Acta Cryst E CRYSTALLOGRAPHIC COMMUNICATIONS
ISSN 2056-9890

# The novel high-pressure/high-temperature compound $Co_{12}P_7$ determined from synchrotron data

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Received 10 August 2020
Accepted 17 September 2020

Edited by M. Weil, Vienna University of Technology, Austria

**Keywords:** crystal structure; synchrotron; high-pressure synthesis; cobalt phosphide; $M_{12}P_7$ phase.

**CCDC references**: 2032430; 2032429

**Supporting information**: this article has supporting information at journals.iucr.org/e

The structural properties of cobalt phosphides were investigated at high pressures and temperatures to better understand the behavior of metal-rich phosphides in Earth and planetary interiors. Using single-crystal X-ray diffraction synchrotron data and a laser-heated diamond anvil cell, we discovered a new high pressure–temperature (*HP–HT*) cobalt phosphide, $Co_{12}P_7$, dodecacobalt heptaphosphide, synthesized at 27 GPa and 1740 K, and at 48 GPa and 1790 K. $Co_{12}P_7$ adopts a structure initially proposed for $Cr_{12}P_7$ (space-group type $P\overline{6}$, $Z$ =1), consisting of chains of edge-sharing $CoP_5$ square pyramids and chains of corner-sharing $CoP_4$ tetrahedra. This arrangement leaves space for trigonal–prismatic channels running parallel to the $c$ axis. Coupled disordering of metal and phosphorus atoms has been observed in this structure for related $M_{12}P_7$ ($M$ = Cr, V) compounds, but all Co and P sites are ordered in $Co_{12}P_7$. All atomic sites in this crystal structure are situated on special positions. Upon decompression to ambient conditions, peak broadening and loss of reflections at high angles was observed, suggesting phase instability.

## 1. Chemical context

Cobalt phosphides have previously been examined in the context of binary phase relations and thermodynamics (Okamoto & Massalski, 1990; Schlesinger, 2002) and have gained attention for their unique conductive properties (Prins & Bussell, 2012; Popczun *et al.*, 2014; Pan *et al.*, 2016; Pramanik *et al.*, 2017), magnetic properties (Fujii *et al.*, 1988; Jeitschko *et al.*, 1978; Jeitschko & Jaberg, 1980; Reehuis & Jeitschko, 1989), and ability to store lanthanide cations (Jeitschko *et al.*, 1978). Cobalt phosphides also serve as structural analogs to iron-rich phosphides and sulfides in planetary core-forming alloys. Previous studies of CoP and $Co_2P$ indicate that their phase relations tend to precede in pressure the stability of isostructural Fe-phosphides and Fe-sulfides (Rundqvist, 1960; Ellner & Mittemeijer, 2001; Dera *et al.*, 2008; Tateno *et al.*, 2019; Rundqvist, 1962; Ono & Kikegawa, 2006; Ono *et al.* 2008). Hence, understanding the behavior of cobalt phosphides at high pressures provides insight into the ultra-high pressure behavior of iron sulfides and phosphides.

There are few structures reported in the literature for transition-metal phosphides with the composition $M_{12}P_7$. Baurecht *et al.* (1971) first examined $Cr_{12}P_7$ and determined that it adopts a hexagonal lattice with space group $P\overline{6}$, $Z$ = 1.

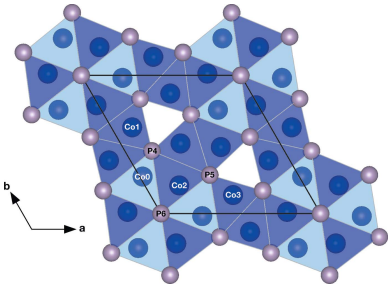

Table 1
Selected structural parameters for $Co_{12}P_7$ at 48 GPa.

| Group | Maximal bond length (Å) | minimal bond length (Å) | Polyhedron volume (Å$^3$) | Distortion index |
|---|---|---|---|---|
| $CoP_4$ (Co0—P4, —P5, —P6) | 2.102 (2) | 2.063 (2) | 4.5433 | 0.00656 |
| $CoP_5$ (Co1—P4, —P5) | 2.220 (4) | 2.147 (4) | 8.1257 | 0.01085 |
| $CoP_5$ (Co2—P4, —P5, —P6) | 2.317 (2) | 2.197 (4) | 9.0766 | 0.01432 |
| $CoP_5$ (Co3—P4, —P5) | 2.219 (3) | 2.194 (3) | 8.3239 | 0.00514 |

The structure consists of columns of alternating tetrahedral and pyramidal polyhedra and columns of stacked triangular–prismatic polyhedra extending along the *c*-axis direction. Chromium atoms occupy half of all possible tetrahedral and pyramidal sites while the triangular–prismatic sites are empty (Baurecht *et al.*, 1971). The polyhedra in the unit cell can be described as $Cr_9{}^{P}Cr_3{}^{T}[]_2{}^{Pr}P_7$ (P = pyramidal, T = tetrahedral, Pr = trigonal–prismatic, [] = empty site) (Maaref *et al.*, 1981). Coupled disordering of two half-atoms of the corresponding metal with two half-atoms of phosphorus within the tetrahedral and pyramidal sites has been observed in this structure for compounds $Th_7S_{12}$, $V_{12}P_7$, and $Cr_{12}P_7$, increasing the symmetry to the $P6_3/m$ space group (Zachariasen, 1949; Olofsson & Ganglberger 1970; Chun & Carpenter, 1979).

At ambient conditions the $M_{12}P_7$ composition is not observed in the binary systems with *M* = Co, Ni, Fe. Dhahri (1996) concluded that $Co_{12}P_7$, $Ni_{12}P_7$ and $Fe_{12}P_7$ do not occur in the $Cr_{12}P_7$ structure type at ambient conditions because, unlike Cr and V, the elements Co, Ni and Fe do not preferentially occupy pyramidal sites. In support of this conclusion, the $Zn_2Fe_{12}P_7$ structure type ($P\overline{6}$, $Z = 1$) with many structural similarities to the $Cr_{12}P_7$ structure type, has been observed in $Ln_2M_{12}P_7$ (*Ln* = rare-earth element; *M* = Co, Ni, Fe) compounds where the pyramidal-to-tetrahedral site ratio is 1:3 (Jeitschko *et al.*, 1978; Jeitschko & Jaberg, 1980; Reehuis & Jeitschko, 1989). Ordering is present in the Co-, Fe-, Ni-rich $Zn_2Fe_{12}P_7$ isomorphs (Jeitschko *et al.*, 1984). No other structure types for the composition $M_{12}P_7$ (*M* = Co, Ni, Fe) have been reported so far.

The effect of pressure and temperature on stabilizing Co in both the tetrahedral and pyramidal sites and ordering of Co and P in the $Cr_{12}P_7$-type structure has not been examined previously. In the current study, we report the synthesis of a $Co_{12}P_7$ phase at 27 GPa and 1750 K, and at 48 GPa and 1790 K; both phases are isostructural and crystallize in space group $P\overline{6}$. Structure refinements revealed that Co and P sites are ordered in the high *P*–*T* structure and Co atoms occupy tetrahedral and pyramidal coordinations. Using single-crystal diffraction techniques, we report refined atomic coordinate sites of $Co_{12}P_7$ at 48 GPa and 15 GPa.

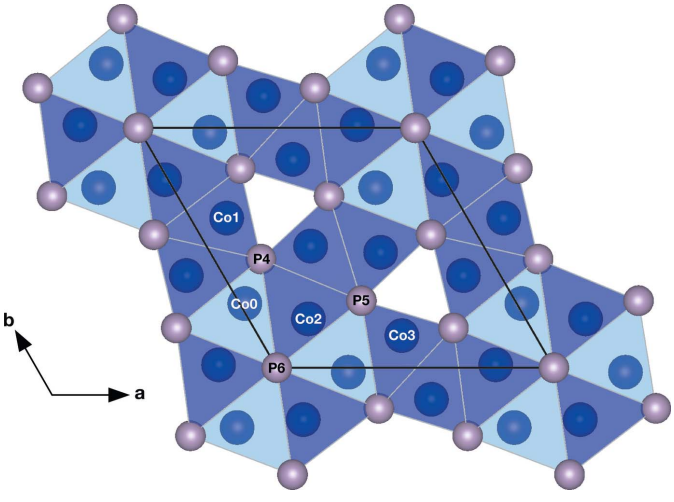


Figure 1
Crystal structure of $Co_{12}P_7$ based on the 48 GPa data set with atoms of the asymmetric unit labeled. $CoP_4$ tetrahedra are shaded in cyan and $CoP_5$ square pyramids are shaded in violet.

## 2. Structural commentary

Refinement of the structure confirms that $Co_{12}P_7$ assumes the ordered $Cr_{12}P_7$ structure type (Baurecht *et al.*, 1971; Chun & Carpenter, 1979). Two of the Co sites (Co0, Co1) occupy Wyckoff position 3 *j* (point group symmetry *m*..), the other two Co sites (Co2, Co3) Wyckoff position 3 *k* (*m*..), one P site (P5) Wyckoff position 3 *j*, one P site (P4) Wyckoff position 3 *k*, and one P site (P6) Wyckoff position 1 *a* ($\overline{6}$..). The Co sites occupy tetrahedral (cyan) and pyramidal (violet) sites as imaged in Fig. 1. Chains of edge-sharing $CoP_5$ square pyramids and chains of corner-sharing $CoP_4$ tetrahedra build up the framework with trigonal–prismatic channels running parallel to the *c* axis.

Ranges of interatomic Co—P distances and polyhedral volumes are provided in Table 1 and Fig. 2 with $CoP_4$ tetrahedra represented by a cyan polyhedron and $CoP_5$ pyramids represented by violet polyhedra. Co0 atoms occupy a distorted tetrahedral site with one P atom at a short distance, two at

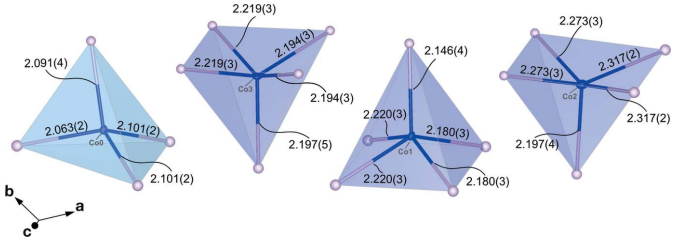


Figure 2
Co—P polyhedra as observed in the $Co_{12}P_7$ structure (48 GPa data set) showing varying degrees of volume and distortion, quantified in Table 1. $CoP_4$ tetrahedra are shaded in cyan and $CoP_5$ square pyramids are shaded in violet. Displacement ellipsoids are drawn at the 50% probability level.

**Table 2**
Experimental details.

| | 48 GPa | 15 GPa |
|---|---|---|
| Crystal data | | |
| Chemical formula | $Co_{12}P_7$ | $Co_{12}P_7$ |
| $M_r$ | 923.95 | 923.95 |
| Crystal system, space group | Hexagonal, $P\overline{6}$ | Hexagonal, $P\overline{6}$ |
| Temperature (K) | 293 | 293 |
| $a$, $c$ (Å) | 7.9700 (14), 3.2034 (4) | 8.253 (5), 3.2902 (18) |
| $V$ (Å$^3$) | 176.22 (7) | 194.1 (3) |
| $Z$ | 1 | 1 |
| Radiation type | Synchrotron, λ = 0.29521 Å | Synchrotron, λ = 0.3344 Å |
| $\mu$ (mm$^{-1}$) | 2.47 | 3.17 |
| Crystal size (mm) | 0.01 × 0.01 × 0.01 | 0.01 × 0.01 × 0.01 |
| Data collection | | |
| Diffractometer | 13IDD @ APS | 13BMD @ APS |
| Absorption correction | Multi-scan (*CrysAlis PRO*; Rigaku OD, 2018) | Multi-scan (*CrysAlis PRO*; Rigaku OD, 2018) |
| $T_{min}$, $T_{max}$ | 0.789, 1.000 | 0.546, 1.000 |
| No. of measured, independent and observed [$I > 2\sigma(I)$] reflections | 336, 292, 279 | 592, 321, 253 |
| $R_{int}$ | 0.006 | 0.055 |
| (sin $\theta/\lambda)_{max}$ (Å$^{-1}$) | 0.874 | 0.762 |
| Refinement | | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, $S$ | 0.037, 0.096, 1.12 | 0.053, 0.105, 1.11 |
| No. of reflections | 292 | 321 |
| No. of parameters | 32 | 32 |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 2.35, −1.81 | 1.70, −1.74 |
| Absolute structure | Flack $x$ determined using 75 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013) | Flack $x$ determined using 78 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013) |
| Absolute structure parameter | 0.42 (6) | 0.4 (2) |

Computer programs: *CrysAlis PRO* (Rigaku OD, 2018), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2014/7* (Sheldrick, 2015*b*), *VESTA* (Momma & Izumi, 2011) and *publCIF* (Westrip, 2010).

intermediate distances and one at a long distance (Table 1, Fig. 2). Co1 and Co2 atoms occupy square pyramids with two intermediate and two long interatomic distances at the base. Co3 atoms occupy a less distorted square pyramid with two elongated and two truncated bonds at the base (Fig. 2). Interatomic distances at 48 GPa range from 2.063 (2)–2.102 (2) Å in the tetrahedral polyhedra, 2.147 (4)–2.220 (4) Å for Co1—P polyhedra, 2.197 (4)–2.317 (2) Å for Co2—P polyhedra and 2.194 (3)–2.219 (3) Å for Co3—P polyhedra (Table 1). These interatomic distances are comparable to those observed in $Co_2P$ and CoP (Rundqvist 1960, 1962).

A grain of $Co_{12}P_7$ was decompressed to ambient conditions where 44 total reflections were identified in reciprocal space and indexed to a unit cell of $a$ = 8.47 (1) Å, $c$ = 3.37 (1) Å. These unit-cell parameters are in agreement with the pressure–volume trend observed, but peak broadening and loss of reflections at high angles may reflect the onset of phase instability on decompression.

## 3. Synthesis and crystallization

The synthesis of $Co_{12}P_7$ was performed at high pressures and temperatures in a laser-heated diamond anvil cell (LHDAC). Two samples were loaded for this study in which $Co_{12}P_7$ was synthesized at 26.9 (8) GPa and 1740 (110) K and 48.2 (5) GPa and 1790 (200) K, respectively. Pressure was generated in BX-90-type (70° angular opening) diamond anvil cells (DACs) with 300 µm culet, Boehler–Almax type diamonds and seats. Co–P samples and a ruby sphere for pressure calibration were loaded into a sample chamber drilled from a rhenium gasket. The chamber was subsequently filled with compressed neon gas (Rivers *et al.*, 2008). Pressure was determined using the ruby fluorescence scale and the Ne equation of state (Mao & Bell, 1976; Fei *et al.*, 2007).

Samples were heated from both sides with 100W Yb-doped fiber lasers at beamline 13-ID-D (GeoSoilEnviroCARS) of the Advanced Photon Source (APS), Argonne National Laboratory. Heating cycles typically lasted ∼15 minutes at target temperatures prior to quench. The lasers were shaped with ∼15 µm flat tops and temperature was measured spectroradiometrically from a 6 µm central region of the laser heated spot using a gray body approximation (Heinz & Jeanloz, 1987). Axial temperature gradients through the sample were accounted for by applying a 3% correction on temperature measurements (Campbell *et al.*, 2007, 2009).

Upon quench from high temperatures, high-pressure samples consisted of agglomerates of $Co_{12}P_7$ and *Pnma* $Co_2P$ (Rundqvist, 1960) crystals of variable grain sizes up to ∼5 µm in diameter. Grains of target phases were identified in reciprocal space and sorted out from the scattering contribution of other grains, neon and diamond. Diffraction data were processed using Dioptas (Prescher & Prakapenka, 2015) and *CrysAlis Pro* (Rigaku OD, 2018). Decompression data were collected for both samples in two experimental stations; here we report two selected refinements of the $Co_{12}P_7$ structure at 48.2 (5) GPa and 15.4 (2) GPa.

## 4. Refinement

Crystal data, data collection and structure refinement details at 48 GPa and 15 GPa are summarized in Table 2.

Monochromatic X-ray diffraction measurements took place at beamlines 13-ID-D (2 μm x 3 μm beam, λ = 0.2952 Å) and 13-BM-D (5 μm × 8 μm beam, λ = 0.3344 Å) at APS (Table 2). Diffraction measurements were collected at synthesis pressures and upon decompression. At target pressure steps, 10 x 10 μm still image maps were collected in 2 μm steps around the heated region. At selected map locations exhibiting the largest crystallites, rotation images were collected spanning ±30° at a rate of 1s per 0.5° step.

Grains of $Co_{12}P_7$ identified in reciprocal space were indexed to a primitive hexagonal lattice. Analysis of systematic absences indicated space group $P\overline{6}$ with $Z = 1$. Two grains from distinct loadings and measured at different beamlines were selected for structural refinements as they showed the largest number of observed reflections and good statistical parameters (Table 2). Structure factors measured in microdiffraction in the LHDAC show some well-known limitations, such as limited resolution and redundancy, reflections overlapped by parasitic scattering, diamond diffraction (Loveday *et al.*, 1990) and, more notably, variable volume of illuminated crystal during rotation. As could be expected, we identified eight and five outlier reflections in the refinements for the 48 GPa and 15 GPa data sets, respectively, and omitted them in the final calculations. Based on the ratio 'observed reflections/refined parameters' and statistical tests (Hamilton, 1965), we concluded that the P sites should be refined with isotropic displacement parameters ($U_{iso}$) whereas the Co sites could be refined with anisotropic displacement parameters. After convergence, site occupancies of Co atoms and P atoms were released in alternate runs. Within uncertainty (< 1.2% for Co and < 1.3% for P), all sites are fully occupied.

## Funding information

Portions of this work were performed at GeoSoilEnviroCARS (The University of Chicago, Sector 13), Advanced Photon Source (APS), Argonne National Laboratory. GeoSoilEnviroCARS is supported by the National Science Foundation – Earth Sciences (EAR – 1634415) and Department of Energy – GeoSciences (DE-FG02–94ER14466). This research used resources of the Advanced Photon Source, a US Department of Energy (DOE) Office of Science User Facility operated for the DOE Office of Science by Argonne National Laboratory under Contract No. DE-AC02–06CH11357. This material is based upon work supported by a National Science Foundation Graduate Research Fellowship to CZ. This work was also supported by the National Science Foundation by grant EAR – 1651017 to AC.

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# supporting information

*Acta Cryst.* (2020). E**76**, 1665-1668 [https://doi.org/10.1107/S2056989020012657]

## The novel high-pressure/high-temperature compound $Co_{12}P_7$ determined from synchrotron data

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### Computing details

For both structures, data collection: *CrysAlis PRO* (Rigaku OD, 2018); cell refinement: *CrysAlis PRO* (Rigaku OD, 2018); data reduction: *CrysAlis PRO* (Rigaku OD, 2018); program(s) used to solve structure: SHELXT (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2014/7* (Sheldrick, 2015b); molecular graphics: *VESTA* (Momma & Izumi, 2011); software used to prepare material for publication: *publCIF* (Westrip, 2010).

### Dodecacobalt heptaphosphide (Co12P7_at_48GPa)

*Crystal data*

$Co_{12}P_7$
$M_r$ = 923.95
Hexagonal, $P\bar{6}$
$a$ = 7.9700 (14) Å
$c$ = 3.2034 (4) Å
$V$ = 176.22 (7) Å$^3$
$Z$ = 1
$F(000)$ = 429
$D_x$ = 8.706 Mg m$^{-3}$
Synchrotron radiation, $\lambda$ = 0.29521 Å
Cell parameters from 292 reflections
$\theta$ = 2.3–14.9°
$\mu$ = 2.47 mm$^{-1}$
$T$ = 293 K
Irregular, black
0.01 × 0.01 × 0.01 mm

*Data collection*

13IDD @ APS diffractometer
Radiation source: synchrotron
$\omega$ scans
Absorption correction: multi-scan (*CrysAlisPro*; Rigaku OD, 2018)
$T_{min}$ = 0.789, $T_{max}$ = 1.000
336 measured reflections
292 independent reflections
279 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.006
$\theta_{max}$ = 15.0°, $\theta_{min}$ = 2.1°
$h$ = −6→8
$k$ = −10→9
$l$ = −5→5

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.096
$S$ = 1.12
292 reflections
32 parameters
0 restraints
$w = 1/[\sigma^2(F_o^2) + (0.0802P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 2.35 e Å$^{-3}$
$\Delta\rho_{min}$ = −1.81 e Å$^{-3}$
Absolute structure: Flack $x$ determined using 75 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: 0.42 (6)

*Special details*

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

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

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Co0 | 0.0185 (3) | 0.2676 (3) | 0.0000 | 0.0047 (4) |
| Co1 | 0.1313 (3) | 0.6239 (3) | 0.0000 | 0.0047 (4) |
| Co2 | 0.2161 (3) | 0.2037 (4) | 0.5000 | 0.0071 (4) |
| Co3 | 0.5185 (3) | 0.1341 (3) | 0.5000 | 0.0051 (4) |
| P4 | 0.1693 (5) | 0.4529 (5) | 0.5000 | 0.0062 (6)* |
| P5 | 0.4454 (5) | 0.2795 (6) | 0.0000 | 0.0050 (6)* |
| P6 | 0.0000 | 0.0000 | 0.0000 | 0.0069 (9)* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Co0 | 0.0044 (8) | 0.0030 (8) | 0.0062 (5) | 0.0015 (7) | 0.000 | 0.000 |
| Co1 | 0.0038 (8) | 0.0024 (7) | 0.0071 (8) | 0.0009 (6) | 0.000 | 0.000 |
| Co2 | 0.0081 (8) | 0.0069 (9) | 0.0079 (6) | 0.0049 (7) | 0.000 | 0.000 |
| Co3 | 0.0038 (8) | 0.0028 (8) | 0.0069 (7) | 0.0005 (6) | 0.000 | 0.000 |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Co0—P6 | 2.0629 (18) | Co2—Co3 | 2.730 (2) |
| Co0—P5$^{i}$ | 2.091 (4) | Co3—P5$^{xi}$ | 2.194 (3) |
| Co0—P4 | 2.102 (2) | Co3—P5$^{xii}$ | 2.194 (3) |
| Co0—P4$^{ii}$ | 2.102 (2) | Co3—P4$^{viii}$ | 2.197 (5) |
| Co0—Co3$^{iii}$ | 2.458 (2) | Co3—P5$^{vii}$ | 2.218 (3) |
| Co0—Co3$^{i}$ | 2.458 (2) | Co3—P5 | 2.219 (3) |
| Co0—Co2$^{ii}$ | 2.4710 (19) | Co3—Co0$^{viii}$ | 2.458 (2) |
| Co0—Co2 | 2.4710 (19) | Co3—Co0$^{ix}$ | 2.458 (2) |
| Co0—Co2$^{iii}$ | 2.497 (2) | Co3—Co3$^{xii}$ | 2.474 (3) |
| Co0—Co2$^{i}$ | 2.497 (2) | Co3—Co3$^{xiii}$ | 2.475 (3) |
| Co0—Co1 | 2.514 (3) | Co3—Co1$^{viii}$ | 2.578 (2) |
| Co0—Co1$^{iv}$ | 2.515 (2) | Co3—Co1$^{ix}$ | 2.578 (2) |
| Co1—P5$^{v}$ | 2.147 (4) | P4—Co0$^{vii}$ | 2.102 (2) |
| Co1—P4$^{v}$ | 2.180 (3) | P4—Co1$^{x}$ | 2.180 (3) |
| Co1—P4$^{vi}$ | 2.180 (3) | P4—Co1$^{iv}$ | 2.180 (3) |
| Co1—P4$^{ii}$ | 2.220 (3) | P4—Co3$^{i}$ | 2.197 (5) |
| Co1—P4 | 2.220 (3) | P4—Co1$^{vii}$ | 2.220 (3) |
| Co1—Co0$^{v}$ | 2.515 (2) | P4—P4$^{iv}$ | 2.674 (6) |
| Co1—Co1$^{v}$ | 2.546 (3) | P4—P4$^{v}$ | 2.674 (6) |
| Co1—Co1$^{iv}$ | 2.546 (3) | P5—Co0$^{viii}$ | 2.091 (4) |
| Co1—Co3$^{iii}$ | 2.578 (2) | P5—Co1$^{iv}$ | 2.147 (4) |

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|---|---|---|---|
| Co1—Co3$^{i}$ | 2.578 (2) | P5—Co3$^{xiii}$ | 2.194 (3) |
| Co1—Co2$^{v}$ | 2.639 (2) | P5—Co3$^{xiv}$ | 2.194 (3) |
| Co2—P4 | 2.197 (4) | P5—Co3$^{ii}$ | 2.218 (3) |
| Co2—P5 | 2.273 (3) | P5—Co2$^{ii}$ | 2.273 (3) |
| Co2—P5$^{vii}$ | 2.273 (3) | P6—Co0$^{i}$ | 2.0629 (18) |
| Co2—P6 | 2.3174 (17) | P6—Co0$^{viii}$ | 2.0629 (18) |
| Co2—P6$^{vii}$ | 2.3174 (17) | P6—Co2$^{xv}$ | 2.3174 (17) |
| Co2—Co0$^{vii}$ | 2.4710 (19) | P6—Co2$^{viii}$ | 2.3174 (17) |
| Co2—Co0$^{viii}$ | 2.497 (2) | P6—Co2$^{ii}$ | 2.3174 (17) |
| Co2—Co0$^{ix}$ | 2.497 (2) | P6—Co2$^{iii}$ | 2.3175 (17) |
| Co2—Co1$^{x}$ | 2.639 (2) | P6—Co2$^{i}$ | 2.3175 (17) |
| Co2—Co1$^{iv}$ | 2.639 (2) | | |

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|---|---|---|---|
| P6—Co0—P5$^{i}$ | 96.84 (13) | P4—Co2—Co3 | 138.57 (14) |
| P6—Co0—P4 | 116.54 (11) | P5—Co2—Co3 | 51.66 (8) |
| P5$^{i}$—Co0—P4 | 114.33 (11) | P5$^{vii}$—Co2—Co3 | 51.66 (8) |
| P6—Co0—P4$^{ii}$ | 116.54 (11) | P6—Co2—Co3 | 106.26 (8) |
| P5$^{i}$—Co0—P4$^{ii}$ | 114.33 (11) | P6$^{vii}$—Co2—Co3 | 106.26 (8) |
| P4—Co0—P4$^{ii}$ | 99.31 (14) | Co0$^{vii}$—Co2—Co3 | 139.47 (4) |
| P6—Co0—Co3$^{iii}$ | 126.74 (6) | Co0—Co2—Co3 | 139.47 (4) |
| P5$^{i}$—Co0—Co3$^{iii}$ | 57.69 (9) | Co0$^{viii}$—Co2—Co3 | 55.89 (7) |
| P4—Co0—Co3$^{iii}$ | 116.61 (12) | Co0$^{ix}$—Co2—Co3 | 55.89 (7) |
| P4$^{ii}$—Co0—Co3$^{iii}$ | 56.96 (11) | Co1$^{x}$—Co2—Co3 | 96.63 (8) |
| P6—Co0—Co3$^{i}$ | 126.74 (6) | Co1$^{iv}$—Co2—Co3 | 96.63 (8) |
| P5$^{i}$—Co0—Co3$^{i}$ | 57.69 (9) | P5$^{xi}$—Co3—P5$^{xii}$ | 93.78 (15) |
| P4—Co0—Co3$^{i}$ | 56.96 (11) | P5$^{xi}$—Co3—P4$^{viii}$ | 107.43 (14) |
| P4$^{ii}$—Co0—Co3$^{i}$ | 116.61 (12) | P5$^{xii}$—Co3—P4$^{viii}$ | 107.43 (14) |
| Co3$^{iii}$—Co0—Co3$^{i}$ | 81.31 (9) | P5$^{xi}$—Co3—P5$^{vii}$ | 77.38 (14) |
| P6—Co0—Co2$^{ii}$ | 60.69 (6) | P5$^{xii}$—Co3—P5$^{vii}$ | 146.69 (16) |
| P5$^{i}$—Co0—Co2$^{ii}$ | 129.60 (8) | P4$^{viii}$—Co3—P5$^{vii}$ | 105.86 (14) |
| P4—Co0—Co2$^{ii}$ | 116.07 (13) | P5$^{xi}$—Co3—P5 | 146.69 (16) |
| P4$^{ii}$—Co0—Co2$^{ii}$ | 56.73 (11) | P5$^{xii}$—Co3—P5 | 77.38 (14) |
| Co3$^{iii}$—Co0—Co2$^{ii}$ | 98.20 (5) | P4$^{viii}$—Co3—P5 | 105.86 (14) |
| Co3$^{i}$—Co0—Co2$^{ii}$ | 170.85 (9) | P5$^{vii}$—Co3—P5 | 92.44 (15) |
| P6—Co0—Co2 | 60.69 (6) | P5$^{xi}$—Co3—Co0$^{viii}$ | 160.35 (15) |
| P5$^{i}$—Co0—Co2 | 129.60 (8) | P5$^{xii}$—Co3—Co0$^{viii}$ | 89.46 (9) |
| P4—Co0—Co2 | 56.73 (11) | P4$^{viii}$—Co3—Co0$^{viii}$ | 53.31 (7) |
| P4$^{ii}$—Co0—Co2 | 116.07 (13) | P5$^{vii}$—Co3—Co0$^{viii}$ | 109.66 (12) |
| Co3$^{iii}$—Co0—Co2 | 170.85 (9) | P5—Co3—Co0$^{viii}$ | 52.82 (11) |
| Co3$^{i}$—Co0—Co2 | 98.20 (5) | P5$^{xi}$—Co3—Co0$^{ix}$ | 89.46 (9) |
| Co2$^{ii}$—Co0—Co2 | 80.81 (8) | P5$^{xii}$—Co3—Co0$^{ix}$ | 160.35 (15) |
| P6—Co0—Co2$^{iii}$ | 60.19 (6) | P4$^{viii}$—Co3—Co0$^{ix}$ | 53.31 (7) |
| P5$^{i}$—Co0—Co2$^{iii}$ | 58.60 (11) | P5$^{vii}$—Co3—Co0$^{ix}$ | 52.82 (11) |
| P4—Co0—Co2$^{iii}$ | 169.97 (10) | P5—Co3—Co0$^{ix}$ | 109.66 (12) |
| P4$^{ii}$—Co0—Co2$^{iii}$ | 90.40 (8) | Co0$^{viii}$—Co3—Co0$^{ix}$ | 81.32 (9) |
| Co3$^{iii}$—Co0—Co2$^{iii}$ | 66.85 (7) | P5$^{xi}$—Co3—Co3$^{xii}$ | 56.36 (10) |
| Co3$^{i}$—Co0—Co2$^{iii}$ | 116.27 (10) | P5$^{xii}$—Co3—Co3$^{xii}$ | 56.36 (10) |
| Co2$^{ii}$—Co0—Co2$^{iii}$ | 71.44 (10) | P4$^{viii}$—Co3—Co3$^{xii}$ | 151.84 (16) |

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| Co2—Co0—Co2$^{iii}$ | 120.88 (10) | P5$^{vii}$—Co3—Co3$^{xii}$ | 93.38 (11) |
| P6—Co0—Co2$^{i}$ | 60.19 (6) | P5—Co3—Co3$^{xii}$ | 93.38 (11) |
| P5$^{i}$—Co0—Co2$^{i}$ | 58.60 (11) | Co0$^{viii}$—Co3—Co3$^{xii}$ | 138.36 (5) |
| P4—Co0—Co2$^{i}$ | 90.40 (8) | Co0$^{ix}$—Co3—Co3$^{xii}$ | 138.36 (5) |
| P4$^{ii}$—Co0—Co2$^{i}$ | 169.97 (10) | P5$^{xi}$—Co3—Co3$^{xiii}$ | 93.99 (11) |
| Co3$^{iii}$—Co0—Co2$^{i}$ | 116.27 (10) | P5$^{xii}$—Co3—Co3$^{xiii}$ | 93.99 (11) |
| Co3$^{i}$—Co0—Co2$^{i}$ | 66.85 (7) | P4$^{viii}$—Co3—Co3$^{xiii}$ | 148.16 (16) |
| Co2$^{ii}$—Co0—Co2$^{i}$ | 120.88 (10) | P5$^{vii}$—Co3—Co3$^{xiii}$ | 55.42 (11) |
| Co2—Co0—Co2$^{i}$ | 71.44 (10) | P5—Co3—Co3$^{xiii}$ | 55.42 (11) |
| Co2$^{iii}$—Co0—Co2$^{i}$ | 79.79 (9) | Co0$^{viii}$—Co3—Co3$^{xiii}$ | 105.12 (10) |
| P6—Co0—Co1 | 165.52 (9) | Co0$^{ix}$—Co3—Co3$^{xiii}$ | 105.12 (10) |
| P5$^{i}$—Co0—Co1 | 97.64 (13) | Co3$^{xii}$—Co3—Co3$^{xiii}$ | 60.0 |
| P4—Co0—Co1 | 56.65 (9) | P5$^{xi}$—Co3—Co1$^{viii}$ | 107.55 (12) |
| P4$^{ii}$—Co0—Co1 | 56.65 (9) | P5$^{xii}$—Co3—Co1$^{viii}$ | 52.72 (10) |
| Co3$^{iii}$—Co0—Co1 | 62.44 (6) | P4$^{viii}$—Co3—Co1$^{viii}$ | 54.71 (8) |
| Co3$^{i}$—Co0—Co1 | 62.44 (6) | P5$^{vii}$—Co3—Co1$^{viii}$ | 160.55 (15) |
| Co2$^{ii}$—Co0—Co1 | 109.16 (7) | P5—Co3—Co1$^{viii}$ | 92.62 (8) |
| Co2—Co0—Co1 | 109.16 (7) | Co0$^{viii}$—Co3—Co1$^{viii}$ | 59.83 (7) |
| Co2$^{iii}$—Co0—Co1 | 128.86 (7) | Co0$^{ix}$—Co3—Co1$^{viii}$ | 107.89 (10) |
| Co2$^{i}$—Co0—Co1 | 128.86 (7) | Co3$^{xii}$—Co3—Co1$^{viii}$ | 105.04 (11) |
| P6—Co0—Co1$^{iv}$ | 104.70 (9) | Co3$^{xiii}$—Co3—Co1$^{viii}$ | 140.36 (4) |
| P5$^{i}$—Co0—Co1$^{iv}$ | 158.46 (14) | P5$^{xi}$—Co3—Co1$^{ix}$ | 52.72 (10) |
| P4—Co0—Co1$^{iv}$ | 55.49 (9) | P5$^{xii}$—Co3—Co1$^{ix}$ | 107.55 (12) |
| P4$^{ii}$—Co0—Co1$^{iv}$ | 55.49 (9) | P4$^{viii}$—Co3—Co1$^{ix}$ | 54.71 (8) |
| Co3$^{iii}$—Co0—Co1$^{iv}$ | 107.42 (7) | P5$^{vii}$—Co3—Co1$^{ix}$ | 92.62 (8) |
| Co3$^{i}$—Co0—Co1$^{iv}$ | 107.42 (7) | P5—Co3—Co1$^{ix}$ | 160.55 (15) |
| Co2$^{ii}$—Co0—Co1$^{iv}$ | 63.90 (7) | Co0$^{viii}$—Co3—Co1$^{ix}$ | 107.89 (10) |
| Co2—Co0—Co1$^{iv}$ | 63.90 (7) | Co0$^{ix}$—Co3—Co1$^{ix}$ | 59.83 (7) |
| Co2$^{iii}$—Co0—Co1$^{iv}$ | 133.74 (7) | Co3$^{xii}$—Co3—Co1$^{ix}$ | 105.04 (11) |
| Co2$^{i}$—Co0—Co1$^{iv}$ | 133.74 (7) | Co3$^{xiii}$—Co3—Co1$^{ix}$ | 140.36 (4) |
| Co1—Co0—Co1$^{iv}$ | 60.82 (8) | Co1$^{viii}$—Co3—Co1$^{ix}$ | 76.82 (8) |
| P5$^{v}$—Co1—P4$^{v}$ | 108.68 (12) | P5$^{xi}$—Co3—Co2 | 130.38 (8) |
| P5$^{v}$—Co1—P4$^{vi}$ | 108.68 (12) | P5$^{xii}$—Co3—Co2 | 130.38 (8) |
| P4$^{v}$—Co1—P4$^{vi}$ | 94.55 (18) | P4$^{viii}$—Co3—Co2 | 82.57 (13) |
| P5$^{v}$—Co1—P4$^{ii}$ | 108.29 (12) | P5$^{vii}$—Co3—Co2 | 53.49 (10) |
| P4$^{v}$—Co1—P4$^{ii}$ | 143.01 (13) | P5—Co3—Co2 | 53.49 (10) |
| P4$^{vi}$—Co1—P4$^{ii}$ | 74.85 (14) | Co0$^{viii}$—Co3—Co2 | 57.26 (7) |
| P5$^{v}$—Co1—P4 | 108.29 (12) | Co0$^{ix}$—Co3—Co2 | 57.26 (7) |
| P4$^{v}$—Co1—P4 | 74.85 (14) | Co3$^{xii}$—Co3—Co2 | 125.59 (11) |
| P4$^{vi}$—Co1—P4 | 143.01 (13) | Co3$^{xiii}$—Co3—Co2 | 65.59 (11) |
| P4$^{ii}$—Co1—P4 | 92.36 (16) | Co1$^{viii}$—Co3—Co2 | 116.75 (8) |
| P5$^{v}$—Co1—Co0 | 89.08 (13) | Co1$^{ix}$—Co3—Co2 | 116.75 (8) |
| P4$^{v}$—Co1—Co0 | 127.10 (9) | Co0—P4—Co0$^{vii}$ | 99.31 (14) |
| P4$^{vi}$—Co1—Co0 | 127.10 (9) | Co0—P4—Co1$^{x}$ | 144.1 (2) |
| P4$^{ii}$—Co1—Co0 | 52.26 (8) | Co0$^{vii}$—P4—Co1$^{x}$ | 71.92 (7) |
| P4—Co1—Co0 | 52.26 (8) | Co0—P4—Co1$^{iv}$ | 71.92 (7) |
| P5$^{v}$—Co1—Co0$^{v}$ | 91.74 (12) | Co0$^{vii}$—P4—Co1$^{iv}$ | 144.1 (2) |
| P4$^{v}$—Co1—Co0$^{v}$ | 52.58 (9) | Co1$^{x}$—P4—Co1$^{iv}$ | 94.55 (17) |

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| P4$^{vi}$—Co1—Co0$^{v}$ | 52.58 (9) | Co0—P4—Co2 | 70.15 (11) |
| P4$^{ii}$—Co1—Co0$^{v}$ | 127.40 (9) | Co0$^{vii}$—P4—Co2 | 70.15 (11) |
| P4—Co1—Co0$^{v}$ | 127.40 (9) | Co1$^{x}$—P4—Co2 | 74.16 (12) |
| Co0—Co1—Co0$^{v}$ | 179.18 (8) | Co1$^{iv}$—P4—Co2 | 74.16 (12) |
| P5$^{v}$—Co1—Co1$^{v}$ | 151.31 (16) | Co0—P4—Co3$^{i}$ | 69.73 (11) |
| P4$^{v}$—Co1—Co1$^{v}$ | 55.38 (11) | Co0$^{vii}$—P4—Co3$^{i}$ | 69.73 (11) |
| P4$^{vi}$—Co1—Co1$^{v}$ | 55.38 (11) | Co1$^{x}$—P4—Co3$^{i}$ | 132.68 (9) |
| P4$^{ii}$—Co1—Co1$^{v}$ | 91.21 (10) | Co1$^{iv}$—P4—Co3$^{i}$ | 132.68 (9) |
| P4—Co1—Co1$^{v}$ | 91.21 (10) | Co2—P4—Co3$^{i}$ | 116.01 (16) |
| Co0—Co1—Co1$^{v}$ | 119.61 (8) | Co0—P4—Co1 | 71.09 (7) |
| Co0$^{v}$—Co1—Co1$^{v}$ | 59.56 (10) | Co0$^{vii}$—P4—Co1 | 140.9 (2) |
| P5$^{v}$—Co1—Co1$^{iv}$ | 148.69 (16) | Co1$^{x}$—P4—Co1 | 136.84 (16) |
| P4$^{v}$—Co1—Co1$^{iv}$ | 92.13 (10) | Co1$^{iv}$—P4—Co1 | 70.69 (9) |
| P4$^{vi}$—Co1—Co1$^{iv}$ | 92.13 (10) | Co2—P4—Co1 | 133.80 (8) |
| P4$^{ii}$—Co1—Co1$^{iv}$ | 53.93 (10) | Co3$^{i}$—P4—Co1 | 71.42 (12) |
| P4—Co1—Co1$^{iv}$ | 53.93 (10) | Co0—P4—Co1$^{vii}$ | 140.9 (2) |
| Co0—Co1—Co1$^{iv}$ | 59.61 (8) | Co0$^{vii}$—P4—Co1$^{vii}$ | 71.09 (7) |
| Co0$^{v}$—Co1—Co1$^{iv}$ | 119.56 (10) | Co1$^{x}$—P4—Co1$^{vii}$ | 70.69 (9) |
| Co1$^{v}$—Co1—Co1$^{iv}$ | 60.0 | Co1$^{iv}$—P4—Co1$^{vii}$ | 136.84 (17) |
| P5$^{v}$—Co1—Co3$^{iii}$ | 54.42 (8) | Co2—P4—Co1$^{vii}$ | 133.80 (8) |
| P4$^{v}$—Co1—Co3$^{iii}$ | 163.07 (13) | Co3$^{i}$—P4—Co1$^{vii}$ | 71.42 (12) |
| P4$^{vi}$—Co1—Co3$^{iii}$ | 92.51 (9) | Co1—P4—Co1$^{vii}$ | 92.36 (16) |
| P4$^{ii}$—Co1—Co3$^{iii}$ | 53.87 (11) | Co0—P4—P4$^{iv}$ | 125.14 (14) |
| P4—Co1—Co3$^{iii}$ | 107.88 (12) | Co0$^{vii}$—P4—P4$^{iv}$ | 125.14 (14) |
| Co0—Co1—Co3$^{iii}$ | 57.72 (8) | Co1$^{x}$—P4—P4$^{iv}$ | 53.25 (12) |
| Co0$^{v}$—Co1—Co3$^{iii}$ | 122.84 (8) | Co1$^{iv}$—P4—P4$^{iv}$ | 53.25 (12) |
| Co1$^{v}$—Co1—Co3$^{iii}$ | 139.67 (4) | Co2—P4—P4$^{iv}$ | 94.4 (2) |
| Co1$^{iv}$—Co1—Co3$^{iii}$ | 102.97 (11) | Co3$^{i}$—P4—P4$^{iv}$ | 149.6 (2) |
| P5$^{v}$—Co1—Co3$^{i}$ | 54.42 (8) | Co1—P4—P4$^{iv}$ | 87.91 (10) |
| P4$^{v}$—Co1—Co3$^{i}$ | 92.51 (9) | Co1$^{vii}$—P4—P4$^{iv}$ | 87.91 (10) |
| P4$^{vi}$—Co1—Co3$^{i}$ | 163.07 (13) | Co0—P4—P4$^{v}$ | 122.98 (14) |
| P4$^{ii}$—Co1—Co3$^{i}$ | 107.88 (12) | Co0$^{vii}$—P4—P4$^{v}$ | 122.98 (14) |
| P4—Co1—Co3$^{i}$ | 53.87 (11) | Co1$^{x}$—P4—P4$^{v}$ | 88.73 (10) |
| Co0—Co1—Co3$^{i}$ | 57.72 (8) | Co1$^{iv}$—P4—P4$^{v}$ | 88.73 (10) |
| Co0$^{v}$—Co1—Co3$^{i}$ | 122.84 (8) | Co2—P4—P4$^{v}$ | 154.4 (2) |
| Co1$^{v}$—Co1—Co3$^{i}$ | 139.67 (4) | Co3$^{i}$—P4—P4$^{v}$ | 89.6 (2) |
| Co1$^{iv}$—Co1—Co3$^{i}$ | 102.97 (11) | Co1—P4—P4$^{v}$ | 51.90 (11) |
| Co3$^{iii}$—Co1—Co3$^{i}$ | 76.82 (8) | Co1$^{vii}$—P4—P4$^{v}$ | 51.90 (11) |
| P5$^{v}$—Co1—Co2$^{v}$ | 55.58 (8) | P4$^{iv}$—P4—P4$^{v}$ | 60.0 |
| P4$^{v}$—Co1—Co2$^{v}$ | 53.20 (10) | Co0$^{viii}$—P5—Co1$^{iv}$ | 126.72 (19) |
| P4$^{vi}$—Co1—Co2$^{v}$ | 107.02 (11) | Co0$^{viii}$—P5—Co3$^{xiii}$ | 132.10 (9) |
| P4$^{ii}$—Co1—Co2$^{v}$ | 163.76 (12) | Co1$^{iv}$—P5—Co3$^{xiii}$ | 72.86 (12) |
| P4—Co1—Co2$^{v}$ | 94.83 (9) | Co0$^{viii}$—P5—Co3$^{xiv}$ | 132.10 (9) |
| Co0—Co1—Co2$^{v}$ | 123.33 (7) | Co1$^{iv}$—P5—Co3$^{xiv}$ | 72.86 (12) |
| Co0$^{v}$—Co1—Co2$^{v}$ | 57.23 (6) | Co3$^{xiii}$—P5—Co3$^{xiv}$ | 93.78 (15) |
| Co1$^{v}$—Co1—Co2$^{v}$ | 103.16 (10) | Co0$^{viii}$—P5—Co3$^{ii}$ | 69.48 (13) |
| Co1$^{iv}$—Co1—Co2$^{v}$ | 140.65 (5) | Co1$^{iv}$—P5—Co3$^{ii}$ | 133.45 (8) |
| Co3$^{iii}$—Co1—Co2$^{v}$ | 109.96 (9) | Co3$^{xiii}$—P5—Co3$^{ii}$ | 133.08 (18) |

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| Co3$^{i}$—Co1—Co2$^{v}$ | 65.62 (7) | Co3$^{xiv}$—P5—Co3$^{ii}$ | 68.22 (10) |
| P4—Co2—P5 | 103.71 (12) | Co0$^{viii}$—P5—Co3 | 69.48 (13) |
| P4—Co2—P5$^{vii}$ | 103.71 (12) | Co1$^{iv}$—P5—Co3 | 133.45 (8) |
| P5—Co2—P5$^{vii}$ | 89.59 (15) | Co3$^{xiii}$—P5—Co3 | 68.22 (10) |
| P4—Co2—P6 | 103.35 (9) | Co3$^{xiv}$—P5—Co3 | 133.08 (18) |
| P5—Co2—P6 | 85.20 (8) | Co3$^{ii}$—P5—Co3 | 92.44 (15) |
| P5$^{vii}$—Co2—P6 | 152.92 (13) | Co0$^{viii}$—P5—Co2 | 69.66 (13) |
| P4—Co2—P6$^{vii}$ | 103.35 (9) | Co1$^{iv}$—P5—Co2 | 73.26 (11) |
| P5—Co2—P6$^{vii}$ | 152.92 (13) | Co3$^{xiii}$—P5—Co2 | 78.50 (8) |
| P5$^{vii}$—Co2—P6$^{vii}$ | 85.20 (8) | Co3$^{xiv}$—P5—Co2 | 146.03 (19) |
| P6—Co2—P6$^{vii}$ | 87.44 (8) | Co3$^{ii}$—P5—Co2 | 139.1 (2) |
| P4—Co2—Co0$^{vii}$ | 53.12 (8) | Co3—P5—Co2 | 74.85 (8) |
| P5—Co2—Co0$^{vii}$ | 155.85 (14) | Co0$^{viii}$—P5—Co2$^{ii}$ | 69.66 (13) |
| P5$^{vii}$—Co2—Co0$^{vii}$ | 89.95 (7) | Co1$^{iv}$—P5—Co2$^{ii}$ | 73.25 (11) |
| P6—Co2—Co0$^{vii}$ | 105.40 (8) | Co3$^{xiii}$—P5—Co2$^{ii}$ | 146.03 (19) |
| P6$^{vii}$—Co2—Co0$^{vii}$ | 50.91 (5) | Co3$^{xiv}$—P5—Co2$^{ii}$ | 78.50 (8) |
| P4—Co2—Co0 | 53.12 (8) | Co3$^{ii}$—P5—Co2$^{ii}$ | 74.85 (8) |
| P5—Co2—Co0 | 89.95 (7) | Co3—P5—Co2$^{ii}$ | 139.1 (2) |
| P5$^{vii}$—Co2—Co0 | 155.85 (14) | Co2—P5—Co2$^{ii}$ | 89.59 (15) |
| P6—Co2—Co0 | 50.91 (5) | Co0$^{i}$—P6—Co0 | 120.0 |
| P6$^{vii}$—Co2—Co0 | 105.40 (8) | Co0$^{i}$—P6—Co0$^{viii}$ | 120.0 |
| Co0$^{vii}$—Co2—Co0 | 80.81 (8) | Co0—P6—Co0$^{viii}$ | 120.0 |
| P4—Co2—Co0$^{viii}$ | 140.08 (4) | Co0$^{i}$—P6—Co2$^{xv}$ | 69.24 (6) |
| P5—Co2—Co0$^{viii}$ | 51.74 (11) | Co0—P6—Co2$^{xv}$ | 136.27 (4) |
| P5$^{vii}$—Co2—Co0$^{viii}$ | 106.53 (11) | Co0$^{viii}$—P6—Co2$^{xv}$ | 68.40 (6) |
| P6—Co2—Co0$^{viii}$ | 50.57 (5) | Co0$^{i}$—P6—Co2$^{viii}$ | 69.24 (6) |
| P6$^{vii}$—Co2—Co0$^{viii}$ | 104.56 (10) | Co0—P6—Co2$^{viii}$ | 136.27 (4) |
| Co0$^{vii}$—Co2—Co0$^{viii}$ | 149.98 (11) | Co0$^{viii}$—P6—Co2$^{viii}$ | 68.40 (6) |
| Co0—Co2—Co0$^{viii}$ | 91.97 (7) | Co2$^{xv}$—P6—Co2$^{viii}$ | 87.45 (8) |
| P4—Co2—Co0$^{ix}$ | 140.08 (4) | Co0$^{i}$—P6—Co2 | 136.27 (4) |
| P5—Co2—Co0$^{ix}$ | 106.54 (11) | Co0—P6—Co2 | 68.40 (6) |
| P5$^{vii}$—Co2—Co0$^{ix}$ | 51.74 (11) | Co0$^{viii}$—P6—Co2 | 69.24 (6) |
| P6—Co2—Co0$^{ix}$ | 104.56 (10) | Co2$^{xv}$—P6—Co2 | 137.63 (3) |
| P6$^{vii}$—Co2—Co0$^{ix}$ | 50.57 (5) | Co2$^{viii}$—P6—Co2 | 77.49 (6) |
| Co0$^{vii}$—Co2—Co0$^{ix}$ | 91.97 (7) | Co0$^{i}$—P6—Co2$^{ii}$ | 136.27 (4) |
| Co0—Co2—Co0$^{ix}$ | 149.98 (11) | Co0—P6—Co2$^{ii}$ | 68.40 (6) |
| Co0$^{viii}$—Co2—Co0$^{ix}$ | 79.79 (9) | Co0$^{viii}$—P6—Co2$^{ii}$ | 69.24 (6) |
| P4—Co2—Co1$^{x}$ | 52.64 (9) | Co2$^{xv}$—P6—Co2$^{ii}$ | 77.49 (6) |
| P5—Co2—Co1$^{x}$ | 103.19 (12) | Co2$^{viii}$—P6—Co2$^{ii}$ | 137.64 (3) |
| P5$^{vii}$—Co2—Co1$^{x}$ | 51.16 (10) | Co2—P6—Co2$^{ii}$ | 87.44 (8) |
| P6—Co2—Co1$^{x}$ | 155.65 (9) | Co0$^{i}$—P6—Co2$^{iii}$ | 68.40 (6) |
| P6$^{vii}$—Co2—Co1$^{x}$ | 94.13 (4) | Co0—P6—Co2$^{iii}$ | 69.24 (6) |
| Co0$^{vii}$—Co2—Co1$^{x}$ | 58.87 (6) | Co0$^{viii}$—P6—Co2$^{iii}$ | 136.27 (4) |
| Co0—Co2—Co1$^{x}$ | 105.65 (9) | Co2$^{xv}$—P6—Co2$^{iii}$ | 77.49 (6) |
| Co0$^{viii}$—Co2—Co1$^{x}$ | 149.97 (10) | Co2$^{viii}$—P6—Co2$^{iii}$ | 137.63 (3) |
| Co0$^{ix}$—Co2—Co1$^{x}$ | 95.00 (6) | Co2—P6—Co2$^{iii}$ | 137.63 (3) |
| P4—Co2—Co1$^{iv}$ | 52.64 (9) | Co2$^{ii}$—P6—Co2$^{iii}$ | 77.49 (6) |
| P5—Co2—Co1$^{iv}$ | 51.16 (10) | Co0$^{i}$—P6—Co2$^{i}$ | 68.40 (6) |

| | | | |
|---|---|---|---|
| P5$^{vii}$—Co2—Co1$^{iv}$ | 103.19 (13) | Co0—P6—Co2$^{i}$ | 69.24 (6) |
| P6—Co2—Co1$^{iv}$ | 94.13 (4) | Co0$^{viii}$—P6—Co2$^{i}$ | 136.27 (4) |
| P6$^{vii}$—Co2—Co1$^{iv}$ | 155.65 (9) | Co2$^{xv}$—P6—Co2$^{i}$ | 137.63 (3) |
| Co0$^{vii}$—Co2—Co1$^{iv}$ | 105.65 (9) | Co2$^{viii}$—P6—Co2$^{i}$ | 77.49 (6) |
| Co0—Co2—Co1$^{iv}$ | 58.87 (6) | Co2—P6—Co2$^{i}$ | 77.49 (6) |
| Co0$^{viii}$—Co2—Co1$^{iv}$ | 95.00 (6) | Co2$^{ii}$—P6—Co2$^{i}$ | 137.63 (3) |
| Co0$^{ix}$—Co2—Co1$^{iv}$ | 149.97 (10) | Co2$^{iii}$—P6—Co2$^{i}$ | 87.44 (8) |
| Co1$^{x}$—Co2—Co1$^{iv}$ | 74.74 (7) | | |

Symmetry codes: (i) −*y*, *x*−*y*, *z*; (ii) *x*, *y*, *z*−1; (iii) −*y*, *x*−*y*, *z*−1; (iv) −*y*+1, *x*−*y*+1, *z*; (v) −*x*+*y*, −*x*+1, *z*; (vi) −*x*+*y*, −*x*+1, *z*−1; (vii) *x*, *y*, *z*+1; (viii) −*x*+*y*, −*x*, *z*; (ix) −*x*+*y*, −*x*, *z*+1; (x) −*y*+1, *x*−*y*+1, *z*+1; (xi) −*y*+1, *x*−*y*, *z*+1; (xii) −*y*+1, *x*−*y*, *z*; (xiii) −*x*+*y*+1, −*x*+1, *z*; (xiv) −*x*+*y*+1, −*x*+1, *z*−1; (xv) −*x*+*y*, −*x*, *z*−1.

**(Co12P7_at_15GPa)**

*Crystal data*

$Co_{12}P_7$
$M_r$ = 923.95
Hexagonal, $P\bar{6}$
*a* = 8.253 (5) Å
*c* = 3.2902 (18) Å
*V* = 194.1 (3) Å$^3$
*Z* = 1
*F*(000) = 429
$D_x$ = 7.905 Mg m$^{-3}$
Synchrotron radiation, $\lambda$ = 0.3344 Å
Cell parameters from 249 reflections
$\theta$ = 2.9–14.7°
$\mu$ = 3.17 mm$^{-1}$
*T* = 293 K
Irregular, black
0.01 × 0.01 × 0.01 mm

*Data collection*

13BMD @ APS diffractometer
Radiation source: synchrotron
/w scan
Absorption correction: multi-scan (*CrysAlisPro*; Rigaku OD, 2018)
$T_{min}$ = 0.546, $T_{max}$ = 1.000
592 measured reflections
321 independent reflections
253 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.055
$\theta_{max}$ = 14.8°, $\theta_{min}$ = 3.2°
*h* = −11→12
*k* = −9→8
*l* = −4→4

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.105
*S* = 1.11
321 reflections
32 parameters
0 restraints
$w = 1/[\sigma^2(F_o^2) + (0.0219P)^2 + 2.8589P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 1.70 e Å$^{-3}$
$\Delta\rho_{min}$ = −1.74 e Å$^{-3}$
Absolute structure: Flack *x* determined using 78 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: 0.4 (2)

*Special details*

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

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

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Co0 | 0.0153 (6) | 0.2651 (6) | 0.0000 | 0.0114 (8) |
| Co1 | 0.1320 (7) | 0.6234 (7) | 0.0000 | 0.0123 (9) |
| Co2 | 0.2135 (6) | 0.2038 (8) | 0.5000 | 0.0151 (9) |
| Co3 | 0.5195 (7) | 0.1363 (7) | 0.5000 | 0.0107 (9) |
| P4 | 0.1656 (11) | 0.4503 (11) | 0.5000 | 0.0102 (15)* |
| P5 | 0.4425 (12) | 0.2809 (13) | 0.0000 | 0.0086 (15)* |
| P6 | 0.0000 | 0.0000 | 0.0000 | 0.012 (3)* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Co0 | 0.014 (2) | 0.016 (2) | 0.0072 (18) | 0.009 (2) | 0.000 | 0.000 |
| Co1 | 0.019 (2) | 0.016 (2) | 0.003 (2) | 0.0101 (18) | 0.000 | 0.000 |
| Co2 | 0.024 (2) | 0.020 (3) | 0.005 (2) | 0.014 (2) | 0.000 | 0.000 |
| Co3 | 0.011 (2) | 0.012 (2) | 0.008 (2) | 0.0052 (16) | 0.000 | 0.000 |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Co0—P6 | 2.128 (5) | Co2—Co1$^{iv}$ | 2.731 (5) |
| Co0—P5$^{i}$ | 2.148 (10) | Co2—Co3 | 2.846 (7) |
| Co0—P4 | 2.165 (6) | Co3—P5$^{xi}$ | 2.263 (7) |
| Co0—P4$^{ii}$ | 2.165 (6) | Co3—P5$^{xii}$ | 2.263 (7) |
| Co0—Co3$^{iii}$ | 2.538 (5) | Co3—P4$^{viii}$ | 2.266 (10) |
| Co0—Co3$^{i}$ | 2.538 (5) | Co3—P5$^{vii}$ | 2.301 (8) |
| Co0—Co2$^{ii}$ | 2.543 (6) | Co3—P5 | 2.301 (8) |
| Co0—Co2 | 2.543 (6) | Co3—Co3$^{xiii}$ | 2.536 (9) |
| Co0—Co2$^{iii}$ | 2.571 (6) | Co3—Co3$^{xii}$ | 2.536 (9) |
| Co0—Co2$^{i}$ | 2.571 (6) | Co3—Co0$^{viii}$ | 2.538 (5) |
| Co0—Co1 | 2.612 (7) | Co3—Co0$^{ix}$ | 2.538 (5) |
| Co0—Co1$^{iv}$ | 2.634 (7) | Co3—Co1$^{viii}$ | 2.674 (5) |
| Co1—P5$^{v}$ | 2.202 (10) | Co3—Co1$^{ix}$ | 2.674 (5) |
| Co1—P4$^{v}$ | 2.266 (7) | P4—Co0$^{vii}$ | 2.165 (6) |
| Co1—P4$^{vi}$ | 2.266 (7) | P4—Co1$^{x}$ | 2.266 (7) |
| Co1—P4$^{ii}$ | 2.284 (7) | P4—Co1$^{iv}$ | 2.266 (7) |
| Co1—P4 | 2.285 (7) | P4—Co3$^{i}$ | 2.266 (10) |
| Co1—Co1$^{v}$ | 2.624 (9) | P4—Co1$^{vii}$ | 2.285 (7) |
| Co1—Co1$^{iv}$ | 2.624 (9) | P5—Co0$^{viii}$ | 2.148 (10) |
| Co1—Co0$^{v}$ | 2.634 (7) | P5—Co1$^{iv}$ | 2.202 (10) |
| Co1—Co3$^{iii}$ | 2.674 (5) | P5—Co3$^{xiii}$ | 2.263 (7) |
| Co1—Co3$^{i}$ | 2.674 (5) | P5—Co3$^{xiv}$ | 2.263 (7) |
| Co1—Co2$^{v}$ | 2.731 (5) | P5—Co3$^{ii}$ | 2.301 (8) |
| Co2—P4 | 2.258 (9) | P5—Co2$^{ii}$ | 2.341 (7) |
| Co2—P5$^{vii}$ | 2.341 (7) | P6—Co0$^{i}$ | 2.128 (5) |
| Co2—P5 | 2.341 (7) | P6—Co0$^{viii}$ | 2.128 (5) |
| Co2—P6 | 2.383 (4) | P6—Co2$^{xv}$ | 2.383 (4) |

| | | | |
|---|---|---|---|
| Co2—P6$^{vii}$ | 2.383 (4) | P6—Co2$^{iii}$ | 2.383 (4) |
| Co2—Co0$^{vii}$ | 2.543 (6) | P6—Co2$^{i}$ | 2.383 (4) |
| Co2—Co0$^{viii}$ | 2.571 (6) | P6—Co2$^{viii}$ | 2.383 (4) |
| Co2—Co0$^{ix}$ | 2.571 (6) | P6—Co2$^{ii}$ | 2.383 (4) |
| Co2—Co1$^{x}$ | 2.731 (5) | | |

| | | | |
|---|---|---|---|
| P6—Co0—P5$^{i}$ | 96.9 (3) | P5$^{vii}$—Co2—Co1$^{iv}$ | 102.3 (3) |
| P6—Co0—P4 | 116.4 (2) | P5—Co2—Co1$^{iv}$ | 50.7 (2) |
| P5$^{i}$—Co0—P4 | 114.7 (3) | P6—Co2—Co1$^{iv}$ | 94.84 (11) |
| P6—Co0—P4$^{ii}$ | 116.4 (2) | P6$^{vii}$—Co2—Co1$^{iv}$ | 156.4 (2) |
| P5$^{i}$—Co0—P4$^{ii}$ | 114.7 (3) | Co0$^{vii}$—Co2—Co1$^{iv}$ | 106.0 (2) |
| P4—Co0—P4$^{ii}$ | 98.9 (4) | Co0—Co2—Co1$^{iv}$ | 59.81 (15) |
| P6—Co0—Co3$^{iii}$ | 127.43 (16) | Co0$^{viii}$—Co2—Co1$^{iv}$ | 94.89 (12) |
| P5$^{i}$—Co0—Co3$^{iii}$ | 58.1 (2) | Co0$^{ix}$—Co2—Co1$^{iv}$ | 148.9 (2) |
| P4—Co0—Co3$^{iii}$ | 116.1 (3) | Co1$^{x}$—Co2—Co1$^{iv}$ | 74.08 (17) |
| P4$^{ii}$—Co0—Co3$^{iii}$ | 56.9 (2) | P4—Co2—Co3 | 138.5 (3) |
| P6—Co0—Co3$^{i}$ | 127.43 (16) | P5$^{vii}$—Co2—Co3 | 51.6 (2) |
| P5$^{i}$—Co0—Co3$^{i}$ | 58.1 (2) | P5—Co2—Co3 | 51.6 (2) |
| P4—Co0—Co3$^{i}$ | 56.9 (2) | P6—Co2—Co3 | 106.1 (2) |
| P4$^{ii}$—Co0—Co3$^{i}$ | 116.1 (3) | P6$^{vii}$—Co2—Co3 | 106.1 (2) |
| Co3$^{iii}$—Co0—Co3$^{i}$ | 80.8 (2) | Co0$^{vii}$—Co2—Co3 | 139.57 (11) |
| P6—Co0—Co2$^{ii}$ | 60.57 (16) | Co0—Co2—Co3 | 139.58 (11) |
| P5$^{i}$—Co0—Co2$^{ii}$ | 129.6 (2) | Co0$^{viii}$—Co2—Co3 | 55.61 (16) |
| P4—Co0—Co2$^{ii}$ | 115.7 (3) | Co0$^{ix}$—Co2—Co3 | 55.61 (16) |
| P4$^{ii}$—Co0—Co2$^{ii}$ | 56.6 (2) | Co1$^{x}$—Co2—Co3 | 95.9 (2) |
| Co3$^{iii}$—Co0—Co2$^{ii}$ | 98.44 (12) | Co1$^{iv}$—Co2—Co3 | 95.9 (2) |
| Co3$^{i}$—Co0—Co2$^{ii}$ | 170.2 (3) | P5$^{xi}$—Co3—P5$^{xii}$ | 93.3 (4) |
| P6—Co0—Co2 | 60.57 (16) | P5$^{xi}$—Co3—P4$^{viii}$ | 106.5 (3) |
| P5$^{i}$—Co0—Co2 | 129.6 (2) | P5$^{xii}$—Co3—P4$^{viii}$ | 106.5 (3) |
| P4—Co0—Co2 | 56.6 (2) | P5$^{xi}$—Co3—P5$^{vii}$ | 79.0 (4) |
| P4$^{ii}$—Co0—Co2 | 115.7 (3) | P5$^{xii}$—Co3—P5$^{vii}$ | 148.1 (4) |
| Co3$^{iii}$—Co0—Co2 | 170.2 (3) | P4$^{viii}$—Co3—P5$^{vii}$ | 105.3 (3) |
| Co3$^{i}$—Co0—Co2 | 98.44 (12) | P5$^{xi}$—Co3—P5 | 148.1 (4) |
| Co2$^{ii}$—Co0—Co2 | 80.6 (2) | P5$^{xii}$—Co3—P5 | 79.0 (4) |
| P6—Co0—Co2$^{iii}$ | 60.07 (15) | P4$^{viii}$—Co3—P5 | 105.3 (3) |
| P5$^{i}$—Co0—Co2$^{iii}$ | 58.7 (2) | P5$^{vii}$—Co3—P5 | 91.3 (4) |
| P4—Co0—Co2$^{iii}$ | 170.1 (3) | P5$^{xi}$—Co3—Co3$^{xiii}$ | 95.1 (3) |
| P4$^{ii}$—Co0—Co2$^{iii}$ | 90.7 (2) | P5$^{xii}$—Co3—Co3$^{xiii}$ | 95.1 (3) |
| Co3$^{iii}$—Co0—Co2$^{iii}$ | 67.70 (14) | P4$^{viii}$—Co3—Co3$^{xiii}$ | 148.1 (4) |
| Co3$^{i}$—Co0—Co2$^{iii}$ | 116.8 (2) | P5$^{vii}$—Co3—Co3$^{xiii}$ | 55.5 (3) |
| Co2$^{ii}$—Co0—Co2$^{iii}$ | 71.4 (2) | P5—Co3—Co3$^{xiii}$ | 55.5 (3) |
| Co2—Co0—Co2$^{iii}$ | 120.6 (2) | P5$^{xi}$—Co3—Co3$^{xii}$ | 57.0 (3) |
| P6—Co0—Co2$^{i}$ | 60.07 (15) | P5$^{xii}$—Co3—Co3$^{xii}$ | 57.0 (3) |
| P5$^{i}$—Co0—Co2$^{i}$ | 58.7 (2) | P4$^{viii}$—Co3—Co3$^{xii}$ | 151.9 (4) |
| P4—Co0—Co2$^{i}$ | 90.7 (2) | P5$^{vii}$—Co3—Co3$^{xii}$ | 94.1 (3) |
| P4$^{ii}$—Co0—Co2$^{i}$ | 170.1 (3) | P5—Co3—Co3$^{xii}$ | 94.1 (3) |
| Co3$^{iii}$—Co0—Co2$^{i}$ | 116.8 (2) | Co3$^{xiii}$—Co3—Co3$^{xii}$ | 60.0 |
| Co3$^{i}$—Co0—Co2$^{i}$ | 67.70 (14) | P5$^{xi}$—Co3—Co0$^{viii}$ | 159.3 (3) |

| | | | |
|---|---|---|---|
| Co2$^{ii}$—Co0—Co2$^{i}$ | 120.6 (2) | P5$^{xii}$—Co3—Co0$^{viii}$ | 89.59 (18) |
| Co2—Co0—Co2$^{i}$ | 71.4 (2) | P4$^{viii}$—Co3—Co0$^{viii}$ | 53.20 (19) |
| Co2$^{iii}$—Co0—Co2$^{i}$ | 79.6 (2) | P5$^{vii}$—Co3—Co0$^{viii}$ | 108.5 (3) |
| P6—Co0—Co1 | 164.3 (3) | P5—Co3—Co0$^{viii}$ | 52.4 (2) |
| P5$^{i}$—Co0—Co1 | 98.8 (3) | Co3$^{xiii}$—Co3—Co0$^{viii}$ | 105.1 (2) |
| P4—Co0—Co1 | 56.2 (2) | Co3$^{xii}$—Co3—Co0$^{viii}$ | 138.58 (11) |
| P4$^{ii}$—Co0—Co1 | 56.2 (2) | P5$^{xi}$—Co3—Co0$^{ix}$ | 89.59 (18) |
| Co3$^{iii}$—Co0—Co1 | 62.53 (14) | P5$^{xii}$—Co3—Co0$^{ix}$ | 159.3 (3) |
| Co3$^{i}$—Co0—Co1 | 62.53 (14) | P4$^{viii}$—Co3—Co0$^{ix}$ | 53.20 (19) |
| Co2$^{ii}$—Co0—Co1 | 108.4 (2) | P5$^{vii}$—Co3—Co0$^{ix}$ | 52.4 (2) |
| Co2—Co0—Co1 | 108.4 (2) | P5—Co3—Co0$^{ix}$ | 108.5 (3) |
| Co2$^{iii}$—Co0—Co1 | 129.67 (15) | Co3$^{xiii}$—Co3—Co0$^{ix}$ | 105.1 (2) |
| Co2$^{i}$—Co0—Co1 | 129.67 (15) | Co3$^{xii}$—Co3—Co0$^{ix}$ | 138.58 (11) |
| P6—Co0—Co1$^{iv}$ | 104.29 (19) | Co0$^{viii}$—Co3—Co0$^{ix}$ | 80.8 (2) |
| P5$^{i}$—Co0—Co1$^{iv}$ | 158.8 (3) | P5$^{xi}$—Co3—Co1$^{viii}$ | 106.4 (3) |
| P4—Co0—Co1$^{iv}$ | 55.3 (2) | P5$^{xii}$—Co3—Co1$^{viii}$ | 52.2 (2) |
| P4$^{ii}$—Co0—Co1$^{iv}$ | 55.3 (2) | P4$^{viii}$—Co3—Co1$^{viii}$ | 54.34 (19) |
| Co3$^{iii}$—Co0—Co1$^{iv}$ | 107.12 (19) | P5$^{vii}$—Co3—Co1$^{viii}$ | 159.6 (3) |
| Co3$^{i}$—Co0—Co1$^{iv}$ | 107.12 (19) | P5—Co3—Co1$^{viii}$ | 93.3 (2) |
| Co2$^{ii}$—Co0—Co1$^{iv}$ | 63.65 (16) | Co3$^{xiii}$—Co3—Co1$^{viii}$ | 140.83 (9) |
| Co2—Co0—Co1$^{iv}$ | 63.65 (16) | Co3$^{xii}$—Co3—Co1$^{viii}$ | 105.3 (2) |
| Co2$^{iii}$—Co0—Co1$^{iv}$ | 133.59 (16) | Co0$^{viii}$—Co3—Co1$^{viii}$ | 60.09 (15) |
| Co2$^{i}$—Co0—Co1$^{iv}$ | 133.59 (16) | Co0$^{ix}$—Co3—Co1$^{viii}$ | 107.4 (2) |
| Co1—Co0—Co1$^{iv}$ | 60.0 (2) | P5$^{xi}$—Co3—Co1$^{ix}$ | 52.2 (2) |
| P5$^{v}$—Co1—P4$^{v}$ | 108.1 (2) | P5$^{xii}$—Co3—Co1$^{ix}$ | 106.4 (3) |
| P5$^{v}$—Co1—P4$^{vi}$ | 108.1 (2) | P4$^{viii}$—Co3—Co1$^{ix}$ | 54.34 (19) |
| P4$^{v}$—Co1—P4$^{vi}$ | 93.1 (4) | P5$^{vii}$—Co3—Co1$^{ix}$ | 93.3 (2) |
| P5$^{v}$—Co1—P4$^{ii}$ | 108.0 (3) | P5—Co3—Co1$^{ix}$ | 159.6 (3) |
| P4$^{v}$—Co1—P4$^{ii}$ | 144.0 (3) | Co3$^{xiii}$—Co3—Co1$^{ix}$ | 140.83 (9) |
| P4$^{vi}$—Co1—P4$^{ii}$ | 76.3 (3) | Co3$^{xii}$—Co3—Co1$^{ix}$ | 105.3 (2) |
| P5$^{v}$—Co1—P4 | 108.0 (3) | Co0$^{viii}$—Co3—Co1$^{ix}$ | 107.4 (2) |
| P4$^{v}$—Co1—P4 | 76.3 (3) | Co0$^{ix}$—Co3—Co1$^{ix}$ | 60.09 (15) |
| P4$^{vi}$—Co1—P4 | 144.0 (3) | Co1$^{viii}$—Co3—Co1$^{ix}$ | 75.95 (16) |
| P4$^{ii}$—Co1—P4 | 92.1 (4) | P5$^{xi}$—Co3—Co2 | 131.18 (19) |
| P5$^{v}$—Co1—Co0 | 89.0 (3) | P5$^{xii}$—Co3—Co2 | 131.18 (19) |
| P4$^{v}$—Co1—Co0 | 128.2 (2) | P4$^{viii}$—Co3—Co2 | 82.0 (3) |
| P4$^{vi}$—Co1—Co0 | 128.2 (2) | P5$^{vii}$—Co3—Co2 | 52.8 (2) |
| P4$^{ii}$—Co1—Co0 | 51.9 (2) | P5—Co3—Co2 | 52.8 (2) |
| P4—Co1—Co0 | 51.9 (2) | Co3$^{xiii}$—Co3—Co2 | 66.1 (3) |
| P5$^{v}$—Co1—Co1$^{v}$ | 150.6 (4) | Co3$^{xii}$—Co3—Co2 | 126.1 (3) |
| P4$^{v}$—Co1—Co1$^{v}$ | 55.1 (2) | Co0$^{viii}$—Co3—Co2 | 56.70 (15) |
| P4$^{vi}$—Co1—Co1$^{v}$ | 55.1 (2) | Co0$^{ix}$—Co3—Co2 | 56.70 (15) |
| P4$^{ii}$—Co1—Co1$^{v}$ | 92.1 (2) | Co1$^{viii}$—Co3—Co2 | 116.37 (18) |
| P4—Co1—Co1$^{v}$ | 92.1 (2) | Co1$^{ix}$—Co3—Co2 | 116.37 (18) |
| Co0—Co1—Co1$^{v}$ | 120.4 (2) | Co0—P4—Co0$^{vii}$ | 98.9 (4) |
| P5$^{v}$—Co1—Co1$^{iv}$ | 149.4 (4) | Co0—P4—Co2 | 70.2 (2) |
| P4$^{v}$—Co1—Co1$^{iv}$ | 92.6 (2) | Co0$^{vii}$—P4—Co2 | 70.2 (2) |
| P4$^{vi}$—Co1—Co1$^{iv}$ | 92.6 (2) | Co0—P4—Co1$^{x}$ | 144.1 (4) |

| | | | |
|---|---|---|---|
| P4$^{ii}$—Co1—Co1$^{iv}$ | 54.4 (2) | Co0$^{vii}$—P4—Co1$^{x}$ | 72.93 (17) |
| P4—Co1—Co1$^{iv}$ | 54.4 (2) | Co2—P4—Co1$^{x}$ | 74.3 (3) |
| Co0—Co1—Co1$^{iv}$ | 60.4 (2) | Co0—P4—Co1$^{iv}$ | 72.93 (17) |
| Co1$^{v}$—Co1—Co1$^{iv}$ | 60.0 | Co0$^{vii}$—P4—Co1$^{iv}$ | 144.1 (4) |
| P5$^{v}$—Co1—Co0$^{v}$ | 91.0 (3) | Co2—P4—Co1$^{iv}$ | 74.3 (3) |
| P4$^{v}$—Co1—Co0$^{v}$ | 51.8 (2) | Co1$^{x}$—P4—Co1$^{iv}$ | 93.1 (4) |
| P4$^{vi}$—Co1—Co0$^{v}$ | 51.8 (2) | Co0—P4—Co3$^{i}$ | 69.9 (3) |
| P4$^{ii}$—Co1—Co0$^{v}$ | 128.0 (2) | Co0$^{vii}$—P4—Co3$^{i}$ | 69.9 (3) |
| P4—Co1—Co0$^{v}$ | 128.0 (2) | Co2—P4—Co3$^{i}$ | 116.5 (4) |
| Co0—Co1—Co0$^{v}$ | 180.0 (2) | Co1$^{x}$—P4—Co3$^{i}$ | 133.35 (18) |
| Co1$^{v}$—Co1—Co0$^{v}$ | 59.6 (2) | Co1$^{iv}$—P4—Co3$^{i}$ | 133.35 (18) |
| Co1$^{iv}$—Co1—Co0$^{v}$ | 119.6 (2) | Co0—P4—Co1 | 71.84 (17) |
| P5$^{v}$—Co1—Co3$^{iii}$ | 54.26 (19) | Co0$^{vii}$—P4—Co1 | 141.5 (4) |
| P4$^{v}$—Co1—Co3$^{iii}$ | 162.3 (3) | Co2—P4—Co1 | 133.94 (18) |
| P4$^{vi}$—Co1—Co3$^{iii}$ | 93.40 (17) | Co1$^{x}$—P4—Co1 | 135.3 (4) |
| P4$^{ii}$—Co1—Co3$^{iii}$ | 53.7 (2) | Co1$^{iv}$—P4—Co1 | 70.4 (2) |
| P4—Co1—Co3$^{iii}$ | 107.1 (3) | Co3$^{i}$—P4—Co1 | 72.0 (3) |
| Co0—Co1—Co3$^{iii}$ | 57.38 (16) | Co0—P4—Co1$^{vii}$ | 141.5 (4) |
| Co1$^{v}$—Co1—Co3$^{iii}$ | 140.25 (9) | Co0$^{vii}$—P4—Co1$^{vii}$ | 71.84 (17) |
| Co1$^{iv}$—Co1—Co3$^{iii}$ | 103.5 (2) | Co2—P4—Co1$^{vii}$ | 133.94 (18) |
| Co0$^{v}$—Co1—Co3$^{iii}$ | 122.64 (18) | Co1$^{x}$—P4—Co1$^{vii}$ | 70.4 (2) |
| P5$^{v}$—Co1—Co3$^{i}$ | 54.26 (19) | Co1$^{iv}$—P4—Co1$^{vii}$ | 135.3 (4) |
| P4$^{v}$—Co1—Co3$^{i}$ | 93.40 (17) | Co3$^{i}$—P4—Co1$^{vii}$ | 72.0 (3) |
| P4$^{vi}$—Co1—Co3$^{i}$ | 162.3 (3) | Co1—P4—Co1$^{vii}$ | 92.1 (4) |
| P4$^{ii}$—Co1—Co3$^{i}$ | 107.1 (3) | Co0$^{viii}$—P5—Co1$^{iv}$ | 127.8 (5) |
| P4—Co1—Co3$^{i}$ | 53.7 (2) | Co0$^{viii}$—P5—Co3$^{xiii}$ | 131.9 (2) |
| Co0—Co1—Co3$^{i}$ | 57.38 (15) | Co1$^{iv}$—P5—Co3$^{xiii}$ | 73.6 (3) |
| Co1$^{v}$—Co1—Co3$^{i}$ | 140.25 (9) | Co0$^{viii}$—P5—Co3$^{xiv}$ | 131.9 (2) |
| Co1$^{iv}$—Co1—Co3$^{i}$ | 103.5 (2) | Co1$^{iv}$—P5—Co3$^{xiv}$ | 73.6 (3) |
| Co0$^{v}$—Co1—Co3$^{i}$ | 122.64 (18) | Co3$^{xiii}$—P5—Co3$^{xiv}$ | 93.3 (4) |
| Co3$^{iii}$—Co1—Co3$^{i}$ | 75.95 (16) | Co0$^{viii}$—P5—Co3 | 69.5 (3) |
| P5$^{v}$—Co1—Co2$^{v}$ | 55.41 (19) | Co1$^{iv}$—P5—Co3 | 133.9 (2) |
| P4$^{v}$—Co1—Co2$^{v}$ | 52.7 (2) | Co3$^{xiii}$—P5—Co3 | 67.5 (2) |
| P4$^{vi}$—Co1—Co2$^{v}$ | 105.6 (3) | Co3$^{xiv}$—P5—Co3 | 131.1 (4) |
| P4$^{ii}$—Co1—Co2$^{v}$ | 163.3 (3) | Co0$^{viii}$—P5—Co3$^{ii}$ | 69.5 (3) |
| P4—Co1—Co2$^{v}$ | 95.17 (19) | Co1$^{iv}$—P5—Co3$^{ii}$ | 133.9 (2) |
| Co0—Co1—Co2$^{v}$ | 123.5 (2) | Co3$^{xiii}$—P5—Co3$^{ii}$ | 131.1 (4) |
| Co1$^{v}$—Co1—Co2$^{v}$ | 102.6 (2) | Co3$^{xiv}$—P5—Co3$^{ii}$ | 67.5 (2) |
| Co1$^{iv}$—Co1—Co2$^{v}$ | 140.73 (11) | Co3—P5—Co3$^{ii}$ | 91.3 (4) |
| Co0$^{v}$—Co1—Co2$^{v}$ | 56.54 (14) | Co0$^{viii}$—P5—Co2 | 69.7 (3) |
| Co3$^{iii}$—Co1—Co2$^{v}$ | 109.6 (2) | Co1$^{iv}$—P5—Co2 | 73.8 (2) |
| Co3$^{i}$—Co1—Co2$^{v}$ | 66.10 (15) | Co3$^{xiii}$—P5—Co2 | 79.62 (16) |
| P4—Co2—P5$^{vii}$ | 103.7 (3) | Co3$^{xiv}$—P5—Co2 | 147.3 (4) |
| P4—Co2—P5 | 103.7 (3) | Co3—P5—Co2 | 75.6 (2) |
| P5$^{vii}$—Co2—P5 | 89.3 (3) | Co3$^{ii}$—P5—Co2 | 139.2 (4) |
| P4—Co2—P6 | 103.6 (2) | Co0$^{viii}$—P5—Co2$^{ii}$ | 69.7 (3) |
| P5$^{vii}$—Co2—P6 | 152.7 (3) | Co1$^{iv}$—P5—Co2$^{ii}$ | 73.8 (2) |
| P5—Co2—P6 | 85.31 (18) | Co3$^{xiii}$—P5—Co2$^{ii}$ | 147.3 (4) |

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|---|---|---|---|
| P4—Co2—P6$^{vii}$ | 103.6 (2) | Co3$^{xiv}$—P5—Co2$^{ii}$ | 79.62 (16) |
| P5$^{vii}$—Co2—P6$^{vii}$ | 85.30 (18) | Co3—P5—Co2$^{ii}$ | 139.2 (4) |
| P5—Co2—P6$^{vii}$ | 152.7 (3) | Co3$^{ii}$—P5—Co2$^{ii}$ | 75.6 (2) |
| P6—Co2—P6$^{vii}$ | 87.33 (17) | Co2—P5—Co2$^{ii}$ | 89.3 (3) |
| P4—Co2—Co0$^{vii}$ | 53.20 (19) | Co0$^{i}$—P6—Co0$^{viii}$ | 120.0 |
| P5$^{vii}$—Co2—Co0$^{vii}$ | 90.21 (18) | Co0$^{i}$—P6—Co0 | 120.0 |
| P5—Co2—Co0$^{vii}$ | 155.9 (3) | Co0$^{viii}$—P6—Co0 | 120.0 |
| P6—Co2—Co0$^{vii}$ | 105.4 (2) | Co0$^{i}$—P6—Co2$^{xv}$ | 69.23 (17) |
| P6$^{vii}$—Co2—Co0$^{vii}$ | 51.06 (12) | Co0$^{viii}$—P6—Co2$^{xv}$ | 68.36 (17) |
| P4—Co2—Co0 | 53.20 (19) | Co0—P6—Co2$^{xv}$ | 136.33 (9) |
| P5$^{vii}$—Co2—Co0 | 155.9 (3) | Co0$^{i}$—P6—Co2$^{iii}$ | 68.36 (17) |
| P5—Co2—Co0 | 90.21 (18) | Co0$^{viii}$—P6—Co2$^{iii}$ | 136.33 (9) |
| P6—Co2—Co0 | 51.06 (12) | Co0—P6—Co2$^{iii}$ | 69.23 (17) |
| P6$^{vii}$—Co2—Co0 | 105.4 (2) | Co2$^{xv}$—P6—Co2$^{iii}$ | 77.58 (13) |
| Co0$^{vii}$—Co2—Co0 | 80.6 (2) | Co0$^{i}$—P6—Co2$^{i}$ | 68.36 (17) |
| P4—Co2—Co0$^{viii}$ | 140.20 (12) | Co0$^{viii}$—P6—Co2$^{i}$ | 136.33 (9) |
| P5$^{vii}$—Co2—Co0$^{viii}$ | 106.2 (3) | Co0—P6—Co2$^{i}$ | 69.23 (17) |
| P5—Co2—Co0$^{viii}$ | 51.6 (2) | Co2$^{xv}$—P6—Co2$^{i}$ | 137.59 (6) |
| P6—Co2—Co0$^{viii}$ | 50.70 (12) | Co2$^{iii}$—P6—Co2$^{i}$ | 87.34 (17) |
| P6$^{vii}$—Co2—Co0$^{viii}$ | 104.5 (2) | Co0$^{i}$—P6—Co2$^{viii}$ | 69.23 (17) |
| Co0$^{vii}$—Co2—Co0$^{viii}$ | 150.1 (2) | Co0$^{viii}$—P6—Co2$^{viii}$ | 68.36 (17) |
| Co0—Co2—Co0$^{viii}$ | 92.22 (16) | Co0—P6—Co2$^{viii}$ | 136.33 (9) |
| P4—Co2—Co0$^{ix}$ | 140.20 (12) | Co2$^{xv}$—P6—Co2$^{viii}$ | 87.34 (17) |
| P5$^{vii}$—Co2—Co0$^{ix}$ | 51.6 (2) | Co2$^{iii}$—P6—Co2$^{viii}$ | 137.59 (6) |
| P5—Co2—Co0$^{ix}$ | 106.2 (3) | Co2$^{i}$—P6—Co2$^{viii}$ | 77.58 (13) |
| P6—Co2—Co0$^{ix}$ | 104.5 (2) | Co0$^{i}$—P6—Co2$^{ii}$ | 136.33 (9) |
| P6$^{vii}$—Co2—Co0$^{ix}$ | 50.70 (12) | Co0$^{viii}$—P6—Co2$^{ii}$ | 69.23 (17) |
| Co0$^{vii}$—Co2—Co0$^{ix}$ | 92.22 (16) | Co0—P6—Co2$^{ii}$ | 68.37 (17) |
| Co0—Co2—Co0$^{ix}$ | 150.1 (2) | Co2$^{xv}$—P6—Co2$^{ii}$ | 77.58 (13) |
| Co0$^{viii}$—Co2—Co0$^{ix}$ | 79.6 (2) | Co2$^{iii}$—P6—Co2$^{ii}$ | 77.58 (13) |
| P4—Co2—Co1$^{x}$ | 52.99 (19) | Co2$^{i}$—P6—Co2$^{ii}$ | 137.59 (6) |
| P5$^{vii}$—Co2—Co1$^{x}$ | 50.7 (2) | Co2$^{viii}$—P6—Co2$^{ii}$ | 137.59 (6) |
| P5—Co2—Co1$^{x}$ | 102.3 (3) | Co0$^{i}$—P6—Co2 | 136.33 (9) |
| P6—Co2—Co1$^{x}$ | 156.4 (2) | Co0$^{viii}$—P6—Co2 | 69.23 (17) |
| P6$^{vii}$—Co2—Co1$^{x}$ | 94.84 (11) | Co0—P6—Co2 | 68.37 (17) |
| Co0$^{vii}$—Co2—Co1$^{x}$ | 59.81 (15) | Co2$^{xv}$—P6—Co2 | 137.59 (6) |
| Co0—Co2—Co1$^{x}$ | 106.0 (2) | Co2$^{iii}$—P6—Co2 | 137.59 (6) |
| Co0$^{viii}$—Co2—Co1$^{x}$ | 148.9 (2) | Co2$^{i}$—P6—Co2 | 77.58 (13) |
| Co0$^{ix}$—Co2—Co1$^{x}$ | 94.89 (12) | Co2$^{viii}$—P6—Co2 | 77.58 (13) |
| P4—Co2—Co1$^{iv}$ | 52.99 (19) | Co2$^{ii}$—P6—Co2 | 87.33 (17) |

Symmetry codes: (i) −*y*, *x*−*y*, *z*; (ii) *x*, *y*, *z*−1; (iii) −*y*, *x*−*y*, *z*−1; (iv) −*y*+1, *x*−*y*+1, *z*; (v) −*x*+*y*, −*x*+1, *z*; (vi) −*x*+*y*, −*x*+1, *z*−1; (vii) *x*, *y*, *z*+1; (viii) −*x*+*y*, −*x*, *z*; (ix) −*x*+*y*, −*x*, *z*+1; (x) −*y*+1, *x*−*y*+1, *z*+1; (xi) −*y*+1, *x*−*y*, *z*+1; (xii) −*y*+1, *x*−*y*, *z*; (xiii) −*x*+*y*+1, −*x*+1, *z*; (xiv) −*x*+*y*+1, −*x*+1, *z*−1; (xv) −*x*+*y*, −*x*, *z*−1.