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[5,10,15,20-Tetrakis(4-*tert*-butylphenyl)-porphyrinato-κ^4N]zinc(II) toluene solvate

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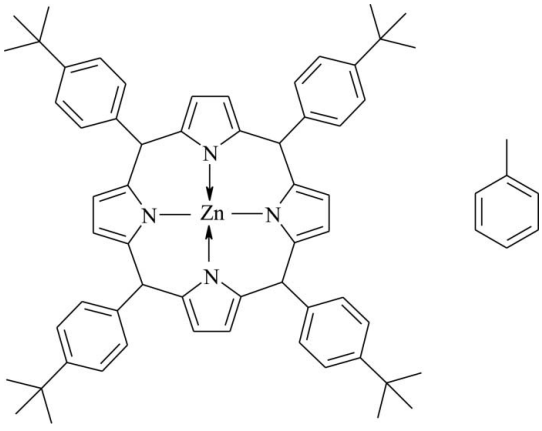
Key indicators: single-crystal X-ray study; T = 85 K; mean σ(C–C) = 0.004 Å; disorder in solvent or counterion; R factor = 0.046; wR factor = 0.122; data-to-parameter ratio = 13.3.

The structure of the title compound, $[Zn(C_{60}H_{60}N_4)]\cdot C_7H_8$, represents a typical clathrate containing a host molecule of [5,10,15,20-tetrakis(4-*tert*-butylphenyl)porphyrinato]zinc(II) and a toluene guest molecule. The Zn atom occupies an inversion center and exhibits ideal square-planar coordination, while the porphyrin group remains perfectly flat. The toluene molecule lies on an inversion center and is disordered.

Related literature

For related literature, see: Berezin (1981); Mele *et al.* (2003, 2007); Allen (2002).



Experimental

Crystal data

$[Zn(C_{60}H_{60}N_4)]\cdot C_7H_8$
M_r = 994.64
Monoclinic, $P2_1/n$
a = 16.0277 (16) Å
b = 9.5884 (14) Å
c = 16.8714 (16) Å
β = 93.892 (8)°
V = 2586.8 (5) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.52 mm^{-1}
T = 85.0 (1) K
0.25 × 0.20 × 0.10 mm

Data collection

Oxford Diffraction Xcalibur diffractometer
Absorption correction: none
14020 measured reflections
4533 independent reflections
3375 reflections with $I > 2\sigma(I)$
R_{int} = 0.060

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.122
S = 1.05
4533 reflections
341 parameters
93 restraints
H-atom parameters not refined
$\Delta\rho_{max}$ = 0.42 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—N2	2.024 (2)	Zn1—N1	2.054 (2)
N2—Zn1—N2^i	180	N2—Zn1—N1	89.94 (8)
N2—Zn1—N1^i	90.06 (8)		

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

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2002); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2006); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 1990); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PV2028).

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  doi:10.1107/S1600536807045953

supplementary materials

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[5,10,15,20-Tetrakis(4-*tert*-butylphenyl)porphyrinato-κ^4N]zinc(II) toluene solvate

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Comment

Physicochemical properties of metallo-porphyrins depend on the complexed metal and the kind of peripherally and/or axially fixed substituents. These factors influence the electronic density distribution within the core of the macrocycle, thus determining both its stability and reactivity (Berezin, 1981). Therefore, structural details are essential in learning the basic chemistry of such compounds featuring unique properties, *e.g.* photocatalytic activity (Mele *et al.*, 2007). 5,10,15,20-Tetrakis(4-*tert*-butylphenyl)porphyrinato zinc(II) (ZnPp), when crystallized from a toluene solution yielded a typical lattice clathrate with ZnPp (host) to toluene (guest) 1:1 stoichiometry. The structure of the title *tert*-butylphenyl *meso*-substituted ZnPp derivative has been solved and reported for the first time in this work.

The crystal lattice consists of discrete centrosymmetrical molecules of ZnPp (Fig. 1) and disordered molecules of toluene, located at the inversion centre. This is a typical case of toluene disorder exhibiting two discrete positions; one molecule is staggered 180° with respect to the other one. The zinc atom is found in a plane defined by the four pyrrole-nitrogen atoms and the N—Zn—N bond angles are *ca* 90°, showing ideal square-planar coordination. The macrocycle itself shows no apparent distortion and one may consider it as "perfectly flat". The *meso* substituted benzene rings are not perpendicular to the plane of the macrocycle, yielding dihedral angles of 78.44 (7)° and 79.17 (7)°. The geometry of the porphyrin core proved typical as for the family of similar zinc porphyrins substituted in their *meso* position by four identical phenyl derivatives (Allen, 2002). The unit cell packing of the title compound is shown in Fig. 2.

Experimental

5,10,15,20-tetrakis(4-*tert*-butylphenyl)porphyrinato zinc(II) was synthesized according to a typical procedure (Mele *et al.*, 2003), applying $ZnCl_2$ as the metal source. Pure monocrystals for X-ray diffraction measurements were obtained by multiple re-crystallization from toluene (reagent grade) at room temperature, yielding the final product in the form of a toluene solvate.

Refinement

The hydrogen atoms were included in the refinement at geometrically idealized positions with C—H distances 0.96 Å for methyl and toluene solvate and 0.93 Å for the rest of the hydrogen atoms and U_{eq} = 1.5 and 1.2 times U_{eq} of the parent atoms, respectively. The toluene solvate was lying about inversion centers and was disordered.

Figures

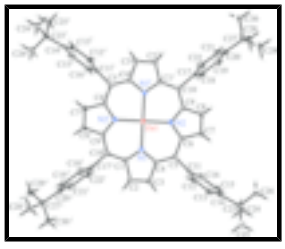


Fig. 1. The molecular structure of the title compound, showing 50% displacement ellipsoids and arbitrary spheres for the H atoms. Symmetry code: (i) −*x* + 1, −*y* + 1, −*z* + 1.

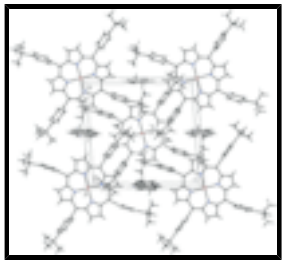


Fig. 2. The packing diagram of the title compound.

[5,10,15,20-Tetrakis(4-*tert*-butylphenyl)porphyrinato-κ^4*N*]zinc(II) toluene solvate

Crystal data

$[Zn(C_{60}H_{60}N_4)]\cdot C_7H_8$	F_{000} = 1056
M_r = 994.64	D_x = 1.277 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 4533 reflections
a = 16.0277 (16) Å	θ = 3.2–25.0º
b = 9.5884 (14) Å	μ = 0.52 mm^{-1}
c = 16.8714 (16) Å	*T* = 85.0 (1) K
β = 93.892 (8)º	Plate, colourless
V = 2586.8 (5) Å^3	0.25 × 0.20 × 0.10 mm
Z = 2	

Data collection

Oxford Diffraction Xcalibur diffractometer	4533 independent reflections
Radiation source: Enhanced (Mo) X-ray Source	3375 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.060
Detector resolution: 1024x1024 with blocks 2x2 pixels mm^{-1}	θ_{max} = 25.0º
T = 85.0(1) K	θ_{min} = 3.2º
ω scans	*h* = −18→19
Absorption correction: none	*k* = −7→11
14020 measured reflections	*l* = −20→19

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.046$	H-atom parameters not refined
$wR(F^2) = 0.122$	$w = 1/[\sigma^2(F_o^2) + (0.0778P)^2 + 0.1154P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.05$	$(\Delta/\sigma)_{max} < 0.001$
4533 reflections	$\Delta\rho_{max} = 0.42$ e Å^{-3}
341 parameters	$\Delta\rho_{min} = -0.37$ e Å^{-3}
93 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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}	Occ. (<1)
Zn1	0.5000	0.5000	0.5000	0.01341 (15)	
N1	0.62401 (12)	0.5020 (2)	0.47623 (12)	0.0138 (4)	
N2	0.46708 (13)	0.5079 (2)	0.38213 (12)	0.0140 (5)	
C1	0.69152 (15)	0.5006 (3)	0.53100 (15)	0.0132 (5)	
C2	0.76805 (15)	0.5049 (3)	0.49013 (15)	0.0141 (5)	
H2A	0.8222	0.5045	0.5136	0.017*	
C3	0.74594 (15)	0.5094 (3)	0.41128 (16)	0.0155 (5)	
H3A	0.7821	0.5131	0.3704	0.019*	
C4	0.65585 (15)	0.5073 (3)	0.40256 (15)	0.0132 (5)	
C5	0.60800 (15)	0.5118 (2)	0.32961 (15)	0.0134 (5)	
C6	0.52031 (15)	0.5115 (2)	0.32132 (15)	0.0134 (5)	
C7	0.47170 (16)	0.5157 (3)	0.24613 (15)	0.0150 (5)	
H7A	0.4924	0.5188	0.1960	0.018*	
C8	0.39000 (16)	0.5143 (3)	0.26257 (15)	0.0158 (6)	
H8A	0.3442	0.5167	0.2257	0.019*	
C9	0.38730 (15)	0.5085 (2)	0.34701 (15)	0.0126 (5)	
C10	0.31249 (15)	0.5036 (3)	0.38640 (15)	0.0132 (5)	

C11	0.65151 (15)	0.5163 (3)	0.25357 (15)	0.0144 (5)	
C12	0.68218 (15)	0.3966 (3)	0.21983 (16)	0.0185 (6)	
H12A	0.6849	0.3143	0.2490	0.022*	
C13	0.70888 (16)	0.3972 (3)	0.14360 (16)	0.0179 (6)	
H13A	0.7290	0.3150	0.1226	0.021*	
C14	0.70640 (15)	0.5172 (3)	0.09771 (15)	0.0161 (6)	
C15	0.68138 (16)	0.6404 (3)	0.13437 (15)	0.0187 (6)	
H15A	0.6832	0.7244	0.1070	0.022*	
C16	0.65410 (16)	0.6393 (3)	0.21022 (16)	0.0199 (6)	
H16A	0.6372	0.7223	0.2327	0.024*	
C17	0.23273 (15)	0.5053 (3)	0.33498 (14)	0.0136 (5)	
C18	0.20367 (16)	0.3871 (3)	0.29459 (16)	0.0194 (6)	
H18A	0.2318	0.3030	0.3031	0.023*	
C19	0.13317 (16)	0.3916 (3)	0.24153 (16)	0.0200 (6)	
H19A	0.1156	0.3108	0.2149	0.024*	
C20	0.08848 (15)	0.5146 (3)	0.22766 (15)	0.0152 (5)	
C21	0.11813 (16)	0.6330 (3)	0.26884 (16)	0.0202 (6)	
H21A	0.0900	0.7172	0.2607	0.024*	
C22	0.18838 (16)	0.6282 (3)	0.32149 (16)	0.0202 (6)	
H22A	0.2061	0.7089	0.3482	0.024*	
C23	0.72525 (16)	0.5201 (3)	0.00997 (15)	0.0169 (6)	
C24	0.74775 (18)	0.3764 (3)	−0.02088 (17)	0.0249 (7)	
H24A	0.7967	0.3423	0.0089	0.037*	
H24B	0.7587	0.3831	−0.0760	0.037*	
H24C	0.7020	0.3134	−0.0149	0.037*	
C25	0.79766 (17)	0.6211 (3)	−0.00308 (16)	0.0224 (6)	
H25A	0.8472	0.5898	0.0268	0.034*	
H25B	0.7833	0.7128	0.0143	0.034*	
H25C	0.8077	0.6238	−0.0585	0.034*	
C26	0.64640 (17)	0.5725 (3)	−0.03894 (16)	0.0245 (7)	
H26A	0.6006	0.5103	−0.0316	0.037*	
H26B	0.6572	0.5755	−0.0942	0.037*	
H26C	0.6324	0.6643	−0.0214	0.037*	
C27	0.01147 (16)	0.5261 (3)	0.16840 (16)	0.0183 (6)	
C28	−0.01266 (18)	0.3852 (3)	0.13143 (17)	0.0258 (7)	
H28A	−0.0257	0.3211	0.1725	0.039*	
H28B	0.0332	0.3494	0.1038	0.039*	
H28C	−0.0607	0.3964	0.0948	0.039*	
C29	0.03216 (18)	0.6284 (3)	0.10215 (17)	0.0253 (7)	
H29A	−0.0153	0.6368	0.0646	0.038*	
H29B	0.0792	0.5939	0.0757	0.038*	
H29C	0.0455	0.7180	0.1249	0.038*	
C30	−0.06321 (17)	0.5829 (4)	0.21073 (18)	0.0303 (7)	
H30A	−0.0765	0.5197	0.2522	0.045*	
H30B	−0.1107	0.5921	0.1732	0.045*	
H30C	−0.0492	0.6725	0.2333	0.045*	
C31	0.9921 (2)	0.5396 (5)	0.4346 (2)	0.0522 (10)	
H31	0.9935	0.5212	0.3788	0.063*	
C32	0.9924 (4)	0.5772 (9)	0.5186 (4)	0.0404 (15)	0.50

C33	0.9924 (4)	0.5879 (8)	0.5862 (4)	0.0391 (16)	0.50
H33	0.9930	0.6022	0.6426	0.047*	0.50
C34	0.9744 (2)	0.7095 (5)	0.5393 (3)	0.0689 (12)	
H34A	0.9773	0.7163	0.5962	0.103*	0.50
H34B	1.0141	0.7724	0.5186	0.103*	0.50
H34C	0.9191	0.7334	0.5184	0.103*	0.50
H34	0.9632	0.8016	0.5582	0.083*	0.50
C35	0.9769 (4)	0.6616 (10)	0.4494 (5)	0.0597 (19)	0.50
H35	0.9667	0.7277	0.4072	0.072*	0.50

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0123 (2)	0.0152 (2)	0.0127 (2)	0.00000 (17)	0.00079 (15)	0.00060 (18)
N1	0.0152 (11)	0.0134 (11)	0.0128 (11)	0.0002 (9)	−0.0001 (8)	0.0003 (9)
N2	0.0113 (10)	0.0149 (11)	0.0159 (11)	0.0009 (9)	0.0011 (8)	0.0009 (9)
C1	0.0151 (12)	0.0092 (12)	0.0153 (13)	−0.0010 (10)	0.0014 (10)	0.0022 (11)
C2	0.0100 (12)	0.0140 (13)	0.0181 (13)	−0.0007 (10)	−0.0005 (10)	0.0005 (11)
C3	0.0141 (12)	0.0137 (13)	0.0190 (14)	0.0005 (11)	0.0046 (10)	0.0003 (11)
C4	0.0133 (12)	0.0111 (12)	0.0154 (13)	0.0003 (10)	0.0022 (10)	0.0001 (11)
C5	0.0163 (13)	0.0078 (12)	0.0162 (13)	0.0002 (10)	0.0002 (10)	−0.0003 (11)
C6	0.0173 (13)	0.0092 (12)	0.0136 (13)	−0.0015 (10)	0.0010 (10)	−0.0011 (11)
C7	0.0177 (13)	0.0161 (13)	0.0113 (13)	−0.0021 (11)	0.0020 (10)	0.0008 (11)
C8	0.0156 (13)	0.0174 (14)	0.0137 (13)	0.0019 (11)	−0.0037 (10)	−0.0011 (11)
C9	0.0158 (13)	0.0070 (12)	0.0146 (13)	0.0000 (10)	−0.0019 (10)	−0.0015 (11)
C10	0.0149 (12)	0.0089 (12)	0.0156 (13)	−0.0005 (10)	−0.0007 (10)	−0.0013 (11)
C11	0.0109 (12)	0.0188 (14)	0.0130 (13)	−0.0024 (10)	−0.0018 (9)	−0.0014 (11)
C12	0.0156 (13)	0.0185 (14)	0.0214 (15)	0.0052 (11)	0.0018 (11)	0.0049 (12)
C13	0.0185 (14)	0.0154 (14)	0.0202 (14)	0.0033 (11)	0.0046 (11)	0.0001 (11)
C14	0.0106 (12)	0.0207 (14)	0.0167 (13)	−0.0010 (11)	−0.0019 (10)	−0.0012 (12)
C15	0.0217 (14)	0.0147 (14)	0.0199 (15)	−0.0017 (11)	0.0032 (11)	0.0016 (12)
C16	0.0210 (14)	0.0164 (14)	0.0226 (15)	−0.0022 (11)	0.0039 (11)	−0.0037 (12)
C17	0.0130 (12)	0.0160 (13)	0.0120 (12)	−0.0005 (11)	0.0035 (10)	0.0011 (11)
C18	0.0208 (14)	0.0144 (14)	0.0223 (15)	0.0036 (11)	−0.0041 (11)	−0.0003 (12)
C19	0.0227 (15)	0.0151 (14)	0.0213 (15)	−0.0020 (11)	−0.0049 (11)	−0.0040 (12)
C20	0.0125 (12)	0.0185 (14)	0.0146 (13)	−0.0016 (11)	0.0002 (10)	0.0022 (11)
C21	0.0200 (14)	0.0153 (14)	0.0248 (15)	0.0043 (11)	−0.0033 (11)	0.0039 (12)
C22	0.0169 (14)	0.0165 (14)	0.0266 (16)	−0.0017 (11)	−0.0037 (11)	−0.0030 (12)
C23	0.0163 (13)	0.0180 (14)	0.0163 (14)	0.0013 (11)	0.0011 (10)	0.0007 (11)
C24	0.0306 (16)	0.0256 (16)	0.0192 (15)	0.0001 (13)	0.0067 (12)	−0.0024 (13)
C25	0.0220 (15)	0.0262 (16)	0.0196 (15)	−0.0001 (12)	0.0054 (11)	0.0011 (13)
C26	0.0236 (15)	0.0333 (17)	0.0160 (15)	0.0008 (13)	−0.0016 (11)	−0.0021 (13)
C27	0.0147 (13)	0.0233 (15)	0.0165 (14)	0.0010 (11)	−0.0023 (10)	−0.0013 (11)
C28	0.0249 (15)	0.0256 (16)	0.0253 (16)	−0.0056 (12)	−0.0094 (12)	0.0000 (13)
C29	0.0240 (15)	0.0263 (16)	0.0245 (16)	−0.0014 (13)	−0.0048 (12)	0.0062 (13)
C30	0.0159 (15)	0.048 (2)	0.0259 (17)	0.0046 (14)	−0.0048 (12)	−0.0033 (15)
C31	0.0228 (18)	0.096 (3)	0.038 (2)	−0.014 (2)	−0.0018 (15)	0.016 (2)
C32	0.013 (3)	0.072 (4)	0.035 (3)	−0.013 (3)	0.002 (3)	−0.001 (3)

C33	0.022 (3)	0.062 (4)	0.033 (3)	−0.012 (3)	0.001 (3)	−0.001 (3)
C34	0.0255 (19)	0.086 (3)	0.095 (3)	−0.011 (2)	0.003 (2)	0.004 (2)
C35	0.031 (4)	0.071 (4)	0.075 (4)	−0.017 (4)	−0.011 (3)	0.044 (4)

Geometric parameters (Å, °)

Zn1—N2	2.024 (2)	C21—H21A	0.9300
Zn1—N1	2.054 (2)	C22—H22A	0.9300
N1—C1	1.374 (3)	C23—C24	1.525 (4)
N1—C4	1.376 (3)	C23—C25	1.539 (4)
N1—N2	2.882 (3)	C23—C26	1.546 (4)
N2—C9	1.372 (3)	C24—H24A	0.9600
N2—C6	1.379 (3)	C24—H24B	0.9600
C1—C10^{i}	1.400 (4)	C24—H24C	0.9600
C1—C2	1.448 (3)	C25—H25A	0.9600
C2—C3	1.354 (4)	C25—H25B	0.9600
C2—H2A	0.9300	C25—H25C	0.9600
C3—C4	1.442 (3)	C26—H26A	0.9600
C3—H3A	0.9300	C26—H26B	0.9600
C4—C5	1.406 (4)	C26—H26C	0.9600
C5—C6	1.403 (4)	C27—C28	1.527 (4)
C5—C11	1.502 (3)	C27—C30	1.535 (4)
C6—C7	1.444 (3)	C27—C29	1.540 (4)
C7—C8	1.357 (4)	C28—H28A	0.9600
C7—H7A	0.9300	C28—H28B	0.9600
C8—C9	1.429 (3)	C28—H28C	0.9600
C8—H8A	0.9300	C29—H29A	0.9600
C9—C10	1.411 (3)	C29—H29B	0.9600
C10—C1^{i}	1.400 (4)	C29—H29C	0.9600
C10—C17	1.496 (3)	C30—H30A	0.9600
C11—C12	1.386 (4)	C30—H30B	0.9600
C11—C16	1.390 (4)	C30—H30C	0.9600
C12—C13	1.383 (4)	C31—C35	1.224 (10)
C12—H12A	0.9300	C31—C33^{ii}	1.300 (9)
C13—C14	1.386 (4)	C31—C32^{ii}	1.383 (9)
C13—H13A	0.9300	C31—C32	1.461 (8)
C14—C15	1.404 (4)	C31—H31	0.9601
C14—C23	1.531 (4)	C32—C33	1.146 (9)
C15—C16	1.380 (4)	C32—C34	1.352 (9)
C15—H15A	0.9300	C32—C31^{ii}	1.383 (9)
C16—H16A	0.9300	C32—C35	1.427 (11)
C17—C18	1.386 (4)	C33—C31^{ii}	1.300 (9)
C17—C22	1.387 (4)	C33—C34	1.428 (9)
C18—C19	1.394 (4)	C33—H33	0.9600
C18—H18A	0.9300	C34—C35	1.588 (11)
C19—C20	1.392 (4)	C34—H34A	0.9600
C19—H19A	0.9300	C34—H34B	0.9600
C20—C21	1.397 (4)	C34—H34C	0.9600

C20—C27	1.539 (3)	C34—H34	0.9600
C21—C22	1.387 (4)	C35—H35	0.9599
N2—Zn1—N2^{i}	180	C23—C25—H25A	109.5
N2—Zn1—N1^{i}	90.06 (8)	C23—C25—H25B	109.5
N2^{i}—Zn1—N1^{i}	89.94 (8)	H25A—C25—H25B	109.5
N2—Zn1—N1	89.94 (8)	C23—C25—H25C	109.5
N2^{i}—Zn1—N1	90.06 (8)	H25A—C25—H25C	109.5
N1^{i}—Zn1—N1	180.000 (1)	H25B—C25—H25C	109.5
C1—N1—C4	106.52 (19)	C23—C26—H26A	109.5
C1—N1—Zn1	126.63 (16)	C23—C26—H26B	109.5
C4—N1—Zn1	126.84 (16)	H26A—C26—H26B	109.5
C1—N1—N2	171.20 (17)	C23—C26—H26C	109.5
C4—N1—N2	82.24 (14)	H26A—C26—H26C	109.5
C9—N2—C6	106.5 (2)	H26B—C26—H26C	109.5
C9—N2—Zn1	126.69 (17)	C28—C27—C30	108.7 (2)
C6—N2—Zn1	126.79 (17)	C28—C27—C29	109.1 (2)
C9—N2—N1	172.12 (17)	C30—C27—C29	109.0 (2)
C6—N2—N1	81.34 (14)	C28—C27—C20	111.8 (2)
Zn1—N2—N1	45.45 (6)	C30—C27—C20	109.9 (2)
C6—N2—N1^{iii}	134.36 (14)	C29—C27—C20	108.3 (2)
Zn1—N2—N1^{iii}	96.26 (6)	C27—C28—H28A	109.5
N1—N2—N1^{iii}	139.30 (6)	C27—C28—H28B	109.5
N1—C1—C10^{i}	125.6 (2)	H28A—C28—H28B	109.5
N1—C1—C2	109.5 (2)	C27—C28—H28C	109.5
C10^{i}—C1—C2	124.9 (2)	H28A—C28—H28C	109.5
C3—C2—C1	107.2 (2)	H28B—C28—H28C	109.5
C3—C2—H2A	126.4	C27—C29—H29A	109.5
C1—C2—H2A	126.4	C27—C29—H29B	109.5
C2—C3—C4	107.1 (2)	H29A—C29—H29B	109.5
C2—C3—H3A	126.5	C27—C29—H29C	109.5
C4—C3—H3A	126.5	H29A—C29—H29C	109.5
N1—C4—C5	125.3 (2)	H29B—C29—H29C	109.5
N1—C4—C3	109.8 (2)	C27—C30—H30A	109.5
C5—C4—C3	124.9 (2)	C27—C30—H30B	109.5
C6—C5—C4	124.8 (2)	H30A—C30—H30B	109.5
C6—C5—C11	115.8 (2)	C27—C30—H30C	109.5
C4—C5—C11	119.4 (2)	H30A—C30—H30C	109.5
N2—C6—C5	126.3 (2)	H30B—C30—H30C	109.5
N2—C6—C7	109.3 (2)	C35—C31—C33^{ii}	176.1 (6)
C5—C6—C7	124.4 (2)	C35—C31—C32^{ii}	133.5 (6)
C8—C7—C6	106.9 (2)	C33^{ii}—C31—C32^{ii}	50.5 (4)
C8—C7—H7A	126.5	C35—C31—C32	63.5 (6)
C6—C7—H7A	126.5	C33^{ii}—C31—C32	120.4 (6)
C7—C8—C9	107.4 (2)	C32^{ii}—C31—C32	70.0 (6)
C7—C8—H8A	126.3	C35—C31—H31	113.2

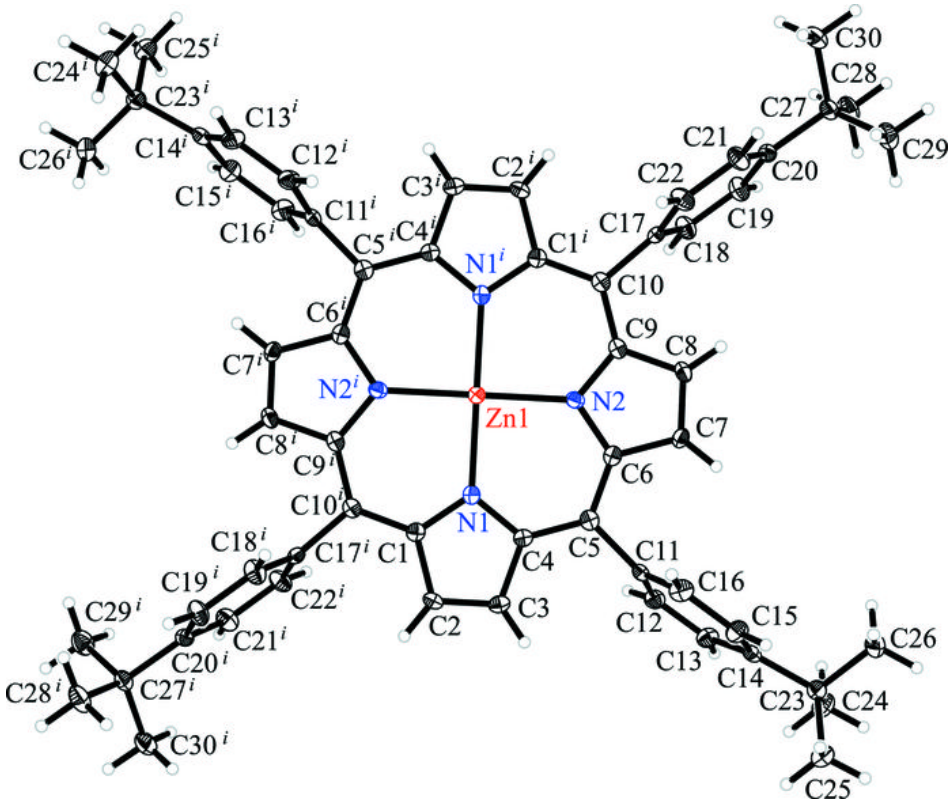
C9—C8—H8A	126.3	C33^{ii}—C31—H31	62.9
N2—C9—C10	126.4 (2)	C32^{ii}—C31—H31	113.3
N2—C9—C8	109.9 (2)	C32—C31—H31	175.9
C10—C9—C8	123.7 (2)	C33—C32—C34	69.1 (6)
C1^{i}—C10—C9	124.6 (2)	C33—C32—C31^{ii}	61.0 (6)
C1^{i}—C10—C17	118.8 (2)	C34—C32—C31^{ii}	130.2 (6)
C9—C10—C17	116.5 (2)	C33—C32—C35	138.8 (9)
C12—C11—C16	117.6 (2)	C34—C32—C35	69.6 (6)
C12—C11—C5	121.7 (2)	C31^{ii}—C32—C35	160.0 (8)
C16—C11—C5	120.4 (2)	C33—C32—C31	170.8 (9)
C11—C12—C13	121.3 (2)	C34—C32—C31	119.7 (6)
C11—C12—H12A	119.4	C31^{ii}—C32—C31	110.0 (6)
C13—C12—H12A	119.4	C35—C32—C31	50.1 (5)
C12—C13—C14	121.6 (2)	C33—C32—C32^{ii}	118.2 (9)
C12—C13—H13A	119.2	C34—C32—C32^{ii}	172.0 (8)
C14—C13—H13A	119.2	C31^{ii}—C32—C32^{ii}	57.2 (5)
C13—C14—C15	116.8 (2)	C35—C32—C32^{ii}	102.9 (8)
C13—C14—C23	123.7 (2)	C31—C32—C32^{ii}	52.7 (4)
C15—C14—C23	119.4 (2)	C32—C33—C31^{ii}	68.5 (6)
C16—C15—C14	121.3 (2)	C32—C33—C34	62.2 (6)
C16—C15—H15A	119.3	C31^{ii}—C33—C34	130.7 (6)
C14—C15—H15A	119.3	C32—C33—H33	176.9
C15—C16—C11	121.1 (2)	C31^{ii}—C33—H33	114.4
C15—C16—H16A	119.4	C34—C33—H33	114.8
C11—C16—H16A	119.4	C32—C33—H34A	103.4
C18—C17—C22	117.5 (2)	C31^{ii}—C33—H34A	171.9
C18—C17—C10	121.4 (2)	H33—C33—H34A	73.7
C22—C17—C10	120.9 (2)	C32—C34—C33	48.6 (4)
C17—C18—C19	121.4 (2)	C32—C34—C35	57.4 (5)
C17—C18—H18A	119.3	C33—C34—C35	106.0 (5)
C19—C18—H18A	119.3	C32—C34—H34A	109.0
C20—C19—C18	121.3 (2)	C33—C34—H34A	60.5
C20—C19—H19A	119.3	C35—C34—H34A	166.4
C18—C19—H19A	119.3	C32—C34—H34B	109.7
C19—C20—C21	116.8 (2)	C33—C34—H34B	127.0
C19—C20—C27	123.4 (2)	C35—C34—H34B	76.9
C21—C20—C27	119.7 (2)	H34A—C34—H34B	109.5
C22—C21—C20	121.7 (2)	C32—C34—H34C	109.7
C22—C21—H21A	119.1	C33—C34—H34C	123.1
C20—C21—H21A	119.1	C35—C34—H34C	78.4
C17—C22—C21	121.2 (2)	H34A—C34—H34C	109.5
C17—C22—H22A	119.4	H34B—C34—H34C	109.5
C21—C22—H22A	119.4	C32—C34—H34	175.5
C24—C23—C14	112.4 (2)	C33—C34—H34	127.0
C24—C23—C25	108.8 (2)	C35—C34—H34	126.9
C14—C23—C25	110.5 (2)	H34A—C34—H34	66.6

C24—C23—C26	108.4 (2)	H34B—C34—H34	71.8
C14—C23—C26	108.3 (2)	H34C—C34—H34	73.3
C25—C23—C26	108.4 (2)	C31—C35—C32	66.4 (5)
C23—C24—H24A	109.5	C31—C35—C34	119.3 (6)
C23—C24—H24B	109.5	C32—C35—C34	52.9 (5)
H24A—C24—H24B	109.5	C31—C35—H35	120.4
C23—C24—H24C	109.5	C32—C35—H35	173.1
H24A—C24—H24C	109.5	C34—C35—H35	120.3
H24B—C24—H24C	109.5		
N2—Zn1—N1—C1	178.9 (2)	C12—C13—C14—C23	−172.5 (2)
$N2^{i}$—Zn1—N1—C1	−1.1 (2)	C13—C14—C15—C16	−5.1 (4)
N2—Zn1—N1—C4	0.1 (2)	C23—C14—C15—C16	172.1 (2)
$N2^{i}$—Zn1—N1—C4	−179.9 (2)	C14—C15—C16—C11	0.9 (4)
$N2^{i}$—Zn1—N1—N2	180.0	C12—C11—C16—C15	3.9 (4)
$N1^{i}$—Zn1—N2—C9	−0.8 (2)	C5—C11—C16—C15	−169.3 (2)
N1—Zn1—N2—C9	179.2 (2)	$C1^{i}$—C10—C17—C18	−103.8 (3)
$N1^{i}$—Zn1—N2—C6	−179.6 (2)	C9—C10—C17—C18	77.2 (3)
N1—Zn1—N2—C6	0.4 (2)	$C1^{i}$—C10—C17—C22	81.0 (3)
$N1^{i}$—Zn1—N2—N1	180.0	C9—C10—C17—C22	−98.0 (3)
$N1^{i}$—Zn1—N2—$N1^{iii}$	−15.84 (6)	C22—C17—C18—C19	0.8 (4)
N1—Zn1—N2—$N1^{iii}$	164.16 (6)	C10—C17—C18—C19	−174.5 (2)
C4—N1—N2—C6	0.37 (18)	C17—C18—C19—C20	−0.8 (4)
Zn1—N1—N2—C6	−179.72 (16)	C18—C19—C20—C21	0.5 (4)
C4—N1—N2—Zn1	−179.92 (16)	C18—C19—C20—C27	178.6 (2)
C4—N1—N2—$N1^{iii}$	155.51 (13)	C19—C20—C21—C22	−0.4 (4)
Zn1—N1—N2—$N1^{iii}$	−24.58 (8)	C27—C20—C21—C22	−178.6 (2)
C4—N1—C1—$C10^{i}$	179.6 (2)	C18—C17—C22—C21	−0.7 (4)
Zn1—N1—C1—$C10^{i}$	0.6 (4)	C10—C17—C22—C21	174.7 (2)
C4—N1—C1—C2	−0.2 (3)	C20—C21—C22—C17	0.5 (4)
Zn1—N1—C1—C2	−179.16 (16)	C13—C14—C23—C24	−0.5 (3)
N1—C1—C2—C3	0.3 (3)	C15—C14—C23—C24	−177.5 (2)
$C10^{i}$—C1—C2—C3	−179.5 (2)	C13—C14—C23—C25	−122.2 (3)
C1—C2—C3—C4	−0.3 (3)	C15—C14—C23—C25	60.8 (3)
C1—N1—C4—C5	−179.3 (2)	C13—C14—C23—C26	119.2 (3)
Zn1—N1—C4—C5	−0.3 (4)	C15—C14—C23—C26	−57.8 (3)
N2—N1—C4—C5	−0.2 (2)	C19—C20—C27—C28	3.7 (4)
C1—N1—C4—C3	0.0 (3)	C21—C20—C27—C28	−178.3 (2)
Zn1—N1—C4—C3	178.98 (15)	C19—C20—C27—C30	124.5 (3)
N2—N1—C4—C3	179.06 (19)	C21—C20—C27—C30	−57.5 (3)
C2—C3—C4—N1	0.2 (3)	C19—C20—C27—C29	−116.6 (3)
C2—C3—C4—C5	179.4 (2)	C21—C20—C27—C29	61.4 (3)
N1—C4—C5—C6	0.0 (4)	C35—C31—C32—C34	1.4 (6)
C3—C4—C5—C6	−179.2 (2)	$C33^{ii}$—C31—C32—C34	−178.6 (5)
N1—C4—C5—C11	−179.5 (2)	$C32^{ii}$—C31—C32—C34	−176.6 (8)
C3—C4—C5—C11	1.3 (4)	C35—C31—C32—$C31^{ii}$	178.1 (6)

C9—N2—C6—C5	−179.8 (2)	C33^{ii}—C31—C32—C31^{ii}	−2.0 (6)
Zn1—N2—C6—C5	−0.7 (4)	C32^{ii}—C31—C32—C31^{ii}	0.0
N1—N2—C6—C5	−0.5 (2)	C33^{ii}—C31—C32—C35	180.0 (6)
N1^{iii}—N2—C6—C5	−157.91 (17)	C32^{ii}—C31—C32—C35	−178.1 (6)
C9—N2—C6—C7	0.5 (3)	C35—C31—C32—C32^{ii}	178.1 (6)
Zn1—N2—C6—C7	179.57 (16)	C33^{ii}—C31—C32—C32^{ii}	−2.0 (6)
N1—N2—C6—C7	179.82 (19)	C34—C32—C33—C31^{ii}	178.7 (4)
N1^{iii}—N2—C6—C7	22.4 (3)	C35—C32—C33—C31^{ii}	176.6 (9)
C4—C5—C6—N2	0.6 (4)	C32^{ii}—C32—C33—C31^{ii}	2.1 (6)
C11—C5—C6—N2	−179.9 (2)	C31^{ii}—C32—C33—C34	−178.7 (4)
C4—C5—C6—C7	−179.8 (2)	C35—C32—C33—C34	−2.0 (8)
C11—C5—C6—C7	−0.3 (4)	C32^{ii}—C32—C33—C34	−176.6 (8)
N2—C6—C7—C8	−0.1 (3)	C31^{ii}—C32—C34—C33	1.5 (5)
C5—C6—C7—C8	−179.8 (2)	C35—C32—C34—C33	178.6 (6)
C6—C7—C8—C9	−0.3 (3)	C31—C32—C34—C33	177.4 (7)
C6—N2—C9—C10	179.0 (2)	C33—C32—C34—C35	−178.6 (6)
Zn1—N2—C9—C10	0.0 (3)	C31^{ii}—C32—C34—C35	−177.0 (8)
N1^{iii}—N2—C9—C10	27.91 (17)	C31—C32—C34—C35	−1.2 (5)
C6—N2—C9—C8	−0.7 (3)	C31^{ii}—C33—C34—C32	−1.6 (6)
Zn1—N2—C9—C8	−179.78 (16)	C32—C33—C34—C35	1.3 (5)
N1^{iii}—N2—C9—C8	−151.8 (3)	C31^{ii}—C33—C34—C35	−0.4 (8)
C7—C8—C9—N2	0.7 (3)	C32^{ii}—C31—C35—C32	2.5 (8)
C7—C8—C9—C10	−179.1 (2)	C32^{ii}—C31—C35—C34	1.3 (10)
N2—C9—C10—C1^{i}	1.0 (4)	C32—C31—C35—C34	−1.2 (5)
C8—C9—C10—C1^{i}	−179.3 (2)	C33—C32—C35—C31	−176.6 (9)
N2—C9—C10—C17	−180.0 (2)	C34—C32—C35—C31	−178.7 (5)
C8—C9—C10—C17	−0.3 (4)	C31^{ii}—C32—C35—C31	−5.3 (17)
C6—C5—C11—C12	−98.2 (3)	C32^{ii}—C32—C35—C31	−1.6 (5)
C4—C5—C11—C12	81.3 (3)	C33—C32—C35—C34	2.0 (8)
C6—C5—C11—C16	74.7 (3)	C31^{ii}—C32—C35—C34	173.3 (17)
C4—C5—C11—C16	−105.8 (3)	C31—C32—C35—C34	178.7 (5)
C16—C11—C12—C13	−4.5 (4)	C32^{ii}—C32—C35—C34	177.1 (7)
C5—C11—C12—C13	168.6 (2)	C32—C34—C35—C31	1.4 (5)
C11—C12—C13—C14	0.2 (4)	C33—C34—C35—C31	0.3 (7)
C12—C13—C14—C15	4.6 (4)	C33—C34—C35—C32	−1.1 (5)

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1; (ii) −*x*+2, −*y*+1, −*z*+1; (iii) −*x*−1, −*y*, −*z*+1.

Fig. 1


C25^i
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C25

Fig. 2