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Hydridotetrakis(triphenylphosphito)cobalt(I)

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Key indicators

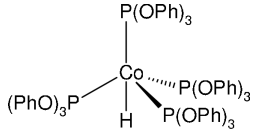
Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.005 Å
Disorder in main residue
R factor = 0.036
wR factor = 0.069
Data-to-parameter ratio = 17.8

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

At 150 K, the coordination geometry of the Co atom in the title compound, $[CoH(C_{18}H_{15}O_3P)_4]$, is monocapped tetrahedral, with the hydride as the face-capping ligand.

Comment

In the title compound, (I), the P atoms of the four triphenylphosphite ligands are disposed in a distorted tetrahedral geometry around the cobalt(I) ion. The location of the face-capping hydride ligand *trans* to P1 was strongly indicated by the long Co1—P1 bond distance of 2.1191 (7) Å caused by the *trans* influence of the hydride, and the pattern of bond angles subtended at the cobalt centre (Table 1). The location was confirmed by the high residual electron density observed at this position in the difference Fourier map and the subsequent successful free refinement of the positional parameters for the hydride ligand, with a Co1—H1 distance of 1.36 (2) Å. This apparent bond shortening relative to the typical value of 1.55 Å for first row transition metal hydrides is characteristic of X-ray crystallography (Teller & Bau, 1981).



(I)

Experimental

The title compound, (I), was prepared by the method of Levison & Robinson (1970). Crystals were grown by the slow diffusion of methanol into a dichloromethane solution of (I) at room temperature. Two crystal morphologies were observed: the majority were thin hexagonal plates which were found to be intractably twinned, and the minority were oblong blocks which were found to be suitable.

Crystal data

$[CoH(C_{18}H_{15}O_3P)_4]$
M_r = 1301.02
Monoclinic, Cc
a = 20.2331 (14) Å
b = 17.2635 (10) Å
c = 18.3682 (11) Å
β = 100.117 (5)°
V = 6316.1 (7) Å^3
Z = 4
D_x = 1.368 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 17065 reflections
θ = 2.0–28.0°
μ = 0.44 mm^{-1}
T = 150 (2) K
Block, pale yellow
0.60 × 0.20 × 0.20 mm

Data collection

Stoe IPDS-II area-detector diffractometer
φ and ω scans
Absorption correction: numerical (*X-SHAPE*; Stoe & Cie, 2001)
T_{min} = 0.803, T_{max} = 0.930
35963 measured reflections
14644 independent reflections
10146 reflections with $I > 2\sigma(I)$
R_{int} = 0.052
θ_{max} = 28.0°
$h = -26 \rightarrow 26$
$k = -22 \rightarrow 22$
$l = -24 \rightarrow 24$

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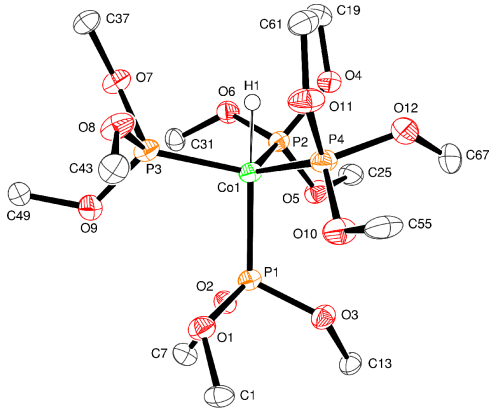

Figure 1
View of the molecule of (I), showing the atom-labelling scheme. For clarity, only the *ipso*-C atoms of the phenyl rings are shown; these rings are numbered sequentially round the ring starting from the *ipso*-C atom. Displacement ellipsoids are drawn at the 50% probability level.

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.069$
$S = 0.80$
14644 reflections
821 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0277P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.31$ e Å^{-3}
$\Delta\rho_{min} = -0.25$ e Å^{-3}
Absolute structure: Flack (1983), 7006 Friedel pairs
Flack parameter = −0.022 (9)

Table 1
Selected geometric parameters (Å, °).

Co1—H1	1.36 (2)	Co1—P3	2.0903 (8)
Co1—P1	2.1191 (7)	Co1—P4	2.0816 (7)
Co1—P2	2.0860 (8)		
P1—Co1—H1	177.6 (11)	P3—Co1—P1	102.89 (3)
P2—Co1—H1	76.4 (11)	P4—Co1—P1	101.41 (3)
P3—Co1—H1	78.6 (11)	P3—Co1—P2	114.86 (3)
P4—Co1—H1	79.5 (11)	P4—Co1—P2	118.38 (3)
P2—Co1—P1	101.19 (3)	P4—Co1—P3	114.50 (3)

The C25–C30 phenyl ring was modelled as disordered over two orientations with a common *ipso*-C atom C25, giving occupancies of 0.725 (17) and 0.275 (17). The displacement parameters for corresponding atoms in the two components were constrained to be the same. All H atoms were initially located in a difference Fourier map. They were then constrained to an ideal geometry, with a C—H distance of 0.95 Å and U_{iso}(H) values set at $1.2U_{eq}$(C). The positional parameters for the hydride ligand were freely refined, but U_{iso}(H) was set to $1.2U_{eq}$(Co).

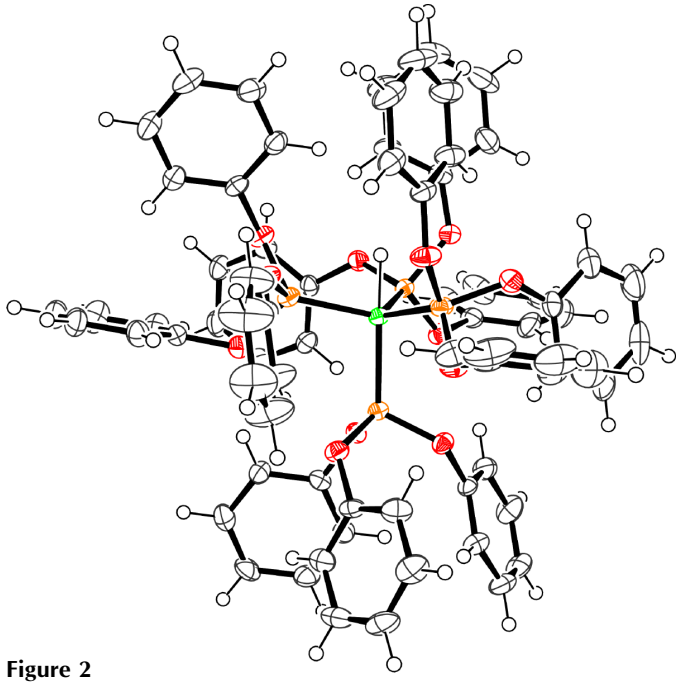

Figure 2
View of the molecule of (I), in the same orientation as Fig. 1, but showing all the atoms. Only the major component of the disordered phenyl ring C25–C30 is shown.

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-RED*32 (Stoe & Cie, 2001); program(s) used to solve structure: *X-STEP*32 (Stoe & Cie, 2001) and *WinGX* (Farrugia, 1999); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON* (Spek, 2001).

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supporting information

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$c = 18.3682\ (11)$ Å
$\beta = 100.117\ (5)°$
$V = 6316.1\ (7)$ Å^3
$Z = 4$
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Cell parameters from 17065 reflections
$\theta = 2.0–28.0°$
$\mu = 0.44$ mm^{-1}
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0.60 × 0.20 × 0.20 mm

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Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: numerical (X-SHAPE; Stoe & Cie, 2001)
$T_{min} = 0.803$, $T_{max} = 0.930$
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14644 independent reflections
10146 reflections with $I > 2\sigma(I)$
$R_{int} = 0.052$
$\theta_{max} = 28.0°$, $\theta_{min} = 2.0°$
$h = -26\rightarrow26$
$k = -22\rightarrow22$
$l = -24\rightarrow24$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.069$
$S = 0.80$
14644 reflections
821 parameters
14 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0277P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.31$ e Å^{-3}
$\Delta\rho_{min} = -0.25$ e Å^{-3}
Absolute structure: Flack (1983), 7006 Friedel pairs
Absolute structure parameter: −0.022 (9)

Special details

Experimental. The crystal was mounted under the perfluoro-polyether PFO-XR75 (Lancaster Synthesis). A total of 150 frames (2 minute exposure) were collected (phi/omega: 0/20–170, delta-omega = 1 °.)

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.

Refinement. 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 $F^2 > \sigma(F^2)$ 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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Co1	0.103899 (17)	0.756339 (19)	−0.021400 (19)	0.01877 (8)	
H1	0.0443 (13)	0.7546 (15)	0.0035 (14)	0.023*	
P1	0.19471 (3)	0.75601 (4)	−0.06392 (4)	0.01935 (14)	
P2	0.04838 (3)	0.67294 (4)	−0.08808 (4)	0.01992 (15)	
P3	0.13500 (4)	0.72342 (4)	0.08881 (4)	0.02127 (15)	
P4	0.07496 (4)	0.87181 (4)	−0.03594 (4)	0.02348 (16)	
O1	0.26053 (9)	0.78802 (11)	−0.00991 (10)	0.0250 (4)	
O2	0.22004 (9)	0.67327 (10)	−0.08955 (10)	0.0219 (4)	
O3	0.19397 (9)	0.80837 (10)	−0.13674 (10)	0.0236 (4)	
O4	−0.03097 (9)	0.68835 (11)	−0.11680 (11)	0.0274 (4)	
O5	0.06847 (10)	0.65581 (11)	−0.16807 (11)	0.0262 (4)	
O6	0.03678 (9)	0.58566 (10)	−0.05793 (11)	0.0237 (4)	
O7	0.08540 (9)	0.66422 (10)	0.12240 (11)	0.0255 (4)	
O8	0.13838 (10)	0.78519 (11)	0.15646 (11)	0.0282 (5)	
O9	0.20639 (9)	0.67837 (11)	0.10904 (11)	0.0272 (4)	
O10	0.13205 (9)	0.93648 (10)	−0.04184 (12)	0.0303 (5)	
O11	0.04527 (10)	0.91427 (10)	0.03008 (12)	0.0307 (5)	
O12	0.01352 (10)	0.89980 (11)	−0.10054 (12)	0.0323 (5)	
C1	0.31024 (14)	0.83781 (16)	−0.02850 (16)	0.0241 (6)	
C2	0.37391 (14)	0.81032 (18)	−0.02789 (16)	0.0296 (7)	
H2	0.3846	0.7577	−0.0161	0.035*	
C3	0.42232 (15)	0.8605 (2)	−0.04477 (18)	0.0368 (8)	
H3	0.4667	0.8420	−0.0437	0.044*	
C4	0.40762 (17)	0.9366 (2)	−0.06304 (19)	0.0411 (9)	
H4	0.4410	0.9700	−0.0762	0.049*	
C5	0.34382 (17)	0.96370 (19)	−0.06186 (19)	0.0406 (8)	
H5	0.3334	1.0163	−0.0738	0.049*	
C6	0.29453 (16)	0.91532 (17)	−0.04352 (18)	0.0344 (7)	
H6	0.2510	0.9347	−0.0413	0.041*	
C7	0.28566 (13)	0.64342 (14)	−0.07817 (16)	0.0217 (6)	
C8	0.30990 (15)	0.60685 (15)	−0.01168 (17)	0.0276 (7)	
H8	0.2837	0.6050	0.0265	0.033*	
C9	0.37274 (15)	0.57318 (17)	−0.00182 (18)	0.0334 (7)	

H9	0.3894	0.5475	0.0434	0.040*	
C10	0.41186 (15)	0.57600 (17)	−0.05613 (19)	0.0352 (7)	
H10	0.4552	0.5530	−0.0485	0.042*	
C11	0.38691 (15)	0.61291 (16)	−0.12176 (18)	0.0330 (7)	
H11	0.4136	0.6155	−0.1594	0.040*	
C12	0.32356 (14)	0.64634 (15)	−0.13385 (17)	0.0273 (6)	
H12	0.3065	0.6708	−0.1796	0.033*	
C13	0.21879 (14)	0.79069 (15)	−0.20141 (15)	0.0221 (6)	
C14	0.18526 (15)	0.73684 (17)	−0.24985 (16)	0.0310 (7)	
H14	0.1468	0.7107	−0.2391	0.037*	
C15	0.20914 (17)	0.72202 (19)	−0.31432 (17)	0.0378 (8)	
H15	0.1871	0.6844	−0.3478	0.045*	
C16	0.26422 (16)	0.76036 (18)	−0.33137 (17)	0.0363 (7)	
H16	0.2798	0.7498	−0.3762	0.044*	
C17	0.29628 (16)	0.81451 (17)	−0.28201 (17)	0.0336 (7)	
H17	0.3342	0.8415	−0.2931	0.040*	
C18	0.27371 (15)	0.82980 (16)	−0.21641 (17)	0.0292 (7)	
H18	0.2960	0.8668	−0.1824	0.035*	
C19	−0.08530 (14)	0.67771 (15)	−0.08145 (17)	0.0249 (6)	
C20	−0.07935 (15)	0.65982 (16)	−0.00686 (18)	0.0292 (7)	
H20	−0.0365	0.6526	0.0231	0.035*	
C21	−0.13725 (18)	0.65270 (18)	0.0227 (2)	0.0408 (8)	
H21	−0.1339	0.6408	0.0738	0.049*	
C22	−0.20006 (18)	0.6625 (2)	−0.0202 (2)	0.0502 (10)	
H22	−0.2394	0.6572	0.0010	0.060*	
C23	−0.20496 (17)	0.6799 (2)	−0.0938 (3)	0.0522 (10)	
H23	−0.2479	0.6869	−0.1237	0.063*	
C24	−0.14745 (15)	0.68737 (18)	−0.1250 (2)	0.0396 (8)	
H24	−0.1510	0.6991	−0.1761	0.047*	
C25	0.02609 (14)	0.61999 (18)	−0.22716 (17)	0.0293 (7)	
C26	0.0033 (4)	0.6650 (4)	−0.2871 (4)	0.0420 (16)	0.724 (17)
H26	0.0143	0.7185	−0.2865	0.050*	0.724 (17)
C27	−0.0357 (5)	0.6329 (5)	−0.3490 (4)	0.0572 (19)	0.724 (17)
H27	−0.0538	0.6640	−0.3904	0.069*	0.724 (17)
C28	−0.0477 (4)	0.5543 (6)	−0.3487 (6)	0.0505 (19)	0.724 (17)
H28	−0.0720	0.5314	−0.3923	0.061*	0.724 (17)
C29	−0.0265 (5)	0.5070 (8)	−0.2886 (6)	0.050 (2)	0.724 (17)
H29	−0.0375	0.4535	−0.2891	0.060*	0.724 (17)
C30	0.0124 (5)	0.5425 (3)	−0.2268 (6)	0.0387 (16)	0.724 (17)
H30	0.0293	0.5124	−0.1843	0.046*	0.724 (17)
C76	−0.0175 (8)	0.6699 (10)	−0.2724 (9)	0.0420 (16)	0.276 (17)
H76	−0.0188	0.7237	−0.2617	0.050*	0.276 (17)
C77	−0.0589 (11)	0.6381 (15)	−0.3336 (10)	0.0572 (19)	0.276 (17)
H77	−0.0874	0.6730	−0.3645	0.069*	0.276 (17)
C78	−0.0629 (13)	0.5606 (16)	−0.3540 (18)	0.0505 (19)	0.276 (17)
H78	−0.0918	0.5396	−0.3957	0.061*	0.276 (17)
C79	−0.0173 (12)	0.519 (2)	−0.3035 (16)	0.050 (2)	0.276 (17)
H79	−0.0161	0.4652	−0.3139	0.060*	0.276 (17)

C80	0.0268 (13)	0.5417 (7)	−0.2404 (15)	0.0387 (16)	0.276 (17)
H80	0.0547	0.5064	−0.2094	0.046*	0.276 (17)
C31	0.08455 (13)	0.53022 (14)	−0.03056 (16)	0.0221 (6)	
C32	0.14181 (15)	0.51687 (15)	−0.06049 (16)	0.0273 (7)	
H32	0.1531	0.5498	−0.0979	0.033*	
C33	0.18210 (15)	0.45452 (17)	−0.03455 (18)	0.0323 (7)	
H33	0.2219	0.4452	−0.0540	0.039*	
C34	0.16591 (16)	0.40610 (18)	0.01851 (18)	0.0364 (8)	
H34	0.1936	0.3628	0.0346	0.044*	
C35	0.10881 (16)	0.42044 (19)	0.04879 (19)	0.0403 (8)	
H35	0.0974	0.3870	0.0858	0.048*	
C36	0.06856 (15)	0.48365 (17)	0.02484 (18)	0.0323 (7)	
H36	0.0303	0.4948	0.0464	0.039*	
C37	0.05452 (14)	0.67947 (15)	0.18360 (15)	0.0238 (6)	
C38	−0.00157 (15)	0.72626 (16)	0.17483 (17)	0.0284 (7)	
H38	−0.0184	0.7491	0.1282	0.034*	
C39	−0.03289 (15)	0.73954 (17)	0.23442 (18)	0.0354 (7)	
H39	−0.0712	0.7722	0.2289	0.043*	
C40	−0.00918 (17)	0.70600 (18)	0.30175 (19)	0.0392 (8)	
H40	−0.0315	0.7147	0.3424	0.047*	
C41	0.04738 (17)	0.65938 (18)	0.31012 (18)	0.0379 (8)	
H41	0.0641	0.6366	0.3568	0.045*	
C42	0.07966 (15)	0.64578 (17)	0.25097 (17)	0.0314 (7)	
H42	0.1185	0.6138	0.2566	0.038*	
C43	0.17956 (15)	0.84901 (16)	0.17300 (17)	0.0261 (6)	
C44	0.16356 (18)	0.8966 (2)	0.2266 (2)	0.0472 (10)	
H44	0.1248	0.8869	0.2478	0.057*	
C45	0.2050 (2)	0.9598 (2)	0.2499 (3)	0.0682 (14)	
H45	0.1940	0.9937	0.2868	0.082*	
C46	0.2611 (2)	0.9732 (2)	0.2200 (2)	0.0602 (11)	
H46	0.2903	1.0147	0.2377	0.072*	
C47	0.2747 (2)	0.9267 (2)	0.1650 (2)	0.0629 (12)	
H47	0.3123	0.9380	0.1422	0.075*	
C48	0.23477 (19)	0.8630 (2)	0.1413 (2)	0.0494 (10)	
H48	0.2456	0.8297	0.1039	0.059*	
C49	0.22635 (14)	0.63535 (17)	0.17413 (16)	0.0259 (6)	
C50	0.25041 (15)	0.67167 (17)	0.24024 (17)	0.0304 (7)	
H50	0.2533	0.7266	0.2429	0.036*	
C51	0.27038 (16)	0.62688 (19)	0.30295 (18)	0.0360 (8)	
H51	0.2862	0.6512	0.3491	0.043*	
C52	0.26734 (17)	0.54701 (19)	0.29842 (19)	0.0375 (8)	
H52	0.2817	0.5164	0.3413	0.045*	
C53	0.24348 (19)	0.5119 (2)	0.2318 (2)	0.0432 (9)	
H53	0.2413	0.4569	0.2290	0.052*	
C54	0.22252 (16)	0.55582 (18)	0.16852 (19)	0.0356 (8)	
H54	0.2060	0.5316	0.1225	0.043*	
C55	0.12062 (15)	1.01700 (16)	−0.03703 (19)	0.0320 (7)	
C56	0.13762 (18)	1.05215 (19)	0.0305 (2)	0.0416 (9)	

H56	0.1548	1.0231	0.0736	0.050*
C57	0.1287 (2)	1.1328 (2)	0.0337 (3)	0.0591 (12)
H57	0.1397	1.1587	0.0799	0.071*
C58	0.1044 (2)	1.17443 (18)	−0.0287 (3)	0.0597 (11)
H58	0.0986	1.2289	−0.0256	0.072*
C59	0.0885 (2)	1.1379 (2)	−0.0952 (3)	0.0600 (12)
H59	0.0722	1.1671	−0.1385	0.072*
C60	0.09606 (18)	1.05783 (18)	−0.1001 (2)	0.0431 (9)
H60	0.0844	1.0320	−0.1462	0.052*
C61	−0.01401 (14)	0.90359 (15)	0.05594 (17)	0.0272 (7)
C62	−0.07014 (15)	0.86666 (16)	0.01733 (19)	0.0322 (7)
H62	−0.0694	0.8443	−0.0298	0.039*
C63	−0.12749 (17)	0.86302 (18)	0.0488 (2)	0.0426 (9)
H63	−0.1659	0.8372	0.0228	0.051*
C64	−0.13066 (19)	0.89497 (18)	0.1154 (2)	0.0495 (10)
H64	−0.1710	0.8926	0.1352	0.059*
C65	−0.0740 (2)	0.93125 (19)	0.1544 (2)	0.0457 (10)
H65	−0.0754	0.9535	0.2014	0.055*
C66	−0.01565 (17)	0.93515 (16)	0.12510 (18)	0.0334 (7)
H66	0.0232	0.9593	0.1522	0.040*
C67	0.00727 (15)	0.88506 (17)	−0.17598 (19)	0.0331 (7)
C68	0.06069 (17)	0.88729 (18)	−0.21262 (19)	0.0370 (8)
H68	0.1049	0.8953	−0.1862	0.044*
C69	0.0493 (2)	0.8776 (2)	−0.2889 (2)	0.0483 (9)
H69	0.0861	0.8785	−0.3147	0.058*
C70	−0.0144 (2)	0.8669 (2)	−0.3275 (2)	0.0606 (12)
H70	−0.0216	0.8612	−0.3797	0.073*
C71	−0.0679 (2)	0.8644 (3)	−0.2904 (3)	0.0679 (13)
H71	−0.1121	0.8564	−0.3168	0.082*
C72	−0.05684 (19)	0.8735 (2)	−0.2144 (2)	0.0553 (10)
H72	−0.0936	0.8718	−0.1885	0.066*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.01937 (17)	0.01814 (17)	0.02013 (19)	−0.00057 (17)	0.00713 (14)	−0.00002 (18)
P1	0.0200 (3)	0.0191 (3)	0.0200 (4)	−0.0007 (3)	0.0064 (3)	−0.0004 (3)
P2	0.0197 (4)	0.0212 (3)	0.0192 (4)	−0.0014 (3)	0.0045 (3)	0.0017 (3)
P3	0.0230 (4)	0.0222 (3)	0.0199 (4)	−0.0033 (3)	0.0072 (3)	−0.0023 (3)
P4	0.0228 (4)	0.0207 (3)	0.0293 (4)	0.0019 (3)	0.0112 (3)	0.0018 (3)
O1	0.0252 (10)	0.0294 (10)	0.0213 (11)	−0.0059 (8)	0.0065 (8)	−0.0028 (9)
O2	0.0208 (10)	0.0207 (9)	0.0238 (11)	0.0007 (8)	0.0026 (8)	−0.0007 (8)
O3	0.0276 (11)	0.0216 (9)	0.0235 (11)	0.0037 (8)	0.0097 (9)	0.0019 (8)
O4	0.0207 (10)	0.0342 (11)	0.0277 (11)	−0.0011 (8)	0.0052 (9)	0.0049 (9)
O5	0.0279 (11)	0.0327 (10)	0.0183 (11)	−0.0054 (9)	0.0050 (8)	−0.0028 (9)
O6	0.0208 (10)	0.0231 (9)	0.0265 (11)	−0.0039 (8)	0.0020 (8)	0.0014 (8)
O7	0.0303 (11)	0.0254 (10)	0.0231 (11)	−0.0058 (8)	0.0106 (9)	−0.0028 (8)
O8	0.0347 (12)	0.0292 (10)	0.0231 (11)	−0.0112 (9)	0.0114 (9)	−0.0091 (9)

O9	0.0241 (10)	0.0345 (10)	0.0227 (11)	0.0011 (9)	0.0030 (8)	0.0015 (9)
O10	0.0303 (12)	0.0197 (9)	0.0446 (13)	0.0019 (8)	0.0165 (10)	0.0008 (9)
O11	0.0309 (11)	0.0230 (10)	0.0430 (13)	−0.0007 (8)	0.0196 (10)	−0.0038 (9)
O12	0.0278 (11)	0.0345 (11)	0.0363 (14)	0.0085 (9)	0.0102 (9)	0.0080 (10)
C1	0.0210 (14)	0.0304 (15)	0.0217 (16)	−0.0095 (12)	0.0061 (12)	−0.0082 (12)
C2	0.0258 (16)	0.0387 (16)	0.0237 (17)	−0.0032 (13)	0.0030 (13)	−0.0095 (13)
C3	0.0217 (15)	0.058 (2)	0.0317 (18)	−0.0080 (14)	0.0084 (13)	−0.0156 (16)
C4	0.039 (2)	0.052 (2)	0.033 (2)	−0.0275 (16)	0.0103 (16)	−0.0103 (16)
C5	0.047 (2)	0.0336 (17)	0.042 (2)	−0.0173 (16)	0.0088 (17)	−0.0075 (15)
C6	0.0331 (17)	0.0282 (15)	0.044 (2)	−0.0059 (13)	0.0114 (15)	−0.0068 (14)
C7	0.0199 (14)	0.0154 (12)	0.0296 (17)	0.0014 (10)	0.0039 (12)	−0.0031 (12)
C8	0.0314 (17)	0.0262 (14)	0.0259 (17)	0.0003 (12)	0.0074 (13)	0.0035 (12)
C9	0.0322 (17)	0.0308 (15)	0.0343 (19)	0.0034 (13)	−0.0022 (14)	0.0043 (14)
C10	0.0234 (16)	0.0326 (16)	0.049 (2)	0.0095 (13)	0.0059 (15)	0.0031 (15)
C11	0.0307 (16)	0.0340 (15)	0.0375 (19)	0.0055 (13)	0.0150 (14)	−0.0006 (14)
C12	0.0292 (16)	0.0255 (14)	0.0281 (17)	0.0036 (12)	0.0080 (13)	0.0013 (12)
C13	0.0244 (15)	0.0236 (13)	0.0204 (15)	0.0056 (11)	0.0099 (12)	0.0031 (12)
C14	0.0293 (15)	0.0360 (17)	0.0278 (17)	−0.0053 (13)	0.0055 (13)	0.0001 (14)
C15	0.052 (2)	0.0393 (18)	0.0221 (17)	−0.0074 (15)	0.0075 (15)	−0.0074 (14)
C16	0.0494 (18)	0.0377 (17)	0.0269 (16)	0.0068 (15)	0.0208 (14)	0.0008 (15)
C17	0.0365 (18)	0.0322 (15)	0.0372 (19)	−0.0015 (13)	0.0206 (15)	0.0043 (14)
C18	0.0336 (16)	0.0256 (15)	0.0314 (18)	−0.0029 (13)	0.0135 (14)	0.0000 (13)
C19	0.0204 (14)	0.0211 (13)	0.0334 (18)	−0.0006 (11)	0.0056 (13)	−0.0025 (13)
C20	0.0276 (16)	0.0301 (15)	0.0321 (18)	−0.0034 (12)	0.0112 (14)	−0.0084 (13)
C21	0.047 (2)	0.0345 (17)	0.047 (2)	−0.0042 (15)	0.0240 (17)	−0.0077 (15)
C22	0.033 (2)	0.044 (2)	0.080 (3)	−0.0033 (16)	0.028 (2)	−0.008 (2)
C23	0.0218 (17)	0.055 (2)	0.079 (3)	0.0043 (16)	0.0052 (18)	0.003 (2)
C24	0.0288 (17)	0.0361 (17)	0.051 (2)	0.0032 (13)	0.0002 (16)	0.0077 (16)
C25	0.0235 (15)	0.0440 (17)	0.0209 (16)	−0.0003 (13)	0.0048 (12)	−0.0036 (14)
C26	0.042 (4)	0.059 (3)	0.025 (3)	−0.009 (3)	0.005 (2)	0.008 (2)
C27	0.048 (5)	0.098 (4)	0.024 (3)	−0.001 (4)	0.000 (3)	0.016 (3)
C28	0.015 (4)	0.106 (4)	0.026 (3)	0.009 (3)	−0.010 (4)	−0.022 (3)
C29	0.037 (3)	0.056 (5)	0.051 (5)	0.004 (3)	−0.004 (3)	−0.026 (4)
C30	0.036 (4)	0.044 (2)	0.033 (4)	0.008 (2)	0.001 (2)	−0.0176 (19)
C76	0.042 (4)	0.059 (3)	0.025 (3)	−0.009 (3)	0.005 (2)	0.008 (2)
C77	0.048 (5)	0.098 (4)	0.024 (3)	−0.001 (4)	0.000 (3)	0.016 (3)
C78	0.015 (4)	0.106 (4)	0.026 (3)	0.009 (3)	−0.010 (4)	−0.022 (3)
C79	0.037 (3)	0.056 (5)	0.051 (5)	0.004 (3)	−0.004 (3)	−0.026 (4)
C80	0.036 (4)	0.044 (2)	0.033 (4)	0.008 (2)	0.001 (2)	−0.0176 (19)
C31	0.0207 (14)	0.0213 (12)	0.0224 (15)	−0.0026 (10)	−0.0013 (12)	0.0011 (12)
C32	0.0313 (16)	0.0246 (14)	0.0266 (18)	−0.0036 (12)	0.0067 (14)	0.0023 (12)
C33	0.0313 (16)	0.0310 (16)	0.0350 (19)	0.0022 (13)	0.0066 (14)	0.0014 (14)
C34	0.0365 (18)	0.0305 (16)	0.040 (2)	0.0026 (13)	0.0005 (15)	0.0108 (14)
C35	0.0367 (19)	0.0408 (19)	0.042 (2)	−0.0021 (15)	0.0046 (16)	0.0228 (16)
C36	0.0241 (15)	0.0404 (17)	0.0328 (19)	−0.0048 (13)	0.0064 (13)	0.0087 (15)
C37	0.0274 (15)	0.0226 (13)	0.0231 (16)	−0.0066 (11)	0.0091 (12)	0.0009 (12)
C38	0.0318 (16)	0.0276 (15)	0.0269 (17)	−0.0027 (12)	0.0081 (13)	0.0056 (12)
C39	0.0373 (17)	0.0323 (16)	0.0407 (19)	0.0027 (14)	0.0180 (14)	0.0038 (15)

C40	0.050 (2)	0.0397 (18)	0.0333 (19)	−0.0034 (16)	0.0231 (17)	−0.0007 (15)
C41	0.048 (2)	0.0401 (17)	0.0272 (18)	−0.0002 (15)	0.0100 (15)	0.0084 (14)
C42	0.0338 (16)	0.0334 (15)	0.0279 (17)	0.0015 (13)	0.0078 (13)	0.0071 (13)
C43	0.0296 (16)	0.0216 (13)	0.0264 (17)	−0.0084 (11)	0.0031 (13)	−0.0033 (12)
C44	0.039 (2)	0.046 (2)	0.060 (3)	−0.0118 (16)	0.0209 (18)	−0.0304 (19)
C45	0.065 (3)	0.058 (2)	0.088 (3)	−0.020 (2)	0.034 (3)	−0.053 (2)
C46	0.064 (3)	0.041 (2)	0.077 (3)	−0.0238 (19)	0.017 (2)	−0.029 (2)
C47	0.065 (3)	0.063 (2)	0.069 (3)	−0.040 (2)	0.034 (2)	−0.026 (2)
C48	0.061 (2)	0.051 (2)	0.044 (2)	−0.0294 (19)	0.0304 (19)	−0.0275 (18)
C49	0.0207 (14)	0.0348 (15)	0.0219 (16)	0.0029 (12)	0.0033 (12)	0.0042 (13)
C50	0.0305 (16)	0.0304 (15)	0.0282 (18)	−0.0020 (13)	−0.0007 (13)	0.0000 (13)
C51	0.0398 (19)	0.0431 (18)	0.0239 (18)	0.0030 (15)	0.0028 (14)	0.0028 (15)
C52	0.041 (2)	0.0392 (18)	0.032 (2)	0.0078 (15)	0.0060 (15)	0.0096 (15)
C53	0.061 (2)	0.0298 (17)	0.040 (2)	0.0070 (16)	0.0113 (18)	0.0003 (15)
C54	0.0418 (19)	0.0344 (17)	0.0313 (19)	0.0036 (14)	0.0084 (15)	−0.0036 (14)
C55	0.0302 (16)	0.0205 (14)	0.052 (2)	−0.0024 (12)	0.0250 (15)	0.0011 (14)
C56	0.047 (2)	0.0358 (18)	0.047 (2)	−0.0114 (16)	0.0227 (18)	−0.0072 (16)
C57	0.067 (3)	0.041 (2)	0.082 (3)	−0.0253 (19)	0.048 (2)	−0.027 (2)
C58	0.065 (2)	0.0210 (15)	0.105 (3)	−0.005 (2)	0.048 (2)	−0.004 (2)
C59	0.068 (3)	0.0240 (17)	0.092 (4)	0.0066 (17)	0.025 (2)	0.012 (2)
C60	0.055 (2)	0.0261 (15)	0.053 (2)	0.0008 (15)	0.0216 (18)	0.0045 (16)
C61	0.0328 (16)	0.0172 (13)	0.0364 (18)	0.0066 (12)	0.0192 (14)	0.0048 (12)
C62	0.0334 (17)	0.0234 (14)	0.044 (2)	−0.0006 (13)	0.0191 (15)	−0.0038 (14)
C63	0.0375 (19)	0.0288 (16)	0.067 (3)	0.0003 (14)	0.0240 (18)	0.0064 (17)
C64	0.054 (2)	0.0293 (16)	0.079 (3)	0.0053 (16)	0.049 (2)	0.0084 (18)
C65	0.068 (3)	0.0324 (17)	0.047 (2)	0.0107 (18)	0.038 (2)	0.0076 (16)
C66	0.0437 (19)	0.0243 (14)	0.0351 (19)	0.0047 (13)	0.0152 (15)	0.0027 (13)
C67	0.0316 (17)	0.0288 (15)	0.038 (2)	0.0072 (13)	0.0045 (15)	0.0130 (14)
C68	0.0386 (19)	0.0312 (16)	0.040 (2)	0.0105 (14)	0.0033 (16)	0.0057 (15)
C69	0.063 (3)	0.043 (2)	0.039 (2)	0.0209 (18)	0.0102 (19)	0.0124 (17)
C70	0.086 (3)	0.048 (2)	0.038 (2)	0.016 (2)	−0.014 (2)	0.0118 (19)
C71	0.050 (3)	0.087 (3)	0.056 (3)	−0.004 (2)	−0.021 (2)	0.026 (3)
C72	0.038 (2)	0.071 (3)	0.053 (3)	0.0021 (19)	−0.0030 (18)	0.028 (2)

Geometric parameters (Å, º)

Co1—H1	1.36 (2)	C76—C77	1.392 (10)
Co1—P1	2.1191 (7)	C76—H76	0.95
Co1—P2	2.0860 (8)	C77—C78	1.388 (10)
Co1—P3	2.0903 (8)	C77—H77	0.95
Co1—P4	2.0816 (7)	C78—C79	1.389 (10)
P1—O1	1.612 (2)	C78—H78	0.95
P1—O3	1.6123 (19)	C79—C80	1.388 (10)
P1—O2	1.6152 (18)	C79—H79	0.95
P2—O5	1.619 (2)	C80—H80	0.95
P2—O4	1.621 (2)	C31—C36	1.379 (4)
P2—O6	1.6365 (19)	C31—C32	1.386 (4)
P3—O9	1.625 (2)	C32—C33	1.383 (4)

P3—O7	1.6279 (19)	C32—H32	0.95
P3—O8	1.6297 (19)	C33—C34	1.367 (4)
P4—O11	1.620 (2)	C33—H33	0.95
P4—O10	1.6237 (19)	C34—C35	1.390 (5)
P4—O12	1.634 (2)	C34—H34	0.95
O1—C1	1.410 (3)	C35—C36	1.386 (4)
O2—C7	1.405 (3)	C35—H35	0.95
O3—C13	1.402 (3)	C36—H36	0.95
O4—C19	1.383 (3)	C37—C38	1.379 (4)
O5—C25	1.403 (3)	C37—C42	1.381 (4)
O6—C31	1.390 (3)	C38—C39	1.377 (4)
O7—C37	1.404 (3)	C38—H38	0.95
O8—C43	1.382 (3)	C39—C40	1.373 (5)
O9—C49	1.405 (3)	C39—H39	0.95
O10—C55	1.414 (3)	C40—C41	1.385 (5)
O11—C61	1.378 (3)	C40—H40	0.95
O12—C67	1.393 (4)	C41—C42	1.383 (4)
C1—C2	1.371 (4)	C41—H41	0.95
C1—C6	1.392 (4)	C42—H42	0.95
C2—C3	1.383 (4)	C43—C44	1.365 (4)
C2—H2	0.95	C43—C48	1.369 (4)
C3—C4	1.377 (5)	C44—C45	1.396 (5)
C3—H3	0.95	C44—H44	0.95
C4—C5	1.376 (5)	C45—C46	1.364 (6)
C4—H4	0.95	C45—H45	0.95
C5—C6	1.387 (4)	C46—C47	1.356 (5)
C5—H5	0.95	C46—H46	0.95
C6—H6	0.95	C47—C48	1.389 (5)
C7—C12	1.383 (4)	C47—H47	0.95
C7—C8	1.386 (4)	C48—H48	0.95
C8—C9	1.381 (4)	C49—C50	1.377 (4)
C8—H8	0.95	C49—C54	1.378 (4)
C9—C10	1.379 (5)	C50—C51	1.387 (4)
C9—H9	0.95	C50—H50	0.95
C10—C11	1.379 (4)	C51—C52	1.382 (5)
C10—H10	0.95	C51—H51	0.95
C11—C12	1.387 (4)	C52—C53	1.375 (5)
C11—H11	0.95	C52—H52	0.95
C12—H12	0.95	C53—C54	1.391 (5)
C13—C18	1.369 (4)	C53—H53	0.95
C13—C14	1.380 (4)	C54—H54	0.95
C14—C15	1.379 (4)	C55—C56	1.370 (5)
C14—H14	0.95	C55—C60	1.372 (5)
C15—C16	1.379 (4)	C56—C57	1.406 (5)
C15—H15	0.95	C56—H56	0.95
C16—C17	1.382 (4)	C57—C58	1.369 (7)
C16—H16	0.95	C57—H57	0.95
C17—C18	1.387 (4)	C58—C59	1.363 (6)

C17—H17	0.95	C58—H58	0.95
C18—H18	0.95	C59—C60	1.395 (4)
C19—C24	1.377 (4)	C59—H59	0.95
C19—C20	1.389 (4)	C60—H60	0.95
C20—C21	1.381 (4)	C61—C62	1.384 (4)
C20—H20	0.95	C61—C66	1.388 (4)
C21—C22	1.384 (5)	C62—C63	1.386 (4)
C21—H21	0.95	C62—H62	0.95
C22—C23	1.371 (6)	C63—C64	1.353 (5)
C22—H22	0.95	C63—H63	0.95
C23—C24	1.390 (5)	C64—C65	1.390 (5)
C23—H23	0.95	C64—H64	0.95
C24—H24	0.95	C65—C66	1.383 (4)
C25—C26	1.361 (6)	C65—H65	0.95
C25—C30	1.367 (7)	C66—H66	0.95
C25—C80	1.374 (10)	C67—C68	1.371 (5)
C25—C76	1.397 (9)	C67—C72	1.378 (5)
C26—C27	1.381 (8)	C68—C69	1.390 (5)
C26—H26	0.95	C68—H68	0.95
C27—C28	1.378 (9)	C69—C70	1.369 (6)
C27—H27	0.95	C69—H69	0.95
C28—C29	1.380 (9)	C70—C71	1.377 (6)
C28—H28	0.95	C70—H70	0.95
C29—C30	1.403 (8)	C71—C72	1.384 (6)
C29—H29	0.95	C71—H71	0.95
C30—H30	0.95	C72—H72	0.95

P1—Co1—H1	177.6 (11)	C77—C76—C25	117.7 (16)
P2—Co1—H1	76.4 (11)	C77—C76—H76	121.2
P3—Co1—H1	78.6 (11)	C25—C76—H76	121.2
P4—Co1—H1	79.5 (11)	C78—C77—C76	127 (2)
P2—Co1—P1	101.19 (3)	C78—C77—H77	116.7
P3—Co1—P1	102.89 (3)	C76—C77—H77	116.7
P4—Co1—P1	101.41 (3)	C77—C78—C79	109 (3)
P3—Co1—P2	114.86 (3)	C77—C78—H78	125.7
P4—Co1—P2	118.38 (3)	C79—C78—H78	125.7
P4—Co1—P3	114.50 (3)	C80—C79—C78	132 (4)
O1—P1—O3	101.81 (10)	C80—C79—H79	114.1
O1—P1—O2	102.26 (10)	C78—C79—H79	114.1
O3—P1—O2	102.19 (10)	C25—C80—C79	114 (3)
O1—P1—Co1	116.64 (7)	C25—C80—H80	123.2
O3—P1—Co1	114.96 (7)	C79—C80—H80	123.2
O2—P1—Co1	116.73 (7)	C36—C31—C32	121.1 (3)
O5—P2—O4	97.28 (10)	C36—C31—O6	115.5 (2)
O5—P2—O6	102.28 (10)	C32—C31—O6	123.2 (2)
O4—P2—O6	93.93 (10)	C33—C32—C31	118.4 (3)
O5—P2—Co1	117.63 (7)	C33—C32—H32	120.8
O4—P2—Co1	118.56 (8)	C31—C32—H32	120.8

O6—P2—Co1	122.09 (8)	C34—C33—C32	121.4 (3)
O9—P3—O7	101.26 (10)	C34—C33—H33	119.3
O9—P3—O8	102.84 (11)	C32—C33—H33	119.3
O7—P3—O8	93.89 (10)	C33—C34—C35	119.8 (3)
O9—P3—Co1	117.12 (8)	C33—C34—H34	120.1
O7—P3—Co1	115.91 (8)	C35—C34—H34	120.1
O8—P3—Co1	121.71 (8)	C36—C35—C34	119.8 (3)
O11—P4—O10	95.77 (10)	C36—C35—H35	120.1
O11—P4—O12	94.30 (11)	C34—C35—H35	120.1
O10—P4—O12	101.99 (11)	C31—C36—C35	119.5 (3)
O11—P4—Co1	118.04 (8)	C31—C36—H36	120.3
O10—P4—Co1	118.66 (7)	C35—C36—H36	120.3
O12—P4—Co1	122.51 (8)	C38—C37—C42	121.2 (3)
C1—O1—P1	127.40 (17)	C38—C37—O7	119.3 (3)
C7—O2—P1	128.38 (16)	C42—C37—O7	119.5 (3)
C13—O3—P1	128.93 (16)	C39—C38—C37	119.3 (3)
C19—O4—P2	130.42 (19)	C39—C38—H38	120.4
C25—O5—P2	124.46 (17)	C37—C38—H38	120.4
C31—O6—P2	128.65 (16)	C40—C39—C38	120.6 (3)
C37—O7—P3	125.21 (16)	C40—C39—H39	119.7
C43—O8—P3	129.19 (18)	C38—C39—H39	119.7
C49—O9—P3	123.95 (17)	C39—C40—C41	119.7 (3)
C55—O10—P4	123.06 (17)	C39—C40—H40	120.1
C61—O11—P4	131.09 (19)	C41—C40—H40	120.1
C67—O12—P4	126.38 (18)	C42—C41—C40	120.4 (3)
C2—C1—C6	121.1 (3)	C42—C41—H41	119.8
C2—C1—O1	119.8 (3)	C40—C41—H41	119.8
C6—C1—O1	119.1 (2)	C37—C42—C41	118.8 (3)
C1—C2—C3	118.9 (3)	C37—C42—H42	120.6
C1—C2—H2	120.6	C41—C42—H42	120.6
C3—C2—H2	120.6	C44—C43—C48	121.0 (3)
C4—C3—C2	121.4 (3)	C44—C43—O8	115.4 (3)
C4—C3—H3	119.3	C48—C43—O8	123.5 (3)
C2—C3—H3	119.3	C43—C44—C45	119.1 (3)
C3—C4—C5	118.9 (3)	C43—C44—H44	120.5
C3—C4—H4	120.5	C45—C44—H44	120.5
C5—C4—H4	120.5	C46—C45—C44	120.4 (3)
C4—C5—C6	121.0 (3)	C46—C45—H45	119.8
C4—C5—H5	119.5	C44—C45—H45	119.8
C6—C5—H5	119.5	C47—C46—C45	119.6 (3)
C5—C6—C1	118.6 (3)	C47—C46—H46	120.2
C5—C6—H6	120.7	C45—C46—H46	120.2
C1—C6—H6	120.7	C46—C47—C48	121.1 (4)
C12—C7—C8	120.8 (3)	C46—C47—H47	119.4
C12—C7—O2	120.6 (2)	C48—C47—H47	119.4
C8—C7—O2	118.5 (2)	C43—C48—C47	118.7 (3)
C9—C8—C7	118.9 (3)	C43—C48—H48	120.6
C9—C8—H8	120.6	C47—C48—H48	120.6

C7—C8—H8	120.6	C50—C49—C54	121.7 (3)
C10—C9—C8	121.5 (3)	C50—C49—O9	120.9 (3)
C10—C9—H9	119.2	C54—C49—O9	117.3 (3)
C8—C9—H9	119.2	C49—C50—C51	119.0 (3)
C11—C10—C9	118.7 (3)	C49—C50—H50	120.5
C11—C10—H10	120.6	C51—C50—H50	120.5
C9—C10—H10	120.6	C52—C51—C50	120.2 (3)
C10—C11—C12	121.2 (3)	C52—C51—H51	119.9
C10—C11—H11	119.4	C50—C51—H51	119.9
C12—C11—H11	119.4	C53—C52—C51	119.9 (3)
C7—C12—C11	118.9 (3)	C53—C52—H52	120.0
C7—C12—H12	120.6	C51—C52—H52	120.0
C11—C12—H12	120.6	C52—C53—C54	120.7 (3)
C18—C13—C14	121.8 (3)	C52—C53—H53	119.6
C18—C13—O3	119.2 (2)	C54—C53—H53	119.6
C14—C13—O3	119.0 (2)	C49—C54—C53	118.5 (3)
C15—C14—C13	118.2 (3)	C49—C54—H54	120.8
C15—C14—H14	120.9	C53—C54—H54	120.8
C13—C14—H14	120.9	C56—C55—C60	122.2 (3)
C16—C15—C14	121.7 (3)	C56—C55—O10	118.3 (3)
C16—C15—H15	119.2	C60—C55—O10	119.4 (3)
C14—C15—H15	119.2	C55—C56—C57	117.5 (4)
C15—C16—C17	118.7 (3)	C55—C56—H56	121.2
C15—C16—H16	120.6	C57—C56—H56	121.2
C17—C16—H16	120.6	C58—C57—C56	121.0 (4)
C16—C17—C18	120.7 (3)	C58—C57—H57	119.5
C16—C17—H17	119.7	C56—C57—H57	119.5
C18—C17—H17	119.7	C59—C58—C57	120.1 (3)
C13—C18—C17	118.9 (3)	C59—C58—H58	120.0
C13—C18—H18	120.5	C57—C58—H58	120.0
C17—C18—H18	120.5	C58—C59—C60	120.3 (4)
C24—C19—O4	115.5 (3)	C58—C59—H59	119.8
C24—C19—C20	120.8 (3)	C60—C59—H59	119.8
O4—C19—C20	123.7 (3)	C55—C60—C59	118.9 (4)
C21—C20—C19	118.4 (3)	C55—C60—H60	120.6
C21—C20—H20	120.8	C59—C60—H60	120.6
C19—C20—H20	120.8	O11—C61—C62	124.8 (3)
C20—C21—C22	121.5 (4)	O11—C61—C66	115.2 (3)
C20—C21—H21	119.3	C62—C61—C66	120.0 (3)
C22—C21—H21	119.3	C61—C62—C63	118.6 (3)
C23—C22—C21	119.3 (3)	C61—C62—H62	120.7
C23—C22—H22	120.4	C63—C62—H62	120.7
C21—C22—H22	120.4	C64—C63—C62	122.3 (3)
C22—C23—C24	120.4 (3)	C64—C63—H63	118.8
C22—C23—H23	119.8	C62—C63—H63	118.8
C24—C23—H23	119.8	C63—C64—C65	118.9 (3)
C19—C24—C23	119.6 (4)	C63—C64—H64	120.5
C19—C24—H24	120.2	C65—C64—H64	120.5

C23—C24—H24	120.2	C66—C65—C64	120.3 (3)
C26—C25—C30	121.5 (6)	C66—C65—H65	119.8
C26—C25—C80	115.5 (13)	C64—C65—H65	119.9
C30—C25—C76	120.0 (9)	C65—C66—C61	119.8 (3)
C80—C25—C76	121.8 (15)	C65—C66—H66	120.1
C26—C25—O5	116.7 (4)	C61—C66—H66	120.1
C30—C25—O5	121.6 (5)	C68—C67—C72	120.4 (4)
C80—C25—O5	123.1 (13)	C68—C67—O12	122.8 (3)
C76—C25—O5	115.1 (8)	C72—C67—O12	116.6 (3)
C25—C26—C27	120.0 (6)	C67—C68—C69	119.1 (3)
C25—C26—H26	120.0	C67—C68—H68	120.4
C27—C26—H26	120.0	C69—C68—H68	120.4
C28—C27—C26	117.9 (8)	C70—C69—C68	120.8 (4)
C28—C27—H27	121.1	C70—C69—H69	119.6
C26—C27—H27	121.1	C68—C69—H69	119.6
C27—C28—C29	123.8 (11)	C69—C70—C71	119.9 (4)
C27—C28—H28	118.1	C69—C70—H70	120.0
C29—C28—H28	118.1	C71—C70—H70	120.0
C28—C29—C30	116.1 (12)	C70—C71—C72	119.6 (4)
C28—C29—H29	121.9	C70—C71—H71	120.2
C30—C29—H29	121.9	C72—C71—H71	120.2
C25—C30—C29	120.6 (9)	C67—C72—C71	120.2 (4)
C25—C30—H30	119.7	C67—C72—H72	119.9
C29—C30—H30	119.7	C71—C72—H72	119.9

P4—Co1—P1—O1	79.83 (9)	O4—C19—C20—C21	178.2 (3)
P2—Co1—P1—O1	−157.88 (8)	C19—C20—C21—C22	0.4 (4)
P3—Co1—P1—O1	−38.87 (9)	C20—C21—C22—C23	−0.2 (5)
P4—Co1—P1—O3	−39.24 (9)	C21—C22—C23—C24	0.2 (5)
P2—Co1—P1—O3	83.05 (9)	O4—C19—C24—C23	−178.3 (3)
P3—Co1—P1—O3	−157.94 (8)	C20—C19—C24—C23	0.6 (5)
P4—Co1—P1—O2	−158.93 (8)	C22—C23—C24—C19	−0.4 (5)
P2—Co1—P1—O2	−36.64 (8)	P2—O5—C25—C26	111.8 (5)
P3—Co1—P1—O2	82.38 (8)	P2—O5—C25—C30	−72.9 (5)
P4—Co1—P2—O5	86.17 (9)	P2—O5—C25—C80	−93.6 (11)
P3—Co1—P2—O5	−133.50 (9)	P2—O5—C25—C76	86.5 (9)
P1—Co1—P2—O5	−23.48 (9)	C30—C25—C26—C27	1.4 (7)
P4—Co1—P2—O4	−30.44 (9)	C80—C25—C26—C27	20.1 (11)
P3—Co1—P2—O4	109.89 (9)	C76—C25—C26—C27	−92 (3)
P1—Co1—P2—O4	−140.09 (9)	O5—C25—C26—C27	176.6 (4)
P4—Co1—P2—O6	−146.13 (9)	C25—C26—C27—C28	−3.0 (8)
P3—Co1—P2—O6	−5.80 (9)	C26—C27—C28—C29	4.1 (10)
P1—Co1—P2—O6	104.23 (9)	C27—C28—C29—C30	−3.4 (10)
P4—Co1—P3—O9	−129.70 (9)	C26—C25—C30—C29	−0.6 (7)
P2—Co1—P3—O9	88.41 (9)	C80—C25—C30—C29	−75 (5)
P1—Co1—P3—O9	−20.59 (9)	C76—C25—C30—C29	25.9 (9)
P4—Co1—P3—O7	110.78 (8)	O5—C25—C30—C29	−175.7 (5)
P2—Co1—P3—O7	−31.10 (9)	C28—C29—C30—C25	1.5 (9)

P1—Co1—P3—O7	−140.11 (8)	C26—C25—C76—C77	78 (3)
P4—Co1—P3—O8	−2.10 (10)	C30—C25—C76—C77	−22.7 (13)
P2—Co1—P3—O8	−143.99 (9)	C80—C25—C76—C77	−2.4 (15)
P1—Co1—P3—O8	107.01 (9)	O5—C25—C76—C77	177.5 (9)
P2—Co1—P4—O11	112.41 (9)	C25—C76—C77—C78	1.6 (18)
P3—Co1—P4—O11	−28.06 (10)	C76—C77—C78—C79	−0.9 (19)
P1—Co1—P4—O11	−138.07 (9)	C77—C78—C79—C80	1 (2)
P2—Co1—P4—O10	−132.69 (10)	C26—C25—C80—C79	−22.6 (15)
P3—Co1—P4—O10	86.84 (10)	C30—C25—C80—C79	92 (6)
P1—Co1—P4—O10	−23.17 (10)	C76—C25—C80—C79	2.5 (16)
P2—Co1—P4—O12	−3.71 (10)	O5—C25—C80—C79	−177.5 (10)
P3—Co1—P4—O12	−144.18 (9)	C78—C79—C80—C25	−2 (2)
P1—Co1—P4—O12	105.82 (10)	P2—O6—C31—C36	145.9 (2)
O3—P1—O1—C1	−10.8 (2)	P2—O6—C31—C32	−39.7 (4)
O2—P1—O1—C1	94.7 (2)	C36—C31—C32—C33	1.3 (4)
Co1—P1—O1—C1	−136.72 (19)	O6—C31—C32—C33	−172.7 (3)
O1—P1—O2—C7	−10.0 (2)	C31—C32—C33—C34	1.0 (5)
O3—P1—O2—C7	95.2 (2)	C32—C33—C34—C35	−1.7 (5)
Co1—P1—O2—C7	−138.5 (2)	C33—C34—C35—C36	0.1 (5)
O1—P1—O3—C13	96.6 (2)	C32—C31—C36—C35	−2.8 (5)
O2—P1—O3—C13	−8.9 (2)	O6—C31—C36—C35	171.6 (3)
Co1—P1—O3—C13	−136.4 (2)	C34—C35—C36—C31	2.1 (5)
O5—P2—O4—C19	151.9 (2)	P3—O7—C37—C38	78.3 (3)
O6—P2—O4—C19	49.0 (2)	P3—O7—C37—C42	−103.4 (3)
Co1—P2—O4—C19	−81.1 (2)	C42—C37—C38—C39	0.0 (4)
O4—P2—O5—C25	−32.9 (2)	O7—C37—C38—C39	178.3 (2)
O6—P2—O5—C25	62.8 (2)	C37—C38—C39—C40	−0.7 (5)
Co1—P2—O5—C25	−160.56 (19)	C38—C39—C40—C41	1.0 (5)
O5—P2—O6—C31	74.8 (2)	C39—C40—C41—C42	−0.7 (5)
O4—P2—O6—C31	173.2 (2)	C38—C37—C42—C41	0.3 (4)
Co1—P2—O6—C31	−59.3 (2)	O7—C37—C42—C41	−177.9 (3)
O9—P3—O7—C37	111.8 (2)	C40—C41—C42—C37	0.0 (5)
O8—P3—O7—C37	7.8 (2)	P3—O8—C43—C44	170.2 (3)
Co1—P3—O7—C37	−120.4 (2)	P3—O8—C43—C48	−12.8 (5)
O9—P3—O8—C43	67.7 (3)	C48—C43—C44—C45	−0.9 (6)
O7—P3—O8—C43	170.2 (2)	O8—C43—C44—C45	176.1 (4)
Co1—P3—O8—C43	−66.0 (3)	C43—C44—C45—C46	−0.8 (7)
O7—P3—O9—C49	−35.9 (2)	C44—C45—C46—C47	3.1 (7)
O8—P3—O9—C49	60.8 (2)	C45—C46—C47—C48	−3.8 (8)
Co1—P3—O9—C49	−162.92 (18)	C44—C43—C48—C47	0.2 (6)
O11—P4—O10—C55	−40.7 (3)	O8—C43—C48—C47	−176.5 (4)
O12—P4—O10—C55	55.0 (3)	C46—C47—C48—C43	2.2 (7)
Co1—P4—O10—C55	−167.1 (2)	P3—O9—C49—C50	−78.6 (3)
O10—P4—O11—C61	164.2 (2)	P3—O9—C49—C54	103.1 (3)
O12—P4—O11—C61	61.7 (3)	C54—C49—C50—C51	−0.9 (5)
Co1—P4—O11—C61	−68.9 (3)	O9—C49—C50—C51	−179.2 (3)
O11—P4—O12—C67	177.9 (2)	C49—C50—C51—C52	1.3 (5)
O10—P4—O12—C67	81.0 (2)	C50—C51—C52—C53	−1.0 (5)

Co1—P4—O12—C67	−54.8 (2)	C51—C52—C53—C54	0.3 (5)
P1—O1—C1—C2	−112.0 (3)	C50—C49—C54—C53	0.2 (5)
P1—O1—C1—C6	71.2 (3)	O9—C49—C54—C53	178.5 (3)
C6—C1—C2—C3	−2.0 (4)	C52—C53—C54—C49	0.1 (5)
O1—C1—C2—C3	−178.7 (3)	P4—O10—C55—C56	94.2 (3)
C1—C2—C3—C4	−0.9 (5)	P4—O10—C55—C60	−88.8 (3)
C2—C3—C4—C5	2.3 (5)	C60—C55—C56—C57	0.4 (5)
C3—C4—C5—C6	−0.8 (5)	O10—C55—C56—C57	177.3 (3)
C4—C5—C6—C1	−2.0 (5)	C55—C56—C57—C58	−0.5 (5)
C2—C1—C6—C5	3.4 (5)	C56—C57—C58—C59	−0.1 (6)
O1—C1—C6—C5	−179.9 (3)	C57—C58—C59—C60	0.8 (6)
P1—O2—C7—C12	−99.6 (3)	C56—C55—C60—C59	0.4 (5)
P1—O2—C7—C8	84.3 (3)	O10—C55—C60—C59	−176.5 (3)
C12—C7—C8—C9	0.0 (4)	C58—C59—C60—C55	−1.0 (6)
O2—C7—C8—C9	176.1 (2)	P4—O11—C61—C62	−18.2 (4)
C7—C8—C9—C10	0.8 (4)	P4—O11—C61—C66	163.7 (2)
C8—C9—C10—C11	−0.5 (5)	O11—C61—C62—C63	−177.2 (3)
C9—C10—C11—C12	−0.4 (5)	C66—C61—C62—C63	0.8 (4)
C8—C7—C12—C11	−0.9 (4)	C61—C62—C63—C64	0.7 (5)
O2—C7—C12—C11	−176.9 (2)	C62—C63—C64—C65	−1.5 (5)
C10—C11—C12—C7	1.1 (4)	C63—C64—C65—C66	0.6 (5)
P1—O3—C13—C18	−111.4 (3)	C64—C65—C66—C61	0.9 (5)
P1—O3—C13—C14	71.6 (3)	O11—C61—C66—C65	176.6 (3)
C18—C13—C14—C15	1.0 (4)	C62—C61—C66—C65	−1.6 (4)
O3—C13—C14—C15	177.9 (3)	P4—O12—C67—C68	−39.5 (4)
C13—C14—C15—C16	−1.1 (5)	P4—O12—C67—C72	145.2 (3)
C14—C15—C16—C17	0.5 (5)	C72—C67—C68—C69	−0.1 (5)
C15—C16—C17—C18	0.3 (5)	O12—C67—C68—C69	−175.2 (3)
C14—C13—C18—C17	−0.3 (4)	C67—C68—C69—C70	0.7 (5)
O3—C13—C18—C17	−177.2 (2)	C68—C69—C70—C71	−1.0 (6)
C16—C17—C18—C13	−0.4 (5)	C69—C70—C71—C72	0.7 (6)
P2—O4—C19—C24	−172.1 (2)	C68—C67—C72—C71	−0.2 (5)
P2—O4—C19—C20	9.0 (4)	O12—C67—C72—C71	175.1 (3)
C24—C19—C20—C21	−0.6 (4)	C70—C71—C72—C67	0.0 (6)