—C32—C33	−179.3 (7)	P6—C103—C104—C105	174.5 (9)
C31—C32—C33—C34	−1.1 (15)	C103—C104—C105—C106	2(2)
C32—C33—C34—C35	−0.4 (16)	C104—C105—C106—C107	0(2)
C33—C34—C35—C36	1.6 (15)	C105—C106—C107—C108	−1(2)
C34—C35—C36—C31	−1.4 (14)	C106—C107—C108—C103	0.6 (18)
C32—C31—C36—C35	−0.1 (13)	C104—C103—C108—C107	0.6 (14)
P2—C31—C36—C35	−179.5 (7)	P6—C103—C108—C107	−175.8 (8)
C49—P3—O3—Co2	−51.2 (9)	C109—P7—O7—Co4	49.4 (7)
C43—P3—O3—Co2	69.5 (9)	C115—P7—O7—Co4	169.3 (6)
C37—P3—O3—Co2	−173.2 (7)	C121—P7—O7—Co4	−73.9 (7)
O4—Co2—O3—P3	−135.9 (7)	O8—Co4—O7—P7	15.7 (7)
Cl3—Co2—O3—P3	−21.2 (8)	Cl7—Co4—O7—P7	128.4 (6)
Cl4—Co2—O3—P3	109.5 (7)	Cl8—Co4—O7—P7	−97.6 (6)
C55—P4—O4—Co2	−30.7 (8)	C127—P8—O8—Co4	155.8 (7)
C61—P4—O4—Co2	−150.8 (6)	C133—P8—O8—Co4	−85.5 (8)
C67—P4—O4—Co2	91.7 (7)	C139—P8—O8—Co4	34.9 (8)
O3—Co2—O4—P4	−28.3 (7)	O7—Co4—O8—P8	156.3 (7)
Cl3—Co2—O4—P4	−147.4 (6)	Cl7—Co4—O8—P8	42.1 (8)
Cl4—Co2—O4—P4	87.5 (7)	Cl8—Co4—O8—P8	−91.9 (7)
O3—P3—C37—C38	−17.4 (8)	O7—P7—C109—C110	43.1 (8)
C49—P3—C37—C38	−140.4 (7)	C115—P7—C109—C110	−78.2 (7)
C43—P3—C37—C38	103.7 (7)	C121—P7—C109—C110	167.3 (7)
O3—P3—C37—C42	167.1 (7)	O7—P7—C109—C114	−141.5 (7)
C49—P3—C37—C42	44.1 (9)	C115—P7—C109—C114	97.2 (8)
C43—P3—C37—C42	−71.8 (8)	C121—P7—C109—C114	−17.2 (8)
C42—C37—C38—C39	1.6 (14)	C114—C109—C110—C111	−1.0 (13)
P3—C37—C38—C39	−174.1 (7)	P7—C109—C110—C111	174.7 (7)
C37—C38—C39—C40	−1.3 (14)	C109—C110—C111—C112	1.3 (14)
C38—C39—C40—C41	0.7 (15)	C110—C111—C112—C113	−0.3 (14)
C39—C40—C41—C42	−0.4 (15)	C111—C112—C113—C114	−1.0 (15)
C40—C41—C42—C37	0.6 (15)	C112—C113—C114—C109	1.3 (15)
C38—C37—C42—C41	−1.2 (14)	C110—C109—C114—C113	−0.3 (13)
P3—C37—C42—C41	174.2 (7)	P7—C109—C114—C113	−175.8 (7)
O3—P3—C43—C48	−62.5 (8)	O7—P7—C115—C120	−132.3 (8)
C49—P3—C43—C48	60.5 (8)	C109—P7—C115—C120	−9.6 (9)
C37—P3—C43—C48	178.0 (7)	C121—P7—C115—C120	107.4 (8)
O3—P3—C43—C44	115.1 (8)	O7—P7—C115—C116	50.4 (8)
C49—P3—C43—C44	−121.8 (8)	C109—P7—C115—C116	173.1 (7)
C37—P3—C43—C44	−4.3 (9)	C121—P7—C115—C116	−69.9 (8)

C48—C43—C44—C45	3.2 (14)	C120—C115—C116—C117	−1.8 (14)
P3—C43—C44—C45	−174.4 (8)	P7—C115—C116—C117	175.6 (8)
C43—C44—C45—C46	−0.5 (15)	C115—C116—C117—C118	1.9 (15)
C44—C45—C46—C47	−2.5 (15)	C116—C117—C118—C119	−1.2 (17)
C45—C46—C47—C48	2.8 (15)	C117—C118—C119—C120	0.5 (18)
C44—C43—C48—C47	−2.8 (14)	C118—C119—C120—C115	−0.3 (18)
P3—C43—C48—C47	174.9 (7)	C116—C115—C120—C119	1.0 (15)
C46—C47—C48—C43	−0.2 (15)	P7—C115—C120—C119	−176.2 (9)
O3—P3—C49—C50	−29.7 (8)	O7—P7—C121—C126	31.2 (9)
C43—P3—C49—C50	−153.1 (7)	C109—P7—C121—C126	−93.6 (8)
C37—P3—C49—C50	92.1 (8)	C115—P7—C121—C126	150.6 (8)
O3—P3—C49—C54	150.5 (7)	O7—P7—C121—C122	−149.6 (8)
C43—P3—C49—C54	27.1 (9)	C109—P7—C121—C122	85.6 (8)
C37—P3—C49—C54	−87.7 (8)	C115—P7—C121—C122	−30.2 (9)
C54—C49—C50—C51	1.7 (14)	C126—C121—C122—C123	−0.5 (15)
P3—C49—C50—C51	−178.2 (8)	P7—C121—C122—C123	−179.7 (9)
C49—C50—C51—C52	−2.0 (16)	C121—C122—C123—C124	−1.1 (17)
C50—C51—C52—C53	1.0 (16)	C122—C123—C124—C125	0.6 (17)
C51—C52—C53—C54	0.4 (16)	C123—C124—C125—C126	1.5 (16)
C52—C53—C54—C49	−0.8 (15)	C122—C121—C126—C125	2.6 (14)
C50—C49—C54—C53	−0.3 (14)	P7—C121—C126—C125	−178.2 (8)
P3—C49—C54—C53	179.6 (7)	C124—C125—C126—C121	−3.1 (16)
O4—P4—C55—C60	135.9 (8)	O8—P8—C127—C132	27.2 (9)
C61—P4—C55—C60	−102.2 (8)	C133—P8—C127—C132	−94.4 (8)
C67—P4—C55—C60	12.2 (9)	C139—P8—C127—C132	149.2 (8)
O4—P4—C55—C56	−46.9 (8)	O8—P8—C127—C128	−155.2 (8)
C61—P4—C55—C56	75.0 (8)	C133—P8—C127—C128	83.2 (9)
C67—P4—C55—C56	−170.6 (7)	C139—P8—C127—C128	−33.2 (9)
C60—C55—C56—C57	0.2 (15)	C132—C127—C128—C129	0.2 (14)
P4—C55—C56—C57	−177.1 (8)	P8—C127—C128—C129	−177.4 (8)
C55—C56—C57—C58	1.1 (18)	C127—C128—C129—C130	0.1 (16)
C56—C57—C58—C59	−1.5 (19)	C128—C129—C130—C131	−0.6 (17)
C57—C58—C59—C60	0.4 (18)	C129—C130—C131—C132	0.9 (17)
C56—C55—C60—C59	−1.2 (14)	C128—C127—C132—C131	0.1 (15)
P4—C55—C60—C59	175.9 (7)	P8—C127—C132—C131	177.8 (8)
C58—C59—C60—C55	0.9 (15)	C130—C131—C132—C127	−0.6 (16)
O4—P4—C61—C66	−36.3 (8)	O8—P8—C133—C134	−116.4 (8)
C55—P4—C61—C66	−159.9 (7)	C127—P8—C133—C134	2.5 (9)
C67—P4—C61—C66	84.2 (8)	C139—P8—C133—C134	120.6 (8)
O4—P4—C61—C62	143.8 (8)	O8—P8—C133—C138	60.1 (8)
C55—P4—C61—C62	20.2 (9)	C127—P8—C133—C138	179.0 (7)
C67—P4—C61—C62	−95.8 (9)	C139—P8—C133—C138	−62.9 (8)
C66—C61—C62—C63	−3.5 (15)	C138—C133—C134—C135	−1.3 (15)
P4—C61—C62—C63	176.5 (8)	P8—C133—C134—C135	175.2 (8)
C61—C62—C63—C64	1.9 (18)	C133—C134—C135—C136	0.8 (16)
C62—C63—C64—C65	−0.6 (19)	C134—C135—C136—C137	0.5 (16)
C63—C64—C65—C66	1.1 (18)	C135—C136—C137—C138	−1.2 (16)
C64—C65—C66—C61	−2.8 (16)	C134—C133—C138—C137	0.6 (14)
C62—C61—C66—C65	4.0 (14)	P8—C133—C138—C137	−176.1 (7)

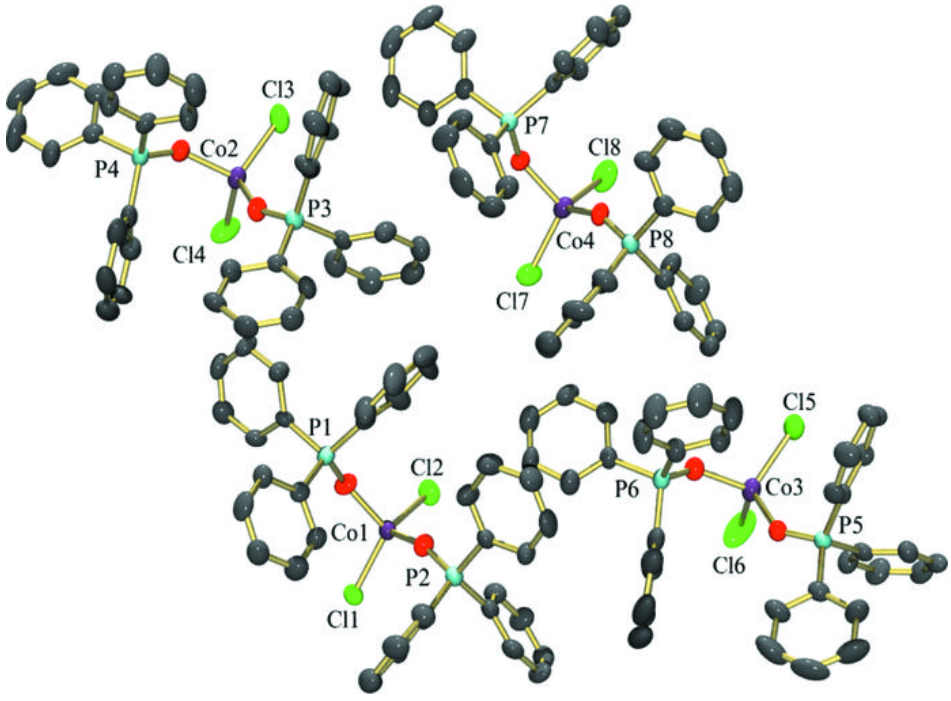
P4—C61—C66—C65	−175.9 (8)	C136—C137—C138—C133	0.7 (15)
O4—P4—C67—C68	148.7 (8)	O8—P8—C139—C144	22.5 (9)
C55—P4—C67—C68	−86.3 (8)	C127—P8—C139—C144	−97.2 (8)
C61—P4—C67—C68	28.7 (9)	C133—P8—C139—C144	146.0 (8)
O4—P4—C67—C72	−29.8 (9)	O8—P8—C139—C140	−156.2 (7)
C55—P4—C67—C72	95.2 (9)	C127—P8—C139—C140	84.0 (8)
C61—P4—C67—C72	−149.9 (8)	C133—P8—C139—C140	−32.8 (9)
C72—C67—C68—C69	−0.5 (15)	C144—C139—C140—C141	1.8 (14)
P4—C67—C68—C69	−179.0 (8)	P8—C139—C140—C141	−179.5 (7)
C67—C68—C69—C70	0.8 (16)	C139—C140—C141—C142	−1.6 (15)
C68—C69—C70—C71	−1.3 (18)	C140—C141—C142—C143	2.3 (16)
C69—C70—C71—C72	1.4 (19)	C141—C142—C143—C144	−3.2 (17)
C70—C71—C72—C67	−1.1 (18)	C140—C139—C144—C143	−2.7 (15)
C68—C67—C72—C71	0.6 (16)	P8—C139—C144—C143	178.5 (8)
P4—C67—C72—C71	179.2 (9)	C142—C143—C144—C139	3.5 (17)

Table 1. Comparison of geometry in $CoCl_2(OPPh_3)_2$ molecules

	(I)* range	(I) average	(IIa)	(IIb)
Co-Cl (Å)	2.221 (3)–2.260 (3)	2.242	2.227 (1)	2.203 (3)
Co-O (Å)	1.952 (6)–1.988 (6)	1.971	1.971 (2)	1.998 (7)
Cl-Co-Cl (°)	116.4 (1)–123.6 (1)	119.7	112.76 (6)	114.1 (1)
O-Co-O (°)	104.3 (3)–107.2 (2)	105.3	97.9 (2)	96.3 (3)
Co-O-P (°)	138.4 (4)–154.3 (4)	145.8	153.6 (2)	152.6 (5)

*(I) refers to the title structure and (II) to the usolvated complex, (IIa) Cotton *et al.* (2002) and (IIb) Marsh (1997) with e.s.ds taken from Mangion *et al.* (1976)

Fig. 1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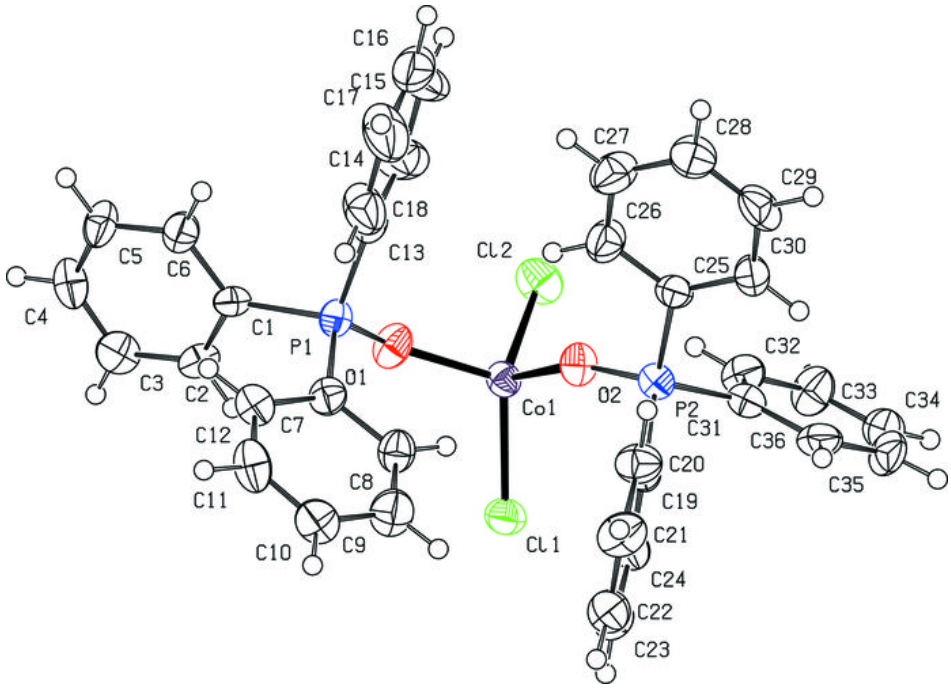
P4
P3
Cl4
P7
Cl8
Co4
P8
Cl7
P1
Cl2
Co1
P2
Cl1
P6
Cl5
Co3
P5
Cl6

Fig. 2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C18
C13
C5
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C1
P1
C3
C2
O1
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C11
C8
C10
C9
Cl2
Co1
Cl1
O2
P2
C27
C28
C29
C26
C30
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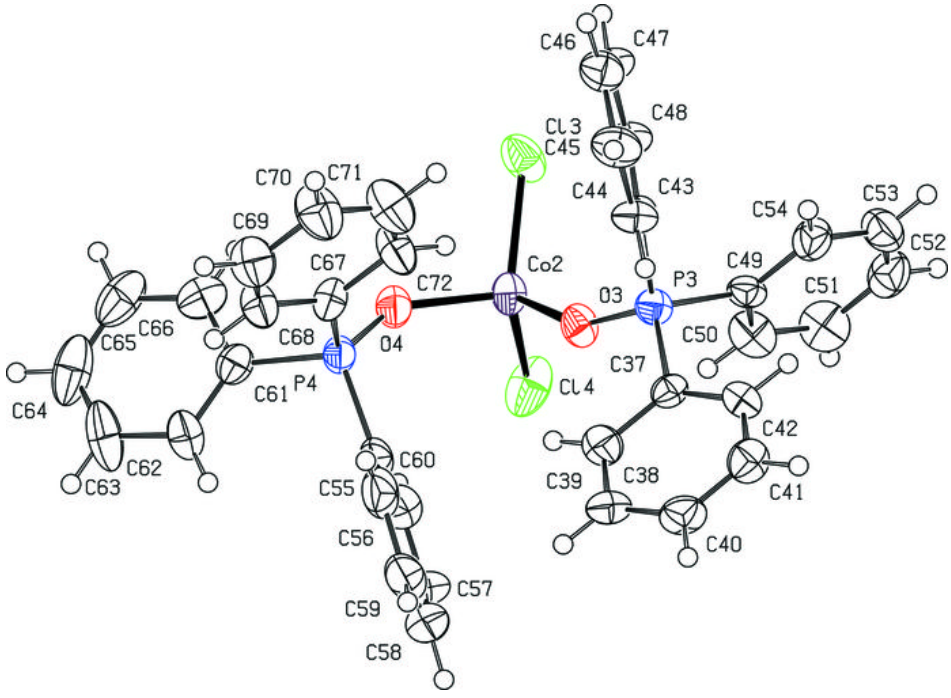
C19
C21
C24
C22
C23

Fig. 3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C43
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C71
C69
C67
C72
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O3
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C53
C52
C49
C51
C50
C66
C65
C68
O4
C37
CL4
C64
C61
P4
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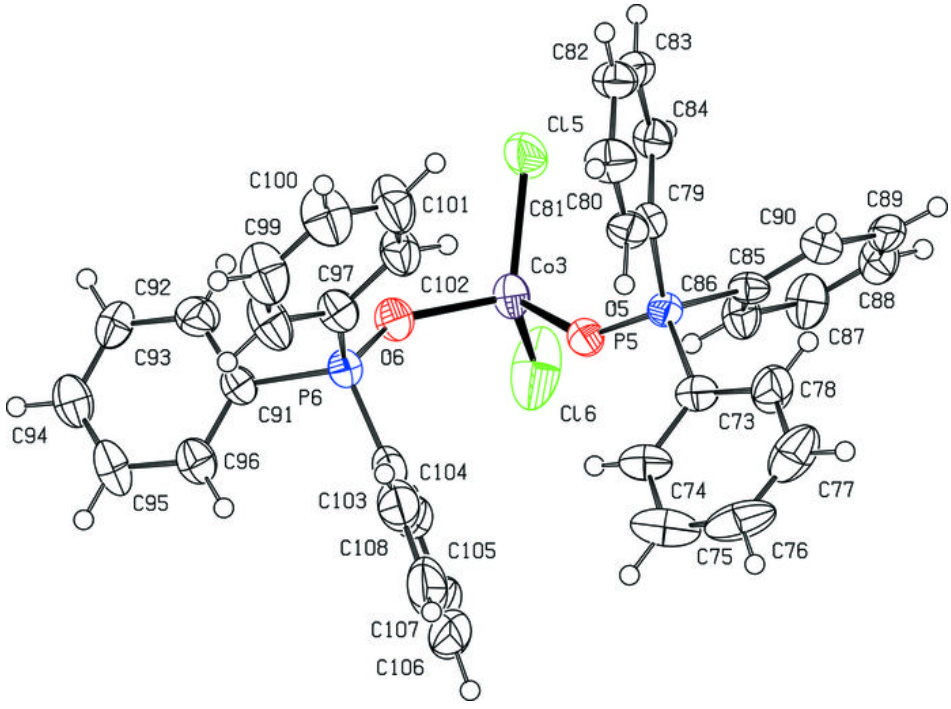
C63
C60
C55
C39
C38
C41
C56
C40
C57
C59
C58

Fig. 4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C81
C80
C79
C100
C101
C99
C97
C102
Co3
C92
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O5
P5
C86
C85
C90
C89
C88
C87
C93
P6
C91
Cl6
C78
C73
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C74
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C95
C103
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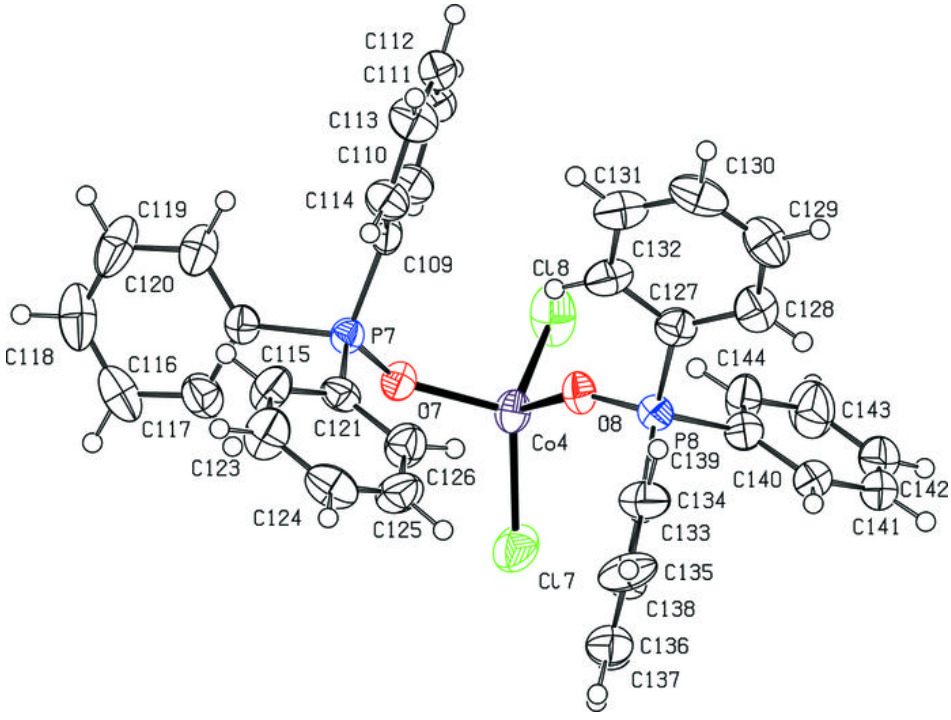
C105
C75
C76
C107
C106

Fig. 5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C128
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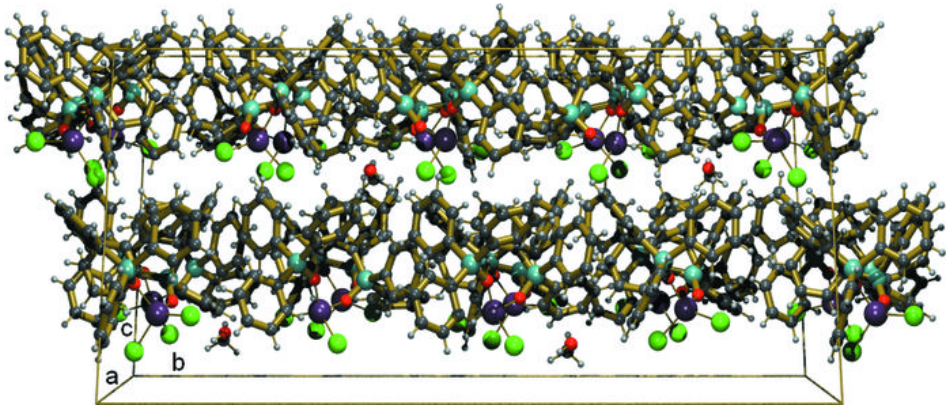
Fig. 6