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# Bis[1,3-bis(diphenylphosphinoylimino)isoindolinato-$\kappa^3O,N,O'$]-calcium(II)

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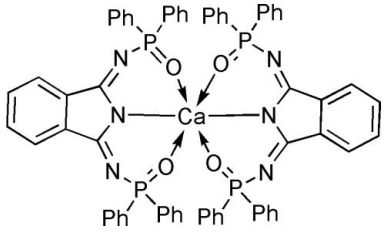
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.007 Å; $R$ factor = 0.050; $wR$ factor = 0.135; data-to-parameter ratio = 13.9.

In the title compound, $[Ca(C_{32}H_{24}N_3O_2P_2)_2]$, the 1,3-bis(diphenylphosphinoylimino)isoindoline ligand adopts a tridentate coordination mode. The compound exhibits a distorted octahedral geometry. The Ca atom lies on a twofold rotation axis.

## Related literature

For a related compound with similar octahedral geometry, see: Cole *et al.* (2006). For related literature, see: Shang (2007).



## Experimental

### *Crystal data*

$[Ca(C_{32}H_{24}N_3O_2P_2)_2]$
$M_r$ = 1129.04
Monoclinic, $C2/c$
$a$ = 26.351 (2) Å
$b$ = 12.4790 (11) Å
$c$ = 21.1997 (19) Å
$\beta$ = 126.1720 (10)°
$V$ = 5627.4 (9) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.28 mm$^{-1}$
$T$ = 293 (2) K
0.20 × 0.15 × 0.10 mm

### *Data collection*

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.837, $T_{max}$ = 0.973
11452 measured reflections
4959 independent reflections
4175 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.019

### *Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.135
$S$ = 1.04
4959 reflections
357 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.40 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.25 e Å$^{-3}$

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| Ca1—O1 | 2.2581 (18) | Ca1—N2 | 2.5513 (18) |
| Ca1—O2 | 2.2646 (18) | | |
| O1—Ca1—O1$^{i}$ | 81.34 (11) | O2—Ca1—N2$^{i}$ | 80.48 (6) |
| O1—Ca1—O2 | 93.49 (8) | O1—Ca1—N2 | 80.81 (6) |
| O1—Ca1—O2$^{i}$ | 157.41 (7) | O2—Ca1—N2 | 90.12 (6) |
| O2—Ca1—O2$^{i}$ | 99.09 (11) | N2$^{i}$—Ca1—N2 | 165.55 (9) |
| O1—Ca1—N2$^{i}$ | 110.51 (6) | | |

Symmetry code: (i) $-x, y, -z+\frac{1}{2}$.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL/PC* (Sheldrick, 1999); software used to prepare material for publication: *SHELXTL/PC*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WW2103).

## References

Bruker (2000). *SMART* (Version 5.0) and *SAINT* (Version 6.02). Bruker AXS Inc., Madison, Wisconsin, USA.
Cole, M. L., Deacon, G. B., Forsyth, C. M., Konstas, K. & Junk, P. C. (2006). *Dalton Trans.* pp. 3360–3367.
Shang, D.-L. (2007). MSc thesis, Shanxi University, People's Republic of China.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.
Sheldrick, G. M. (1999). *SHELXTL/PC*. Version 6.10. Bruker AXS Inc., Madison, Wisconsin, USA.

# supporting information

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## Bis[1,3-bis(diphenylphosphinoylimino)isoindolinato-$\kappa^3O,N,O'$]calcium(II)

**Zhiying Li, Donglin Shang and Jianping Guo**

### S1. Comment

The bis(*N*-diphenylphosphinato)-isoindoline-1,3-diimine ligand is a new type of tridentate ligand (Shang, 2007). There are six atoms coordinated to calcium ion, the four oxygen atoms are approximately in an equatorial plane with calcium(II), the mean deviation from the plane is 0.3218Å and the two nitrogen atoms are in axial positions [N2—Ca—N2$^{i}$ 165.55 (9)° (symmetry code $^{i}$: -*x*, *y*, 1/2 - *z*)]. Because the calcium ion is coordinated *via* two oxygen of the tridentate ligand, two six-membered rings of O1—P1—N1—C13—N2—Ca1 and O2$^{i}$—P2$^{i}$—N3$^{i}$—C20—N2—Ca1 are formed. The dihedral angles between the two six-membered rings and the isoindoline ring are 12.5° and 14.0° respectively. The Ca—O and Ca—N bond lengths of the compound are 2.2581 (18) [Ca1—O1], 2.2646 (18) [Ca1—O2] and 2.5513 (18) [Ca1—N2] Å, respectively. The values are comparable to the octahedral compound [Ca(*o*-TolForm)$_2$(thf)$_2$], which can provide four nitrogen and two oxygen atoms to coordinate calcium(II), the average bond length of Ca—O is 2.368 (2) and Ca—N is 2.43 (2)Å (Cole *et al.*, 2006).

### S2. Experimental

The red crystal of bis(*N*-diphenylphosphinato)-isoindoline-1,3-diimine (Shang, 2007) (0.287 g, 0.53 mmol) was dissolved in absolute ethanol (20 ml), the calcium chloride (0.060 g, 0.53 mmol) was added to the solution in room temperature and the mixture was reacted for 24 h before getting the clear yellow solution, the solvent was evaporated slowly to give pink crystals of title compund. Yield: 0.14 g, 47%. Spectroscopic analysis, $^{1}$H NMR (300 MHz, $CDCl_3$, $\delta$): 7.73–7.88(m, 16H, phenyl; 4H, isoindoline); 7.51–7.54 (t, 4H, J=8.1, isoindoline); 7.10–7.27 (m, 24H, phenyl). $^{31}$P-{$^{1}$H} NMR (300 MHz, $CDCl_3$, $\delta$): 20.2(*s*).

### S3. Refinement

H atoms were placed in their idealized positions and allowed to ride on the respective parent atoms with C—H 0.93 Å, and with $U_{iso}$(H) = 1.2$U_{eq}$ (parent atom).

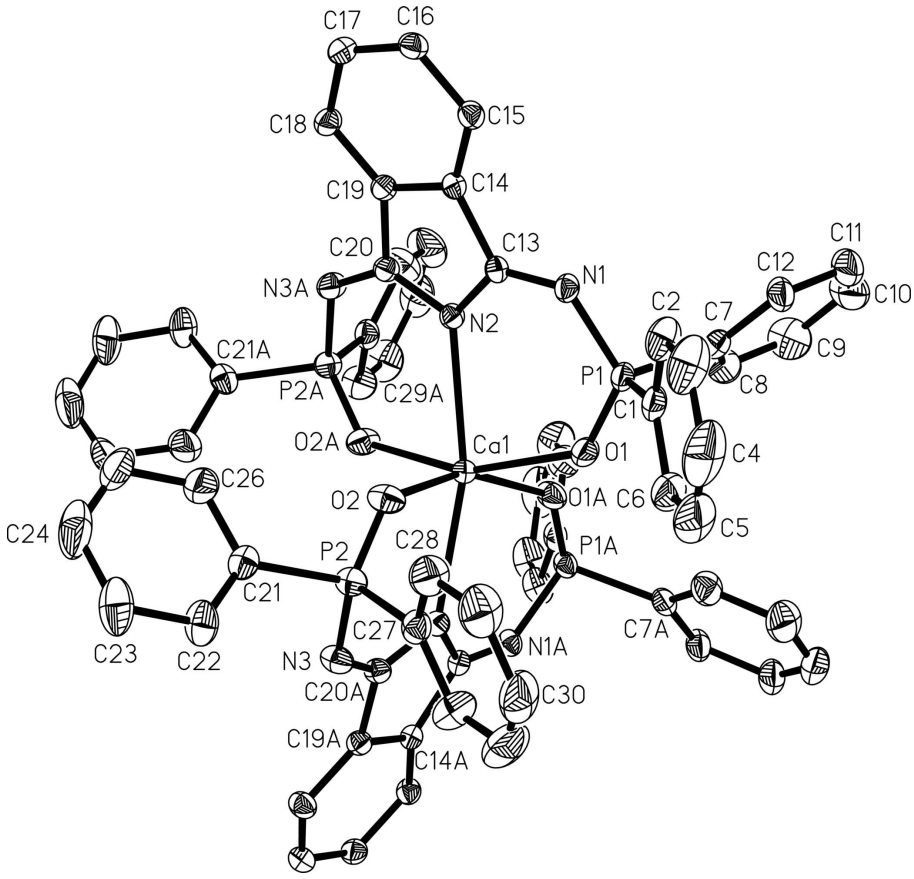


**Figure 1**

Molecular structure of I, showing the atom-labeling scheme and 20% probability displacement ellipsoids. Symmetry codes: (i) -*x*, *y*, -*z* + 1/2.

**Bis[1,3-bis(diphenylphosphinoylimino)isoindolinato-$\kappa^3O,N,O'$]calcium(II)**

*Crystal data*

$[Ca(C_{32}H_{24}N_3O_2P_2)_2]$
$M_r$ = 1129.04
Monoclinic, *C*2/*c*
Hall symbol: -C 2yc
*a* = 26.351 (2) Å
*b* = 12.4790 (11) Å
*c* = 21.1997 (19) Å
$\beta$ = 126.172 (1)°
*V* = 5627.4 (9) Å$^3$
*Z* = 4
*F*(000) = 2344
$D_x$ = 1.333 Mg m$^{-3}$
Mo *K*$\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 4426 reflections
$\theta$ = 2.4–25.9°
$\mu$ = 0.28 mm$^{-1}$
*T* = 293 K
Block, pink
0.20 × 0.15 × 0.10 mm

*Data collection*

Bruker SMART CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega$ scan
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.837, $T_{max}$ = 0.973
11452 measured reflections
4959 independent reflections
4175 reflections with $I > 2\sigma(I)$

$R_{int}$ = 0.019
$\theta_{max}$ = 25.0°, $\theta_{min}$ = 1.9°
$h$ = −31→17
$k$ = −14→14
$l$ = −22→25

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.135
$S$ = 1.04
4959 reflections
357 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.075P)^2 + 4.1489P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.40 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.

**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)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Ca1 | 0.0000 | 0.39576 (5) | 0.2500 | 0.03918 (18) |
| P1 | 0.12637 (3) | 0.56655 (5) | 0.33048 (4) | 0.04665 (19) |
| P2 | 0.02345 (3) | 0.23193 (6) | 0.13903 (4) | 0.0498 (2) |
| O1 | 0.06204 (8) | 0.53300 (15) | 0.26479 (10) | 0.0621 (5) |
| O2 | 0.04545 (8) | 0.27801 (16) | 0.21607 (10) | 0.0620 (5) |
| N1 | 0.16798 (9) | 0.49240 (15) | 0.40938 (11) | 0.0447 (5) |
| N2 | 0.09048 (8) | 0.37004 (14) | 0.39391 (10) | 0.0401 (4) |
| N3 | −0.05179 (10) | 0.22572 (18) | 0.06938 (12) | 0.0553 (6) |
| C1 | 0.17484 (14) | 0.57710 (19) | 0.29706 (17) | 0.0566 (7) |
| C2 | 0.23898 (16) | 0.5685 (3) | 0.3464 (2) | 0.0778 (9) |
| H2B | 0.2592 | 0.5583 | 0.3996 | 0.093* |
| C3 | 0.2736 (2) | 0.5750 (4) | 0.3164 (4) | 0.1129 (15) |
| H3B | 0.3171 | 0.5684 | 0.3502 | 0.135* |
| C4 | 0.2464 (4) | 0.5902 (4) | 0.2414 (5) | 0.137 (2) |
| H4A | 0.2707 | 0.5947 | 0.2228 | 0.164* |
| C5 | 0.1831 (4) | 0.5992 (4) | 0.1915 (3) | 0.1284 (19) |
| H5A | 0.1641 | 0.6105 | 0.1386 | 0.154* |
| C6 | 0.1460 (2) | 0.5919 (3) | 0.2183 (2) | 0.0868 (10) |
| H6A | 0.1025 | 0.5970 | 0.1836 | 0.104* |
| C7 | 0.12490 (12) | 0.6964 (2) | 0.36669 (15) | 0.0547 (6) |
| C8 | 0.07017 (16) | 0.7308 (3) | 0.3552 (2) | 0.0752 (9) |
| H8A | 0.0340 | 0.6891 | 0.3269 | 0.090* |

| | | | | |
|---|---|---|---|---|
| C9 | 0.0699 (2) | 0.8278 (4) | 0.3864 (3) | 0.1074 (14) |
| H9A | 0.0330 | 0.8513 | 0.3784 | 0.129* |
| C10 | 0.1221 (2) | 0.8895 (3) | 0.4283 (3) | 0.1118 (15) |
| H10A | 0.1211 | 0.9539 | 0.4496 | 0.134* |
| C11 | 0.1762 (2) | 0.8569 (3) | 0.4391 (2) | 0.0951 (12) |
| H11A | 0.2120 | 0.8996 | 0.4672 | 0.114* |
| C12 | 0.17765 (14) | 0.7608 (2) | 0.40839 (18) | 0.0681 (8) |
| H12A | 0.2146 | 0.7390 | 0.4158 | 0.082* |
| C13 | 0.14975 (10) | 0.41314 (16) | 0.43053 (13) | 0.0380 (5) |
| C14 | 0.19536 (10) | 0.35340 (17) | 0.50380 (12) | 0.0391 (5) |
| C15 | 0.25946 (11) | 0.36174 (19) | 0.55869 (14) | 0.0460 (5) |
| H15A | 0.2823 | 0.4153 | 0.5553 | 0.055* |
| C16 | 0.28879 (12) | 0.2881 (2) | 0.61895 (14) | 0.0513 (6) |
| H16A | 0.3321 | 0.2919 | 0.6566 | 0.062* |
| C17 | 0.25463 (13) | 0.2089 (2) | 0.62393 (14) | 0.0547 (6) |
| H17A | 0.2752 | 0.1603 | 0.6651 | 0.066* |
| C18 | 0.19053 (12) | 0.2007 (2) | 0.56887 (14) | 0.0508 (6) |
| H18A | 0.1675 | 0.1473 | 0.5721 | 0.061* |
| C19 | 0.16168 (11) | 0.27412 (18) | 0.50904 (13) | 0.0415 (5) |
| C20 | 0.09548 (11) | 0.28795 (18) | 0.44013 (13) | 0.0426 (5) |
| C21 | 0.05040 (12) | 0.0949 (2) | 0.15292 (17) | 0.0561 (7) |
| C22 | 0.05167 (16) | 0.0416 (2) | 0.0977 (2) | 0.0803 (9) |
| H22A | 0.0369 | 0.0756 | 0.0508 | 0.096* |
| C23 | 0.0743 (2) | −0.0612 (3) | 0.1100 (3) | 0.1070 (15) |
| H23A | 0.0739 | −0.0961 | 0.0710 | 0.128* |
| C24 | 0.0965 (2) | −0.1109 (4) | 0.1762 (4) | 0.136 (2) |
| H24A | 0.1124 | −0.1800 | 0.1842 | 0.163* |
| C25 | 0.0960 (2) | −0.0614 (4) | 0.2325 (3) | 0.127 (2) |
| H25A | 0.1112 | −0.0970 | 0.2790 | 0.152* |
| C26 | 0.07300 (17) | 0.0426 (3) | 0.2215 (2) | 0.0937 (12) |
| H26A | 0.0730 | 0.0764 | 0.2606 | 0.112* |
| C27 | 0.05800 (14) | 0.2982 (2) | 0.09748 (17) | 0.0580 (7) |
| C28 | 0.12267 (17) | 0.2995 (3) | 0.1398 (2) | 0.0836 (10) |
| H28A | 0.1472 | 0.2687 | 0.1893 | 0.100* |
| C29 | 0.1514 (2) | 0.3465 (4) | 0.1089 (3) | 0.1113 (14) |
| H29A | 0.1949 | 0.3460 | 0.1374 | 0.134* |
| C30 | 0.1164 (3) | 0.3927 (4) | 0.0380 (3) | 0.1186 (17) |
| H30A | 0.1358 | 0.4242 | 0.0175 | 0.142* |
| C31 | 0.0531 (3) | 0.3935 (4) | −0.0037 (3) | 0.1218 (16) |
| H31A | 0.0292 | 0.4266 | −0.0523 | 0.146* |
| C32 | 0.0238 (2) | 0.3460 (3) | 0.0250 (2) | 0.0955 (11) |
| H32A | −0.0199 | 0.3459 | −0.0050 | 0.115* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Ca1 | 0.0386 (4) | 0.0401 (3) | 0.0360 (3) | 0.000 | 0.0204 (3) | 0.000 |
| P1 | 0.0463 (4) | 0.0371 (3) | 0.0518 (4) | −0.0034 (3) | 0.0263 (3) | 0.0065 (3) |

| | | | | | | |
|---|---|---|---|---|---|---|
| P2 | 0.0419 (4) | 0.0577 (4) | 0.0489 (4) | 0.0108 (3) | 0.0264 (3) | −0.0027 (3) |
| O1 | 0.0561 (11) | 0.0557 (11) | 0.0553 (10) | −0.0095 (9) | 0.0223 (9) | 0.0121 (8) |
| O2 | 0.0436 (10) | 0.0838 (13) | 0.0508 (10) | 0.0106 (9) | 0.0235 (8) | −0.0090 (9) |
| N1 | 0.0411 (10) | 0.0383 (10) | 0.0520 (11) | −0.0033 (8) | 0.0259 (9) | 0.0042 (8) |
| N2 | 0.0379 (10) | 0.0403 (10) | 0.0422 (10) | −0.0024 (8) | 0.0236 (9) | 0.0005 (8) |
| N3 | 0.0466 (12) | 0.0641 (13) | 0.0494 (12) | 0.0124 (10) | 0.0252 (10) | −0.0099 (10) |
| C1 | 0.0760 (19) | 0.0373 (12) | 0.0700 (17) | −0.0044 (12) | 0.0506 (15) | 0.0060 (12) |
| C2 | 0.078 (2) | 0.073 (2) | 0.107 (3) | 0.0026 (16) | 0.068 (2) | 0.0189 (18) |
| C3 | 0.115 (3) | 0.099 (3) | 0.179 (5) | 0.010 (2) | 0.117 (4) | 0.033 (3) |
| C4 | 0.209 (6) | 0.100 (3) | 0.214 (7) | 0.000 (4) | 0.188 (6) | 0.021 (4) |
| C5 | 0.230 (7) | 0.102 (3) | 0.125 (4) | −0.022 (4) | 0.145 (5) | 0.002 (3) |
| C6 | 0.123 (3) | 0.073 (2) | 0.079 (2) | −0.011 (2) | 0.068 (2) | 0.0041 (17) |
| C7 | 0.0567 (15) | 0.0437 (13) | 0.0543 (14) | 0.0071 (12) | 0.0276 (13) | 0.0102 (11) |
| C8 | 0.0617 (19) | 0.074 (2) | 0.083 (2) | 0.0110 (15) | 0.0385 (17) | 0.0006 (17) |
| C9 | 0.092 (3) | 0.108 (3) | 0.121 (3) | 0.033 (3) | 0.062 (3) | −0.007 (3) |
| C10 | 0.123 (4) | 0.075 (2) | 0.100 (3) | 0.025 (3) | 0.045 (3) | −0.020 (2) |
| C11 | 0.097 (3) | 0.0507 (18) | 0.093 (2) | 0.0058 (18) | 0.032 (2) | −0.0062 (17) |
| C12 | 0.0599 (17) | 0.0423 (14) | 0.0785 (19) | 0.0003 (12) | 0.0277 (15) | 0.0001 (13) |
| C13 | 0.0405 (12) | 0.0342 (11) | 0.0434 (12) | −0.0013 (9) | 0.0271 (10) | −0.0025 (9) |
| C14 | 0.0411 (12) | 0.0358 (11) | 0.0413 (12) | −0.0008 (9) | 0.0247 (10) | −0.0031 (9) |
| C15 | 0.0409 (13) | 0.0422 (12) | 0.0499 (13) | −0.0036 (10) | 0.0240 (11) | −0.0022 (10) |
| C16 | 0.0417 (13) | 0.0513 (14) | 0.0450 (13) | 0.0003 (11) | 0.0168 (11) | −0.0042 (11) |
| C17 | 0.0599 (16) | 0.0496 (14) | 0.0438 (13) | 0.0060 (12) | 0.0246 (13) | 0.0061 (11) |
| C18 | 0.0520 (15) | 0.0495 (13) | 0.0479 (13) | −0.0043 (11) | 0.0277 (12) | 0.0077 (11) |
| C19 | 0.0439 (13) | 0.0428 (12) | 0.0404 (11) | −0.0031 (10) | 0.0262 (10) | −0.0004 (10) |
| C20 | 0.0435 (13) | 0.0458 (12) | 0.0399 (12) | −0.0051 (10) | 0.0254 (10) | 0.0002 (10) |
| C21 | 0.0401 (14) | 0.0548 (15) | 0.0686 (17) | 0.0039 (11) | 0.0294 (13) | 0.0092 (13) |
| C22 | 0.094 (2) | 0.0589 (18) | 0.116 (3) | 0.0194 (17) | 0.078 (2) | 0.0013 (18) |
| C23 | 0.097 (3) | 0.062 (2) | 0.186 (5) | 0.015 (2) | 0.097 (3) | −0.006 (3) |
| C24 | 0.082 (3) | 0.058 (2) | 0.201 (6) | 0.013 (2) | 0.046 (4) | 0.018 (3) |
| C25 | 0.122 (4) | 0.066 (3) | 0.110 (3) | −0.002 (2) | 0.023 (3) | 0.035 (2) |
| C26 | 0.093 (3) | 0.075 (2) | 0.077 (2) | −0.0154 (19) | 0.030 (2) | 0.0097 (18) |
| C27 | 0.0699 (18) | 0.0457 (14) | 0.0656 (16) | 0.0075 (12) | 0.0440 (15) | −0.0001 (12) |
| C28 | 0.075 (2) | 0.091 (2) | 0.089 (2) | −0.0115 (18) | 0.0504 (19) | 0.0041 (19) |
| C29 | 0.111 (3) | 0.110 (3) | 0.145 (4) | −0.030 (3) | 0.093 (3) | −0.004 (3) |
| C30 | 0.185 (5) | 0.087 (3) | 0.144 (4) | −0.023 (3) | 0.130 (4) | 0.002 (3) |
| C31 | 0.161 (5) | 0.121 (4) | 0.110 (3) | 0.015 (3) | 0.095 (4) | 0.040 (3) |
| C32 | 0.103 (3) | 0.103 (3) | 0.083 (2) | 0.023 (2) | 0.056 (2) | 0.029 (2) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Ca1—O1 | 2.2581 (18) | C10—H10A | 0.9300 |
| Ca1—O1$^{i}$ | 2.2581 (18) | C11—C12 | 1.376 (4) |
| Ca1—O2 | 2.2646 (18) | C11—H11A | 0.9300 |
| Ca1—O2$^{i}$ | 2.2646 (18) | C12—H12A | 0.9300 |
| Ca1—N2$^{i}$ | 2.5513 (18) | C13—C14 | 1.486 (3) |
| Ca1—N2 | 2.5513 (18) | C14—C19 | 1.377 (3) |
| Ca1—P2 | 3.4369 (8) | C14—C15 | 1.377 (3) |

| | | | |
|---|---|---|---|
| Ca1—P2$^{i}$ | 3.4369 (8) | C15—C16 | 1.381 (3) |
| Ca1—P1 | 3.4403 (7) | C15—H15A | 0.9300 |
| Ca1—P1$^{i}$ | 3.4403 (7) | C16—C17 | 1.382 (4) |
| P1—O1 | 1.4837 (18) | C16—H16A | 0.9300 |
| P1—N1 | 1.6406 (19) | C17—C18 | 1.378 (4) |
| P1—C1 | 1.794 (3) | C17—H17A | 0.9300 |
| P1—C7 | 1.803 (3) | C18—C19 | 1.374 (3) |
| P2—O2 | 1.4888 (19) | C18—H18A | 0.9300 |
| P2—N3 | 1.631 (2) | C19—C20 | 1.483 (3) |
| P2—C27 | 1.799 (3) | C20—N3$^{i}$ | 1.302 (3) |
| P2—C21 | 1.808 (3) | C21—C22 | 1.363 (4) |
| N1—C13 | 1.290 (3) | C21—C26 | 1.367 (4) |
| N2—C20 | 1.369 (3) | C22—C23 | 1.373 (5) |
| N2—C13 | 1.378 (3) | C22—H22A | 0.9300 |
| N3—C20$^{i}$ | 1.302 (3) | C23—C24 | 1.313 (7) |
| C1—C2 | 1.369 (4) | C23—H23A | 0.9300 |
| C1—C6 | 1.379 (4) | C24—C25 | 1.351 (8) |
| C2—C3 | 1.388 (5) | C24—H24A | 0.9300 |
| C2—H2B | 0.9300 | C25—C26 | 1.393 (6) |
| C3—C4 | 1.316 (8) | C25—H25A | 0.9300 |
| C3—H3B | 0.9300 | C26—H26A | 0.9300 |
| C4—C5 | 1.354 (7) | C27—C32 | 1.377 (4) |
| C4—H4A | 0.9300 | C27—C28 | 1.380 (4) |
| C5—C6 | 1.393 (6) | C28—C29 | 1.390 (5) |
| C5—H5A | 0.9300 | C28—H28A | 0.9300 |
| C6—H6A | 0.9300 | C29—C30 | 1.344 (7) |
| C7—C8 | 1.382 (4) | C29—H29A | 0.9300 |
| C7—C12 | 1.382 (4) | C30—C31 | 1.350 (7) |
| C8—C9 | 1.381 (5) | C30—H30A | 0.9300 |
| C8—H8A | 0.9300 | C31—C32 | 1.366 (6) |
| C9—C10 | 1.353 (6) | C31—H31A | 0.9300 |
| C9—H9A | 0.9300 | C32—H32A | 0.9300 |
| C10—C11 | 1.365 (6) | | |

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| O1—Ca1—O1$^{i}$ | 81.34 (11) | C4—C5—H5A | 119.5 |
| O1—Ca1—O2 | 93.49 (8) | C6—C5—H5A | 119.5 |
| O1$^{i}$—Ca1—O2 | 157.41 (7) | C1—C6—C5 | 119.0 (4) |
| O1—Ca1—O2$^{i}$ | 157.41 (7) | C1—C6—H6A | 120.5 |
| O1$^{i}$—Ca1—O2$^{i}$ | 93.49 (8) | C5—C6—H6A | 120.5 |
| O2—Ca1—O2$^{i}$ | 99.09 (11) | C8—C7—C12 | 118.9 (3) |
| O1—Ca1—N2$^{i}$ | 110.51 (6) | C8—C7—P1 | 119.1 (2) |
| O1$^{i}$—Ca1—N2$^{i}$ | 80.81 (6) | C12—C7—P1 | 121.9 (2) |
| O2—Ca1—N2$^{i}$ | 80.48 (6) | C9—C8—C7 | 119.2 (3) |
| O2$^{i}$—Ca1—N2$^{i}$ | 90.12 (6) | C9—C8—H8A | 120.4 |
| O1—Ca1—N2 | 80.81 (6) | C7—C8—H8A | 120.4 |
| O1$^{i}$—Ca1—N2 | 110.51 (6) | C10—C9—C8 | 121.5 (4) |
| O2—Ca1—N2 | 90.12 (6) | C10—C9—H9A | 119.2 |
| O2$^{i}$—Ca1—N2 | 80.48 (6) | C8—C9—H9A | 119.2 |

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| N2$^{i}$—Ca1—N2 | 165.55 (9) | C9—C10—C11 | 119.8 (4) |
| O1—Ca1—P2 | 97.95 (6) | C9—C10—H10A | 120.1 |
| O1$^{i}$—Ca1—P2 | 139.82 (5) | C11—C10—H10A | 120.1 |
| O2—Ca1—P2 | 18.93 (4) | C10—C11—C12 | 119.9 (4) |
| O2$^{i}$—Ca1—P2 | 100.02 (6) | C10—C11—H11A | 120.0 |
| N2$^{i}$—Ca1—P2 | 61.66 (4) | C12—C11—H11A | 120.0 |
| N2—Ca1—P2 | 108.97 (4) | C11—C12—C7 | 120.7 (3) |
| O1—Ca1—P2$^{i}$ | 139.82 (5) | C11—C12—H12A | 119.6 |
| O1$^{i}$—Ca1—P2$^{i}$ | 97.95 (6) | C7—C12—H12A | 119.6 |
| O2—Ca1—P2$^{i}$ | 100.02 (6) | N1—C13—N2 | 129.4 (2) |
| O2$^{i}$—Ca1—P2$^{i}$ | 18.93 (4) | N1—C13—C14 | 120.7 (2) |
| N2$^{i}$—Ca1—P2$^{i}$ | 108.97 (5) | N2—C13—C14 | 109.96 (18) |
| N2—Ca1—P2$^{i}$ | 61.66 (4) | C19—C14—C15 | 120.9 (2) |
| P2—Ca1—P2$^{i}$ | 107.00 (3) | C19—C14—C13 | 106.42 (19) |
| O1—Ca1—P1 | 18.51 (4) | C15—C14—C13 | 132.6 (2) |
| O1$^{i}$—Ca1—P1 | 90.49 (5) | C14—C15—C16 | 118.0 (2) |
| O2—Ca1—P1 | 91.20 (5) | C14—C15—H15A | 121.0 |
| O2$^{i}$—Ca1—P1 | 141.54 (5) | C16—C15—H15A | 121.0 |
| N2$^{i}$—Ca1—P1 | 128.23 (4) | C15—C16—C17 | 120.8 (2) |
| N2—Ca1—P1 | 62.42 (4) | C15—C16—H16A | 119.6 |
| P2—Ca1—P1 | 101.274 (17) | C17—C16—H16A | 119.6 |
| P2$^{i}$—Ca1—P1 | 122.787 (15) | C18—C17—C16 | 121.1 (2) |
| O1—Ca1—P1$^{i}$ | 90.49 (5) | C18—C17—H17A | 119.5 |
| O1$^{i}$—Ca1—P1$^{i}$ | 18.51 (4) | C16—C17—H17A | 119.5 |
| O2—Ca1—P1$^{i}$ | 141.54 (5) | C19—C18—C17 | 117.8 (2) |
| O2$^{i}$—Ca1—P1$^{i}$ | 91.20 (5) | C19—C18—H18A | 121.1 |
| N2$^{i}$—Ca1—P1$^{i}$ | 62.42 (4) | C17—C18—H18A | 121.1 |
| N2—Ca1—P1$^{i}$ | 128.23 (4) | C18—C19—C14 | 121.4 (2) |
| P2—Ca1—P1$^{i}$ | 122.787 (15) | C18—C19—C20 | 132.5 (2) |
| P2$^{i}$—Ca1—P1$^{i}$ | 101.274 (17) | C14—C19—C20 | 106.04 (19) |
| P1—Ca1—P1$^{i}$ | 103.44 (3) | N3$^{i}$—C20—N2 | 129.2 (2) |
| O1—P1—N1 | 120.24 (10) | N3$^{i}$—C20—C19 | 120.1 (2) |
| O1—P1—C1 | 109.60 (13) | N2—C20—C19 | 110.65 (18) |
| N1—P1—C1 | 103.94 (12) | C22—C21—C26 | 117.6 (3) |
| O1—P1—C7 | 110.69 (12) | C22—C21—P2 | 121.9 (2) |
| N1—P1—C7 | 104.01 (11) | C26—C21—P2 | 120.4 (3) |
| C1—P1—C7 | 107.54 (12) | C21—C22—C23 | 121.3 (4) |
| N1—P1—Ca1 | 91.43 (7) | C21—C22—H22A | 119.3 |
| C1—P1—Ca1 | 123.78 (9) | C23—C22—H22A | 119.3 |
| C7—P1—Ca1 | 120.67 (9) | C24—C23—C22 | 120.9 (5) |
| O2—P2—N3 | 119.32 (10) | C24—C23—H23A | 119.5 |
| O2—P2—C27 | 112.18 (13) | C22—C23—H23A | 119.5 |
| N3—P2—C27 | 105.94 (13) | C23—C24—C25 | 119.8 (4) |
| O2—P2—C21 | 108.99 (13) | C23—C24—H24A | 120.1 |
| N3—P2—C21 | 104.66 (12) | C25—C24—H24A | 120.1 |
| C27—P2—C21 | 104.56 (12) | C24—C25—C26 | 120.5 (4) |
| N3—P2—Ca1 | 91.97 (7) | C24—C25—H25A | 119.7 |
| C27—P2—Ca1 | 114.13 (9) | C26—C25—H25A | 119.7 |

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| C21—P2—Ca1 | 131.54 (10) | C21—C26—C25 | 119.7 (4) |
| P1—O1—Ca1 | 132.60 (10) | C21—C26—H26A | 120.1 |
| P2—O2—Ca1 | 131.50 (10) | C25—C26—H26A | 120.1 |
| C13—N1—P1 | 128.67 (17) | C32—C27—C28 | 117.7 (3) |
| C20—N2—C13 | 106.88 (18) | C32—C27—P2 | 124.0 (3) |
| C20—N2—Ca1 | 125.26 (14) | C28—C27—P2 | 118.3 (2) |
| C13—N2—Ca1 | 124.95 (14) | C27—C28—C29 | 120.3 (4) |
| C20$^{i}$—N3—P2 | 127.09 (18) | C27—C28—H28A | 119.9 |
| C2—C1—C6 | 119.0 (3) | C29—C28—H28A | 119.9 |
| C2—C1—P1 | 122.6 (2) | C30—C29—C28 | 120.3 (4) |
| C6—C1—P1 | 118.4 (3) | C30—C29—H29A | 119.9 |
| C1—C2—C3 | 119.6 (4) | C28—C29—H29A | 119.9 |
| C1—C2—H2B | 120.2 | C29—C30—C31 | 120.1 (4) |
| C3—C2—H2B | 120.2 | C29—C30—H30A | 120.0 |
| C4—C3—C2 | 121.7 (5) | C31—C30—H30A | 120.0 |
| C4—C3—H3B | 119.1 | C30—C31—C32 | 120.7 (4) |
| C2—C3—H3B | 119.1 | C30—C31—H31A | 119.7 |
| C3—C4—C5 | 119.8 (4) | C32—C31—H31A | 119.7 |
| C3—C4—H4A | 120.1 | C31—C32—C27 | 121.0 (4) |
| C5—C4—H4A | 120.1 | C31—C32—H32A | 119.5 |
| C4—C5—C6 | 120.9 (5) | C27—C32—H32A | 119.5 |

Symmetry code: (i) $-x, y, -z+1/2$.