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# Crystal structure of bis(acetonyltriphenylphosphonium) tetrachloridocobaltate(II)

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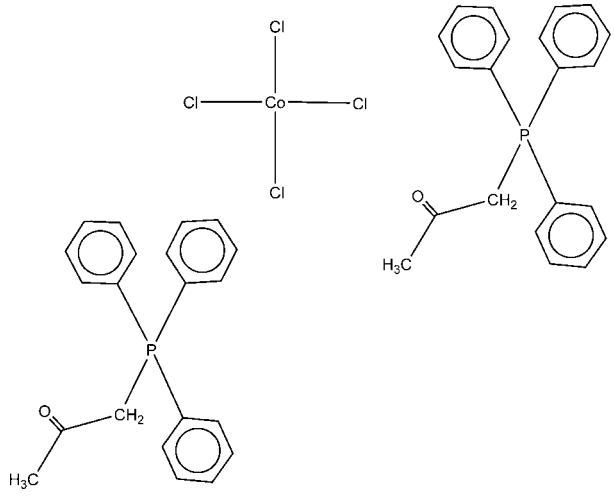
The complex title salt, $(C_{21}H_{20}OP)_2[CoCl_4]$, is the reaction product of $CoCl_2$ with acetonyltriphenylphosphonium chloride in acetonitrile. In the anion, the $Co^{II}$ atom exhibits a typical tetrahedral environment, with Co—Cl distances ranging from 2.2721 (6) to 2.2901 (6) Å, and with Cl—Co—Cl angles ranging from 106.12 (2) to 112.24 (2)°. The two phosphonium cations likewise show the expected tetrahedral configuration, with P—C distances ranging from 1.785 (2) to 1.8059 (18) Å and C—P—C angles ranging from 106.98 (8) to 112.85 (15)°. The molecules interact in the lattice mainly through Coulombic and van der Waals forces because there is no particular polarity to the charges carried by the cations or anion. In the crystal, the cations and anions are arranged in sheets parallel to (001).

**Keywords:** crystal structure; tetrachloridocobaltate dianion; acetonyltriphenylphosphonium cation; alkyltriphenylphosphonium.

**CCDC reference**: 1430699

## 1. Related literature

Cobalt(II) and cobalt(III) compounds can show a variety of extended structural arrangements and are used as metal catalysts (Adams *et al.*, 2008; Boudraa *et al.*, 2015; Bronova *et al.*, 2013; Dhieb *et al.*, 2014; Lassahn *et al.*, 2003; Luo *et al.*, 2013; Merola *et al.*, 2013). Alkyltriphenylphosphonium cations have been employed as stabilizing cations for a variety of different anions, such as nitrate, tetraphenylborate and bromide (Diop *et al.*, 2013; Evans, 2010; Kavitha *et al.*, 2012). For other structures containing the tetrahedral $[CoCl_4]^{2-}$ anion, see: Diop *et al.* (2015); Gueddar *et al.* (2013).




## 2. Experimental

### 2.1. Crystal data

$(C_{21}H_{20}OP)_2[CoCl_4]$
$M_r$ = 839.41
Orthorhombic, *Pbca*
*a* = 18.758 (3) Å
*b* = 15.769 (2) Å
*c* = 27.157 (4) Å
*V* = 8033 (2) Å$^3$
*Z* = 8
Mo *Kα* radiation
$\mu$ = 0.81 mm$^{-1}$
*T* = 120 K
0.24 × 0.16 × 0.10 mm

### 2.2. Data collection

Bruker Kappa X8-APEXII diffractometer
Absorption correction: numerical (*SADABS*; Krause *et al.*, 2015)
$T_{min}$ = 0.813, $T_{max}$ = 0.920
148135 measured reflections
10073 independent reflections
8207 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.061

### 2.3. Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.097
*S* = 1.06
10073 reflections
462 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.76 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.25 e Å$^{-3}$

Data collection: *APEX2* (Bruker, 2014); cell refinement: *SAINT* (Bruker, 2014); data reduction: *SAINT*; program(s) used to solve structure: *SHELXT* (Sheldrick, 2015*a*); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015*b*); molecular graphics: *XP* in *SHELXTL* (Sheldrick, 2008) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *CIFTAB* (Sheldrick, 2008) and *publCIF* (Westrip, 2010).

## Acknowledgements

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Supporting information for this paper is available from the IUCr electronic archives (Reference: WM5224).

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# supporting information

*Acta Cryst.* (2015). E**71**, m209–m210 [https://doi.org/10.1107/S2056989015019180]

## Crystal structure of bis(acetonyltriphenylphosphonium) tetrachloridocobaltate(II)

**Mouhamadou Birame Diop, Libasse Diop and Allen G. Oliver**

### S1. Synthesis and crystallization

All chemicals were purchased from Aldrich-Germany and were used as received. Acetonyl triphenylphosphonium chloride was mixed in acetonitrile with $CoCl_2·6H_2O$ in a 2:1 ratio. Blue crystals suitable for a single-crystal X-ray diffraction study were obtained after slow solvent evaporation at room temperature.

### S2. Refinement

Hydrogen atoms were included in idealized positions with $U_{iso}(H) = 1.2U_{eq}(C_{aromatic/methylene})$ or $1.5U_{eq}(C_{methyl})$. C—H distances were set to 0.95 (aromatic), 0.98 (methyl) and 0.99 Å (methylene).

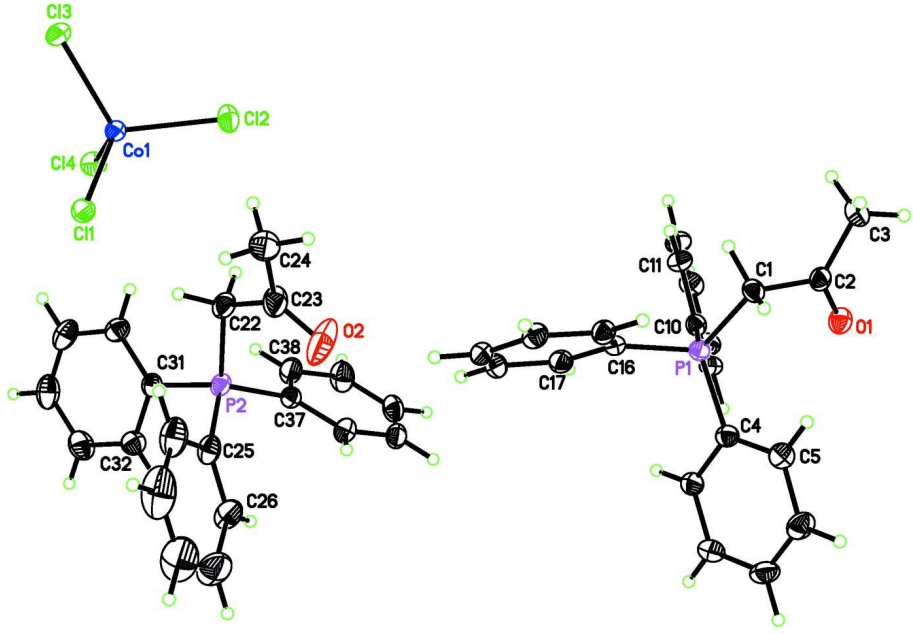


**Figure 1**

The molecular components of the title compound. Displacement ellipsoids are drawn at the 50% probability level.

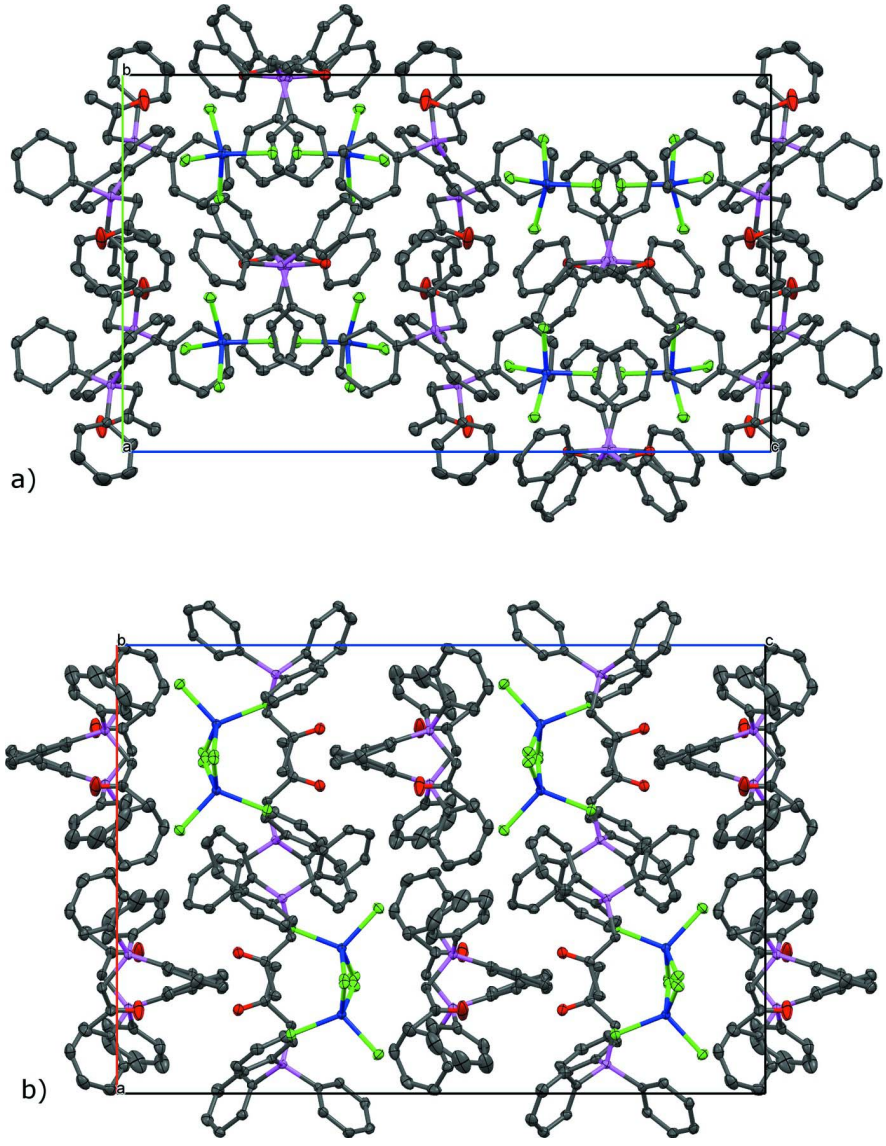


**Figure 2**

Packing views of the title compound *a*) along [100] and *b*) along [010]. Hydrogen atoms were omitted for clarity. Displacement ellipsoids are drawn at the 50% probability level.

### Bis(acetonyltriphenylphosphonium) tetrachloridocobaltate(II)

*Crystal data*

$(C_{21}H_{20}OP)_2[CoCl_4]$
$M_r$ = 839.41
Orthorhombic, *Pbca*
*a* = 18.758 (3) Å
*b* = 15.769 (2) Å
*c* = 27.157 (4) Å
*V* = 8033 (2) Å$^3$
*Z* = 8
*F*(000) = 3464
$D_x$ = 1.388 Mg m$^{-3}$
Mo *Kα* radiation, $\lambda$ = 0.71073 Å
Cell parameters from 9962 reflections
$\theta$ = 2.3–28.3°
$\mu$ = 0.81 mm$^{-1}$
*T* = 120 K
Tablet, blue
0.24 × 0.16 × 0.10 mm

*Data collection*

Bruker Kappa X8-APEXII diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 8.33 pixels mm$^{-1}$
combination of $\omega$ and $\varphi$–scans
Absorption correction: numerical (*SADABS*; Krause *et al.*, 2015)
$T_{min}$ = 0.813, $T_{max}$ = 0.920

148135 measured reflections
10073 independent reflections
8207 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.061
$\theta_{max}$ = 28.4°, $\theta_{min}$ = 1.5°
$h$ = −25→25
$k$ = −21→21
$l$ = −36→36

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.097
$S$ = 1.06
10073 reflections
462 parameters
0 restraints
Primary atom site location: real-space vector search
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.047P)^2 + 5.1834P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.76 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.25 e Å$^{-3}$

*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$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Co1 | 0.67585 (2) | 0.78995 (2) | 0.34640 (2) | 0.01815 (7) |
| Cl1 | 0.74555 (3) | 0.67130 (3) | 0.35096 (2) | 0.02314 (10) |
| Cl2 | 0.58678 (3) | 0.77319 (3) | 0.40325 (2) | 0.02611 (11) |
| Cl3 | 0.63163 (3) | 0.79320 (3) | 0.26854 (2) | 0.02741 (11) |
| Cl4 | 0.73968 (3) | 0.90911 (3) | 0.36500 (2) | 0.02644 (11) |
| P1 | 0.43467 (2) | 0.50603 (3) | 0.74508 (2) | 0.01730 (10) |
| O1 | 0.31362 (7) | 0.50028 (9) | 0.81285 (5) | 0.0253 (3) |
| C1 | 0.34791 (9) | 0.46217 (12) | 0.73157 (7) | 0.0205 (4) |
| H1A | 0.3308 | 0.4851 | 0.6998 | 0.025* |
| H1B | 0.3520 | 0.3998 | 0.7282 | 0.025* |
| C2 | 0.29400 (10) | 0.48277 (11) | 0.77155 (7) | 0.0205 (4) |
| C3 | 0.21765 (10) | 0.48012 (13) | 0.75622 (8) | 0.0268 (4) |
| H3A | 0.2090 | 0.4289 | 0.7367 | 0.040* |
| H3B | 0.2066 | 0.5304 | 0.7364 | 0.040* |
| H3C | 0.1872 | 0.4794 | 0.7855 | 0.040* |
| C4 | 0.48127 (10) | 0.44742 (12) | 0.79153 (7) | 0.0201 (4) |
| C5 | 0.45435 (11) | 0.37160 (12) | 0.80994 (7) | 0.0243 (4) |
| H5 | 0.4095 | 0.3509 | 0.7990 | 0.029* |
| C6 | 0.49371 (12) | 0.32628 (13) | 0.84449 (8) | 0.0293 (4) |

| | | | | |
|---|---|---|---|---|
| H6 | 0.4757 | 0.2743 | 0.8571 | 0.035* |
| C7 | 0.55904 (12) | 0.35646 (13) | 0.86060 (8) | 0.0295 (4) |
| H7 | 0.5853 | 0.3254 | 0.8845 | 0.035* |
| C8 | 0.58631 (11) | 0.43149 (13) | 0.84208 (7) | 0.0261 (4) |
| H8 | 0.6311 | 0.4519 | 0.8533 | 0.031* |
| C9 | 0.54805 (10) | 0.47700 (12) | 0.80697 (7) | 0.0228 (4) |
| H9 | 0.5671 | 0.5278 | 0.7936 | 0.027* |
| C10 | 0.42343 (9) | 0.61523 (11) | 0.76149 (7) | 0.0189 (3) |
| C11 | 0.38399 (11) | 0.66634 (13) | 0.72936 (7) | 0.0244 (4) |
| H11 | 0.3648 | 0.6432 | 0.6999 | 0.029* |
| C12 | 0.37310 (11) | 0.75082 (13) | 0.74080 (8) | 0.0281 (4) |
| H12 | 0.3460 | 0.7857 | 0.7193 | 0.034* |
| C13 | 0.40164 (11) | 0.78474 (13) | 0.78367 (8) | 0.0269 (4) |
| H13 | 0.3949 | 0.8431 | 0.7911 | 0.032* |
| C14 | 0.43982 (11) | 0.73370 (13) | 0.81562 (7) | 0.0256 (4) |
| H14 | 0.4588 | 0.7571 | 0.8451 | 0.031* |
| C15 | 0.45054 (10) | 0.64892 (12) | 0.80503 (7) | 0.0217 (4) |
| H15 | 0.4762 | 0.6139 | 0.8273 | 0.026* |
| C16 | 0.48683 (9) | 0.49899 (12) | 0.68965 (6) | 0.0187 (3) |
| C17 | 0.54246 (10) | 0.55695 (13) | 0.68207 (7) | 0.0233 (4) |
| H17 | 0.5488 | 0.6035 | 0.7039 | 0.028* |
| C18 | 0.58806 (10) | 0.54562 (14) | 0.64240 (7) | 0.0264 (4) |
| H18 | 0.6261 | 0.5844 | 0.6371 | 0.032* |
| C19 | 0.57847 (11) | 0.47806 (13) | 0.61039 (7) | 0.0256 (4) |
| H19 | 0.6102 | 0.4704 | 0.5835 | 0.031* |
| C20 | 0.52278 (11) | 0.42182 (12) | 0.61749 (7) | 0.0235 (4) |
| H20 | 0.5158 | 0.3764 | 0.5950 | 0.028* |
| C21 | 0.47709 (10) | 0.43131 (12) | 0.65729 (7) | 0.0215 (4) |
| H21 | 0.4394 | 0.3920 | 0.6625 | 0.026* |
| P2 | 0.81009 (3) | 0.67681 (3) | 0.51792 (2) | 0.02010 (10) |
| O2 | 0.68507 (12) | 0.56656 (15) | 0.53292 (6) | 0.0650 (7) |
| C22 | 0.73531 (11) | 0.66612 (14) | 0.47682 (7) | 0.0291 (4) |
| H22A | 0.7082 | 0.7199 | 0.4765 | 0.035* |
| H22B | 0.7532 | 0.6559 | 0.4430 | 0.035* |
| C23 | 0.68560 (12) | 0.59424 (16) | 0.49123 (8) | 0.0339 (5) |
| C24 | 0.64020 (12) | 0.55970 (15) | 0.45136 (8) | 0.0338 (5) |
| H24A | 0.6195 | 0.6066 | 0.4325 | 0.051* |
| H24B | 0.6019 | 0.5254 | 0.4657 | 0.051* |
| H24C | 0.6692 | 0.5242 | 0.4295 | 0.051* |
| C25 | 0.85355 (11) | 0.57674 (12) | 0.52453 (7) | 0.0257 (4) |
| C26 | 0.89525 (13) | 0.56012 (14) | 0.56578 (8) | 0.0346 (5) |
| H26 | 0.8976 | 0.6002 | 0.5918 | 0.041* |
| C27 | 0.93322 (17) | 0.48528 (18) | 0.56879 (10) | 0.0547 (8) |
| H27 | 0.9618 | 0.4738 | 0.5969 | 0.066* |
| C28 | 0.9295 (2) | 0.42738 (18) | 0.53091 (12) | 0.0666 (10) |
| H28 | 0.9554 | 0.3758 | 0.5332 | 0.080* |
| C29 | 0.8887 (2) | 0.44340 (17) | 0.48981 (11) | 0.0613 (9) |
| H29 | 0.8866 | 0.4029 | 0.4640 | 0.074* |

| | | | | |
|---|---|---|---|---|
| C30 | 0.85083 (15) | 0.51835 (15) | 0.48610 (9) | 0.0396 (6) |
| H30 | 0.8232 | 0.5299 | 0.4576 | 0.048* |
| C31 | 0.87237 (10) | 0.74834 (12) | 0.49010 (7) | 0.0207 (4) |
| C32 | 0.94058 (11) | 0.75279 (13) | 0.51041 (7) | 0.0262 (4) |
| H32 | 0.9520 | 0.7204 | 0.5388 | 0.031* |
| C33 | 0.99159 (12) | 0.80463 (15) | 0.48902 (9) | 0.0341 (5) |
| H33 | 1.0381 | 0.8078 | 0.5027 | 0.041* |
| C34 | 0.97468 (13) | 0.85188 (14) | 0.44761 (8) | 0.0361 (5) |
| H34 | 1.0099 | 0.8869 | 0.4328 | 0.043* |
| C35 | 0.90704 (13) | 0.84835 (13) | 0.42767 (8) | 0.0329 (5) |
| H35 | 0.8959 | 0.8815 | 0.3995 | 0.039* |
| C36 | 0.85523 (11) | 0.79668 (12) | 0.44854 (7) | 0.0251 (4) |
| H36 | 0.8087 | 0.7942 | 0.4348 | 0.030* |
| C37 | 0.78322 (10) | 0.71941 (12) | 0.57609 (7) | 0.0208 (4) |
| C38 | 0.77556 (12) | 0.80730 (13) | 0.58000 (8) | 0.0294 (4) |
| H38 | 0.7870 | 0.8429 | 0.5529 | 0.035* |
| C39 | 0.75113 (13) | 0.84223 (14) | 0.62383 (8) | 0.0348 (5) |
| H39 | 0.7453 | 0.9019 | 0.6267 | 0.042* |
| C40 | 0.73537 (11) | 0.79010 (14) | 0.66319 (8) | 0.0290 (4) |
| H40 | 0.7190 | 0.8143 | 0.6932 | 0.035* |
| C41 | 0.74312 (11) | 0.70303 (13) | 0.65961 (7) | 0.0257 (4) |
| H41 | 0.7325 | 0.6679 | 0.6871 | 0.031* |
| C42 | 0.76634 (10) | 0.66707 (12) | 0.61586 (7) | 0.0237 (4) |
| H42 | 0.7707 | 0.6073 | 0.6130 | 0.028* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Co1 | 0.01844 (13) | 0.01928 (13) | 0.01673 (12) | 0.00064 (9) | −0.00024 (9) | −0.00037 (9) |
| Cl1 | 0.0255 (2) | 0.0228 (2) | 0.0212 (2) | 0.00573 (18) | 0.00104 (17) | −0.00089 (16) |
| Cl2 | 0.0239 (2) | 0.0303 (2) | 0.0241 (2) | −0.00433 (19) | 0.00580 (18) | −0.00585 (18) |
| Cl3 | 0.0284 (2) | 0.0360 (3) | 0.0178 (2) | 0.0041 (2) | −0.00300 (17) | 0.00000 (18) |
| Cl4 | 0.0277 (2) | 0.0213 (2) | 0.0303 (2) | −0.00336 (18) | −0.00315 (19) | 0.00061 (18) |
| P1 | 0.0163 (2) | 0.0186 (2) | 0.0170 (2) | −0.00126 (17) | −0.00101 (17) | −0.00021 (17) |
| O1 | 0.0276 (7) | 0.0272 (7) | 0.0210 (7) | −0.0022 (6) | 0.0019 (5) | −0.0008 (5) |
| C1 | 0.0171 (8) | 0.0241 (9) | 0.0203 (9) | −0.0038 (7) | −0.0007 (7) | −0.0018 (7) |
| C2 | 0.0221 (9) | 0.0166 (8) | 0.0229 (9) | −0.0008 (7) | 0.0018 (7) | 0.0037 (7) |
| C3 | 0.0198 (9) | 0.0299 (10) | 0.0308 (10) | −0.0007 (8) | 0.0028 (8) | −0.0013 (8) |
| C4 | 0.0207 (9) | 0.0203 (9) | 0.0192 (8) | 0.0020 (7) | −0.0008 (7) | −0.0005 (7) |
| C5 | 0.0253 (9) | 0.0210 (9) | 0.0266 (10) | −0.0001 (8) | 0.0000 (8) | −0.0007 (8) |
| C6 | 0.0364 (12) | 0.0196 (9) | 0.0320 (11) | 0.0028 (8) | 0.0007 (9) | 0.0058 (8) |
| C7 | 0.0320 (11) | 0.0278 (10) | 0.0288 (10) | 0.0105 (9) | −0.0038 (8) | 0.0041 (8) |
| C8 | 0.0216 (9) | 0.0284 (10) | 0.0285 (10) | 0.0027 (8) | −0.0041 (8) | −0.0011 (8) |
| C9 | 0.0208 (9) | 0.0226 (9) | 0.0250 (9) | 0.0009 (7) | 0.0005 (7) | 0.0023 (7) |
| C10 | 0.0182 (8) | 0.0172 (8) | 0.0213 (9) | −0.0006 (7) | 0.0013 (7) | 0.0001 (7) |
| C11 | 0.0259 (10) | 0.0271 (10) | 0.0201 (9) | 0.0012 (8) | −0.0043 (7) | 0.0013 (7) |
| C12 | 0.0296 (11) | 0.0251 (10) | 0.0295 (10) | 0.0054 (8) | −0.0028 (8) | 0.0060 (8) |
| C13 | 0.0251 (10) | 0.0197 (9) | 0.0358 (11) | 0.0014 (8) | 0.0010 (8) | 0.0003 (8) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C14 | 0.0248 (10) | 0.0247 (10) | 0.0272 (10) | 0.0001 (8) | −0.0046 (8) | −0.0053 (8) |
| C15 | 0.0200 (9) | 0.0222 (9) | 0.0229 (9) | 0.0015 (7) | −0.0037 (7) | 0.0014 (7) |
| C16 | 0.0173 (8) | 0.0224 (9) | 0.0165 (8) | 0.0017 (7) | −0.0009 (7) | 0.0021 (7) |
| C17 | 0.0221 (9) | 0.0262 (10) | 0.0215 (9) | −0.0040 (8) | −0.0033 (7) | 0.0010 (7) |
| C18 | 0.0190 (9) | 0.0330 (11) | 0.0273 (10) | −0.0055 (8) | 0.0002 (7) | 0.0059 (8) |
| C19 | 0.0231 (10) | 0.0330 (11) | 0.0209 (9) | 0.0066 (8) | 0.0032 (7) | 0.0075 (8) |
| C20 | 0.0287 (10) | 0.0227 (9) | 0.0192 (9) | 0.0044 (8) | 0.0010 (7) | −0.0012 (7) |
| C21 | 0.0226 (9) | 0.0206 (9) | 0.0214 (9) | −0.0014 (7) | −0.0001 (7) | 0.0016 (7) |
| P2 | 0.0219 (2) | 0.0232 (2) | 0.0152 (2) | −0.00295 (19) | −0.00015 (17) | −0.00036 (18) |
| O2 | 0.0754 (14) | 0.0948 (16) | 0.0248 (9) | −0.0567 (13) | −0.0012 (9) | 0.0086 (9) |
| C22 | 0.0260 (10) | 0.0428 (12) | 0.0185 (9) | −0.0090 (9) | −0.0017 (8) | 0.0017 (8) |
| C23 | 0.0287 (11) | 0.0486 (13) | 0.0244 (10) | −0.0140 (10) | 0.0014 (8) | −0.0022 (9) |
| C24 | 0.0311 (11) | 0.0371 (12) | 0.0333 (11) | −0.0074 (9) | −0.0039 (9) | −0.0041 (9) |
| C25 | 0.0348 (11) | 0.0201 (9) | 0.0222 (9) | −0.0018 (8) | 0.0061 (8) | −0.0016 (7) |
| C26 | 0.0506 (14) | 0.0274 (11) | 0.0257 (10) | 0.0107 (10) | 0.0044 (10) | 0.0005 (8) |
| C27 | 0.076 (2) | 0.0447 (15) | 0.0433 (15) | 0.0297 (14) | 0.0098 (14) | 0.0113 (12) |
| C28 | 0.098 (3) | 0.0351 (14) | 0.067 (2) | 0.0279 (16) | 0.0277 (19) | 0.0062 (14) |
| C29 | 0.097 (2) | 0.0298 (13) | 0.0571 (18) | −0.0002 (15) | 0.0307 (17) | −0.0183 (12) |
| C30 | 0.0544 (15) | 0.0327 (12) | 0.0318 (12) | −0.0071 (11) | 0.0118 (11) | −0.0096 (9) |
| C31 | 0.0231 (9) | 0.0201 (9) | 0.0187 (8) | −0.0006 (7) | 0.0024 (7) | −0.0022 (7) |
| C32 | 0.0251 (10) | 0.0263 (10) | 0.0272 (10) | −0.0025 (8) | −0.0019 (8) | 0.0007 (8) |
| C33 | 0.0257 (11) | 0.0365 (12) | 0.0400 (12) | −0.0076 (9) | 0.0024 (9) | −0.0040 (10) |
| C34 | 0.0423 (13) | 0.0297 (11) | 0.0364 (12) | −0.0119 (10) | 0.0138 (10) | −0.0011 (9) |
| C35 | 0.0504 (14) | 0.0245 (10) | 0.0237 (10) | −0.0044 (9) | 0.0043 (9) | 0.0030 (8) |
| C36 | 0.0304 (10) | 0.0225 (9) | 0.0223 (9) | 0.0012 (8) | −0.0015 (8) | −0.0005 (7) |
| C37 | 0.0198 (9) | 0.0249 (9) | 0.0176 (8) | 0.0003 (7) | 0.0003 (7) | −0.0010 (7) |
| C38 | 0.0345 (11) | 0.0275 (10) | 0.0263 (10) | 0.0039 (9) | 0.0065 (8) | 0.0033 (8) |
| C39 | 0.0421 (13) | 0.0268 (11) | 0.0355 (12) | 0.0041 (9) | 0.0116 (10) | −0.0046 (9) |
| C40 | 0.0275 (11) | 0.0341 (11) | 0.0255 (10) | 0.0012 (9) | 0.0076 (8) | −0.0063 (8) |
| C41 | 0.0250 (10) | 0.0320 (11) | 0.0202 (9) | −0.0034 (8) | 0.0031 (8) | 0.0001 (8) |
| C42 | 0.0274 (10) | 0.0234 (9) | 0.0202 (9) | −0.0022 (8) | 0.0011 (7) | −0.0004 (7) |

*Geometric parameters (Å, º)*

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|---|---|---|---|
| Co1—Cl3 | 2.2721 (6) | C20—H20 | 0.9500 |
| Co1—Cl4 | 2.2845 (6) | C21—H21 | 0.9500 |
| Co1—Cl1 | 2.2859 (6) | P2—C25 | 1.785 (2) |
| Co1—Cl2 | 2.2901 (6) | P2—C37 | 1.7892 (19) |
| P1—C10 | 1.7912 (19) | P2—C31 | 1.7912 (19) |
| P1—C4 | 1.7914 (19) | P2—C22 | 1.801 (2) |
| P1—C16 | 1.7988 (18) | O2—C23 | 1.213 (3) |
| P1—C1 | 1.8059 (18) | C22—C23 | 1.519 (3) |
| O1—C2 | 1.212 (2) | C22—H22A | 0.9900 |
| C1—C2 | 1.519 (3) | C22—H22B | 0.9900 |
| C1—H1A | 0.9900 | C23—C24 | 1.481 (3) |
| C1—H1B | 0.9900 | C24—H24A | 0.9800 |
| C2—C3 | 1.492 (3) | C24—H24B | 0.9800 |
| C3—H3A | 0.9800 | C24—H24C | 0.9800 |

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| C3—H3B | 0.9800 | C25—C26 | 1.391 (3) |
| C3—H3C | 0.9800 | C25—C30 | 1.393 (3) |
| C4—C5 | 1.391 (3) | C26—C27 | 1.381 (3) |
| C4—C9 | 1.401 (3) | C26—H26 | 0.9500 |
| C5—C6 | 1.391 (3) | C27—C28 | 1.377 (4) |
| C5—H5 | 0.9500 | C27—H27 | 0.9500 |
| C6—C7 | 1.386 (3) | C28—C29 | 1.377 (5) |
| C6—H6 | 0.9500 | C28—H28 | 0.9500 |
| C7—C8 | 1.384 (3) | C29—C30 | 1.382 (4) |
| C7—H7 | 0.9500 | C29—H29 | 0.9500 |
| C8—C9 | 1.392 (3) | C30—H30 | 0.9500 |
| C8—H8 | 0.9500 | C31—C32 | 1.395 (3) |
| C9—H9 | 0.9500 | C31—C36 | 1.399 (3) |
| C10—C15 | 1.392 (3) | C32—C33 | 1.386 (3) |
| C10—C11 | 1.399 (3) | C32—H32 | 0.9500 |
| C11—C12 | 1.383 (3) | C33—C34 | 1.386 (3) |
| C11—H11 | 0.9500 | C33—H33 | 0.9500 |
| C12—C13 | 1.389 (3) | C34—C35 | 1.381 (3) |
| C12—H12 | 0.9500 | C34—H34 | 0.9500 |
| C13—C14 | 1.383 (3) | C35—C36 | 1.389 (3) |
| C13—H13 | 0.9500 | C35—H35 | 0.9500 |
| C14—C15 | 1.382 (3) | C36—H36 | 0.9500 |
| C14—H14 | 0.9500 | C37—C42 | 1.396 (3) |
| C15—H15 | 0.9500 | C37—C38 | 1.397 (3) |
| C16—C21 | 1.394 (3) | C38—C39 | 1.389 (3) |
| C16—C17 | 1.402 (3) | C38—H38 | 0.9500 |
| C17—C18 | 1.387 (3) | C39—C40 | 1.380 (3) |
| C17—H17 | 0.9500 | C39—H39 | 0.9500 |
| C18—C19 | 1.387 (3) | C40—C41 | 1.384 (3) |
| C18—H18 | 0.9500 | C40—H40 | 0.9500 |
| C19—C20 | 1.384 (3) | C41—C42 | 1.387 (3) |
| C19—H19 | 0.9500 | C41—H41 | 0.9500 |
| C20—C21 | 1.387 (3) | C42—H42 | 0.9500 |

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|---|---|---|---|
| Cl3—Co1—Cl4 | 112.24 (2) | C20—C21—C16 | 119.51 (18) |
| Cl3—Co1—Cl1 | 106.12 (2) | C20—C21—H21 | 120.2 |
| Cl4—Co1—Cl1 | 111.19 (2) | C16—C21—H21 | 120.2 |
| Cl3—Co1—Cl2 | 111.32 (2) | C25—P2—C37 | 111.83 (9) |
| Cl4—Co1—Cl2 | 109.17 (2) | C25—P2—C31 | 107.53 (9) |
| Cl1—Co1—Cl2 | 106.64 (2) | C37—P2—C31 | 108.65 (9) |
| C10—P1—C4 | 112.22 (8) | C25—P2—C22 | 109.59 (10) |
| C10—P1—C16 | 109.37 (9) | C37—P2—C22 | 111.29 (10) |
| C4—P1—C16 | 106.98 (8) | C31—P2—C22 | 107.79 (9) |
| C10—P1—C1 | 108.21 (9) | C23—C22—P2 | 112.85 (15) |
| C4—P1—C1 | 112.66 (9) | C23—C22—H22A | 109.0 |
| C16—P1—C1 | 107.25 (8) | P2—C22—H22A | 109.0 |
| C2—C1—P1 | 111.90 (13) | C23—C22—H22B | 109.0 |
| C2—C1—H1A | 109.2 | P2—C22—H22B | 109.0 |

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|---|---|---|---|
| P1—C1—H1A | 109.2 | H22A—C22—H22B | 107.8 |
| C2—C1—H1B | 109.2 | O2—C23—C24 | 123.0 (2) |
| P1—C1—H1B | 109.2 | O2—C23—C22 | 120.91 (19) |
| H1A—C1—H1B | 107.9 | C24—C23—C22 | 116.03 (18) |
| O1—C2—C3 | 123.76 (18) | C23—C24—H24A | 109.5 |
| O1—C2—C1 | 120.53 (17) | C23—C24—H24B | 109.5 |
| C3—C2—C1 | 115.71 (16) | H24A—C24—H24B | 109.5 |
| C2—C3—H3A | 109.5 | C23—C24—H24C | 109.5 |
| C2—C3—H3B | 109.5 | H24A—C24—H24C | 109.5 |
| H3A—C3—H3B | 109.5 | H24B—C24—H24C | 109.5 |
| C2—C3—H3C | 109.5 | C26—C25—C30 | 120.0 (2) |
| H3A—C3—H3C | 109.5 | C26—C25—P2 | 120.28 (15) |
| H3B—C3—H3C | 109.5 | C30—C25—P2 | 119.50 (18) |
| C5—C4—C9 | 120.21 (17) | C27—C26—C25 | 119.9 (2) |
| C5—C4—P1 | 121.30 (14) | C27—C26—H26 | 120.0 |
| C9—C4—P1 | 118.38 (14) | C25—C26—H26 | 120.0 |
| C4—C5—C6 | 119.42 (19) | C28—C27—C26 | 119.7 (3) |
| C4—C5—H5 | 120.3 | C28—C27—H27 | 120.1 |
| C6—C5—H5 | 120.3 | C26—C27—H27 | 120.1 |
| C7—C6—C5 | 120.39 (19) | C29—C28—C27 | 120.8 (3) |
| C7—C6—H6 | 119.8 | C29—C28—H28 | 119.6 |
| C5—C6—H6 | 119.8 | C27—C28—H28 | 119.6 |
| C8—C7—C6 | 120.40 (19) | C28—C29—C30 | 120.1 (2) |
| C8—C7—H7 | 119.8 | C28—C29—H29 | 120.0 |
| C6—C7—H7 | 119.8 | C30—C29—H29 | 120.0 |
| C7—C8—C9 | 119.93 (19) | C29—C30—C25 | 119.5 (3) |
| C7—C8—H8 | 120.0 | C29—C30—H30 | 120.3 |
| C9—C8—H8 | 120.0 | C25—C30—H30 | 120.3 |
| C8—C9—C4 | 119.62 (18) | C32—C31—C36 | 120.16 (18) |
| C8—C9—H9 | 120.2 | C32—C31—P2 | 117.58 (14) |
| C4—C9—H9 | 120.2 | C36—C31—P2 | 122.23 (15) |
| C15—C10—C11 | 120.19 (17) | C33—C32—C31 | 119.79 (19) |
| C15—C10—P1 | 122.35 (14) | C33—C32—H32 | 120.1 |
| C11—C10—P1 | 117.43 (14) | C31—C32—H32 | 120.1 |
| C12—C11—C10 | 119.52 (18) | C34—C33—C32 | 120.0 (2) |
| C12—C11—H11 | 120.2 | C34—C33—H33 | 120.0 |
| C10—C11—H11 | 120.2 | C32—C33—H33 | 120.0 |
| C11—C12—C13 | 120.16 (18) | C35—C34—C33 | 120.5 (2) |
| C11—C12—H12 | 119.9 | C35—C34—H34 | 119.8 |
| C13—C12—H12 | 119.9 | C33—C34—H34 | 119.8 |
| C14—C13—C12 | 120.10 (19) | C34—C35—C36 | 120.4 (2) |
| C14—C13—H13 | 120.0 | C34—C35—H35 | 119.8 |
| C12—C13—H13 | 120.0 | C36—C35—H35 | 119.8 |
| C15—C14—C13 | 120.50 (18) | C35—C36—C31 | 119.20 (19) |
| C15—C14—H14 | 119.8 | C35—C36—H36 | 120.4 |
| C13—C14—H14 | 119.8 | C31—C36—H36 | 120.4 |
| C14—C15—C10 | 119.51 (17) | C42—C37—C38 | 120.29 (18) |
| C14—C15—H15 | 120.2 | C42—C37—P2 | 121.68 (15) |

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| C10—C15—H15 | 120.2 | C38—C37—P2 | 117.94 (14) |
| C21—C16—C17 | 120.25 (17) | C39—C38—C37 | 119.49 (19) |
| C21—C16—P1 | 120.22 (14) | C39—C38—H38 | 120.3 |
| C17—C16—P1 | 119.17 (14) | C37—C38—H38 | 120.3 |
| C18—C17—C16 | 119.27 (18) | C40—C39—C38 | 119.9 (2) |
| C18—C17—H17 | 120.4 | C40—C39—H39 | 120.1 |
| C16—C17—H17 | 120.4 | C38—C39—H39 | 120.1 |
| C19—C18—C17 | 120.39 (18) | C39—C40—C41 | 120.92 (19) |
| C19—C18—H18 | 119.8 | C39—C40—H40 | 119.5 |
| C17—C18—H18 | 119.8 | C41—C40—H40 | 119.5 |
| C20—C19—C18 | 120.18 (18) | C40—C41—C42 | 119.92 (19) |
| C20—C19—H19 | 119.9 | C40—C41—H41 | 120.0 |
| C18—C19—H19 | 119.9 | C42—C41—H41 | 120.0 |
| C19—C20—C21 | 120.39 (18) | C41—C42—C37 | 119.50 (18) |
| C19—C20—H20 | 119.8 | C41—C42—H42 | 120.2 |
| C21—C20—H20 | 119.8 | C37—C42—H42 | 120.2 |

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| C10—P1—C1—C2 | −48.98 (15) | C25—P2—C22—C23 | 51.93 (18) |
| C4—P1—C1—C2 | 75.68 (15) | C37—P2—C22—C23 | −72.28 (18) |
| C16—P1—C1—C2 | −166.87 (13) | C31—P2—C22—C23 | 168.68 (15) |
| P1—C1—C2—O1 | −22.6 (2) | P2—C22—C23—O2 | 21.0 (3) |
| P1—C1—C2—C3 | 157.19 (14) | P2—C22—C23—C24 | −157.50 (18) |
| C10—P1—C4—C5 | 129.00 (16) | C37—P2—C25—C26 | −33.4 (2) |
| C16—P1—C4—C5 | −111.05 (16) | C31—P2—C25—C26 | 85.80 (19) |
| C1—P1—C4—C5 | 6.56 (19) | C22—P2—C25—C26 | −157.29 (18) |
| C10—P1—C4—C9 | −54.84 (17) | C37—P2—C25—C30 | 152.48 (17) |
| C16—P1—C4—C9 | 65.11 (16) | C31—P2—C25—C30 | −88.33 (19) |
| C1—P1—C4—C9 | −177.28 (14) | C22—P2—C25—C30 | 28.6 (2) |
| C9—C4—C5—C6 | 1.2 (3) | C30—C25—C26—C27 | −0.8 (4) |
| P1—C4—C5—C6 | 177.30 (15) | P2—C25—C26—C27 | −174.9 (2) |
| C4—C5—C6—C7 | 0.2 (3) | C25—C26—C27—C28 | −0.1 (4) |
| C5—C6—C7—C8 | −0.8 (3) | C26—C27—C28—C29 | 0.5 (5) |
| C6—C7—C8—C9 | −0.1 (3) | C27—C28—C29—C30 | 0.0 (5) |
| C7—C8—C9—C4 | 1.6 (3) | C28—C29—C30—C25 | −0.9 (4) |
| C5—C4—C9—C8 | −2.1 (3) | C26—C25—C30—C29 | 1.2 (4) |
| P1—C4—C9—C8 | −178.31 (15) | P2—C25—C30—C29 | 175.4 (2) |
| C4—P1—C10—C15 | 1.85 (18) | C25—P2—C31—C32 | −49.08 (17) |
| C16—P1—C10—C15 | −116.70 (16) | C37—P2—C31—C32 | 72.13 (17) |
| C1—P1—C10—C15 | 126.77 (16) | C22—P2—C31—C32 | −167.16 (15) |
| C4—P1—C10—C11 | −176.27 (14) | C25—P2—C31—C36 | 128.93 (16) |
| C16—P1—C10—C11 | 65.18 (16) | C37—P2—C31—C36 | −109.86 (16) |
| C1—P1—C10—C11 | −51.35 (17) | C22—P2—C31—C36 | 10.86 (19) |
| C15—C10—C11—C12 | 1.0 (3) | C36—C31—C32—C33 | −0.6 (3) |
| P1—C10—C11—C12 | 179.16 (16) | P2—C31—C32—C33 | 177.42 (16) |
| C10—C11—C12—C13 | 0.5 (3) | C31—C32—C33—C34 | 0.1 (3) |
| C11—C12—C13—C14 | −1.4 (3) | C32—C33—C34—C35 | 0.6 (3) |
| C12—C13—C14—C15 | 0.6 (3) | C33—C34—C35—C36 | −0.7 (3) |
| C13—C14—C15—C10 | 0.9 (3) | C34—C35—C36—C31 | 0.1 (3) |

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| C11—C10—C15—C14 | −1.7 (3) | C32—C31—C36—C35 | 0.5 (3) |
| P1—C10—C15—C14 | −179.79 (15) | P2—C31—C36—C35 | −177.42 (15) |
| C10—P1—C16—C21 | −150.60 (15) | C25—P2—C37—C42 | −28.81 (19) |
| C4—P1—C16—C21 | 87.64 (16) | C31—P2—C37—C42 | −147.34 (16) |
| C1—P1—C16—C21 | −33.46 (17) | C22—P2—C37—C42 | 94.13 (18) |
| C10—P1—C16—C17 | 36.28 (17) | C25—P2—C37—C38 | 154.75 (16) |
| C4—P1—C16—C17 | −85.48 (16) | C31—P2—C37—C38 | 36.22 (19) |
| C1—P1—C16—C17 | 153.41 (15) | C22—P2—C37—C38 | −82.31 (18) |
| C21—C16—C17—C18 | −0.7 (3) | C42—C37—C38—C39 | 0.1 (3) |
| P1—C16—C17—C18 | 172.39 (15) | P2—C37—C38—C39 | 176.59 (17) |
| C16—C17—C18—C19 | 0.4 (3) | C37—C38—C39—C40 | 0.7 (3) |
| C17—C18—C19—C20 | 0.7 (3) | C38—C39—C40—C41 | −0.4 (4) |
| C18—C19—C20—C21 | −1.5 (3) | C39—C40—C41—C42 | −0.6 (3) |
| C19—C20—C21—C16 | 1.2 (3) | C40—C41—C42—C37 | 1.4 (3) |
| C17—C16—C21—C20 | −0.1 (3) | C38—C37—C42—C41 | −1.1 (3) |
| P1—C16—C21—C20 | −173.14 (14) | P2—C37—C42—C41 | −177.50 (15) |