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Bis[1,3-bis(diphenylphosphinoylimino)isoindolinato-κ^3O,N,O']-calcium(II)

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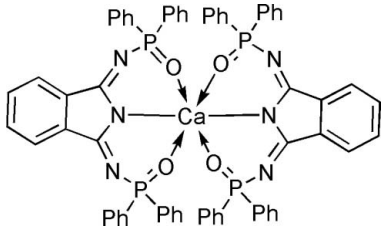
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.007 Å; R factor = 0.050; wR factor = 0.135; data-to-parameter ratio = 13.9.

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
β = 126.1720 (10)°
V = 5627.4 (9) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 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

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supplementary materials

Acta Cryst. (2008). E**64**, m160 [**doi:10.1107/S1600536807065440**]

Bis[1,3-bis(diphenylphosphinoylimino)isoindolinato-κ^3O,N,O']calcium(II)

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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).

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, $CDCl_3$, δ): 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, $CDCl_3$, δ): 20.2(*s*).

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) = 1.2U_{eq} (parent atom).

Figures

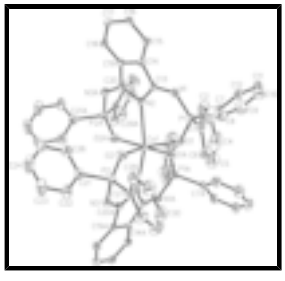


Fig. 1. Molecular structure of I, showing the atom-labeling scheme and 20% probability displacement ellipsoids. Symmetry codes: (i) -*x*, *y*, -*z* + 1/2.

Bis[1,3-bis(diphenylphosphinoylimino)isoindolinato-κ^3O,N,O^1]calcium(II)

Crystal data

$[Ca(C_{32}H_{24}N_3O_2P_2)_2]$	F_{000} = 2344
M_r = 1129.04	D_x = 1.333 Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -C 2yc	Cell parameters from 4426 reflections
a = 26.351 (2) Å	θ = 2.4–25.9º
b = 12.4790 (11) Å	μ = 0.28 mm^{-1}
c = 21.1997 (19) Å	*T* = 293 (2) K
β = 126.1720 (10)º	Block, pink
V = 5627.4 (9) Å^3	0.20 × 0.15 × 0.10 mm
Z = 4	

Data collection

Bruker SMART CCD diffractometer	4959 independent reflections
Radiation source: fine-focus sealed tube	4175 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.019
T = 293(2) K	θ_{max} = 25.0º
ω scan	θ_{min} = 1.9º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	*h* = −31→17
T_{min} = 0.837, T_{max} = 0.973	*k* = −14→14
11452 measured reflections	*l* = −22→25

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.050	H-atom parameters constrained
$wR(F^2)$ = 0.135	$w = 1/[\sigma^2(F_o^2) + (0.075P)^2 + 4.1489P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.04	$(\Delta/\sigma)_{max}$ = 0.001
4959 reflections	$\Delta\rho_{max}$ = 0.40 e Å^{-3}
357 parameters	$\Delta\rho_{min}$ = −0.25 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 ($Å^2$)

	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 (Å^2)

	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, °)

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)

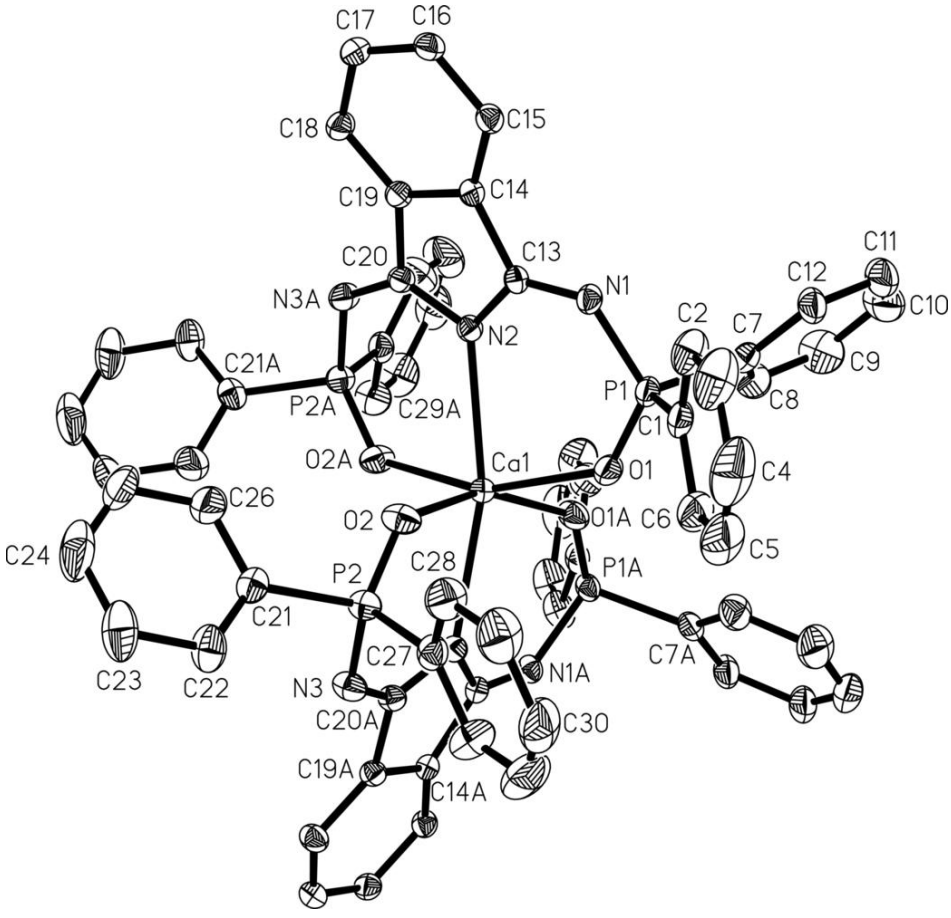
N1—C13	1.290 (3)	C21—C26	1.367 (4)
N2—C20	1.369 (3)	C22—C23	1.373 (5)
N2—C13	1.378 (3)	C22—H22A	0.9300
N3—C20^{i}	1.302 (3)	C23—C24	1.313 (7)
C1—C2	1.369 (4)	C23—H23A	0.9300
C1—C6	1.379 (4)	C24—C25	1.351 (8)
C2—C3	1.388 (5)	C24—H24A	0.9300
C2—H2B	0.9300	C25—C26	1.393 (6)
C3—C4	1.316 (8)	C25—H25A	0.9300
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)		
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
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
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 codes: (i) −*x*, *y*, −*z*+1/2.

Fig. 1


C17
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C12
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C9
C21A
P2A
C29A
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Ca1
O1
C4
C26
O2
O1A
C6
C24
C5
P2
C28
P1A
C21
C27
C7A
C23
C22
N3
N1A
C20A
C30
C19A
C14A