

[meso-Tetrakis(4-pentyloxyphenyl)-porphyrinato]silver(II)

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Received 31 March 2007; accepted 13 April 2007

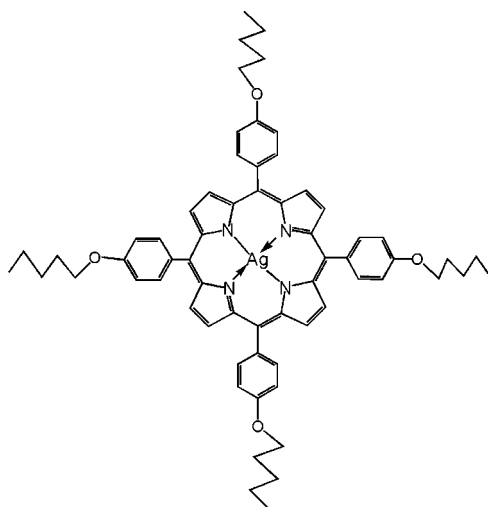
Key indicators: single-crystal X-ray study; $T = 187$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.027; wR factor = 0.075; data-to-parameter ratio = 15.7.

In the title compound, $[\text{Ag}(\text{C}_{64}\text{H}_{68}\text{N}_4\text{O}_4)]$, the planar 24-membered porphyrin ring is located across on an inversion center; the four-coordinate Ag^{II} ion is located at the inversion center, with $\text{Ag}-\text{N}$ distances of 2.0930 (13) and 2.1037 (13) Å. The 4-pentyloxyphenyl groups are twisted with respect to the porphyrin mean plane, the dihedral angles being 65.73 (9) and 58.42 (8)°.

Related literature

The corresponding silver(II) tetraphenylporphyrinate (Scheidt *et al.*, 1986) crystallizes in the triclinic system with $\text{Ag}-\text{N}$ distances of 2.082 (3) and 2.101 (3) Å, respectively.

For related literature, see: Davila & Harriman (1990); Milgrom (1984); Ostovic & Bruce (1989); Tabushi & Kugimiya (1986).



Experimental

Crystal data

$[\text{Ag}(\text{C}_{64}\text{H}_{68}\text{N}_4\text{O}_4)]$
 $M_r = 1065.09$
 Monoclinic, $P2_1/c$
 $a = 13.678$ (2) Å
 $b = 16.164$ (3) Å
 $c = 12.396$ (2) Å
 $\beta = 93.788$ (2)°

$V = 2734.7$ (8) Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 0.42$ mm⁻¹
 $T = 187$ (2) K
 $0.36 \times 0.30 \times 0.12$ mm

Data collection

Bruker SMART APEX CCD diffractometer
 Absorption correction: multi-scan (SADABS; Sheldrick, 2002)
 $T_{\text{min}} = 0.864$, $T_{\text{max}} = 0.952$

14680 measured reflections
 5226 independent reflections
 4753 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.015$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.027$
 $wR(F^2) = 0.075$
 $S = 1.05$
 5226 reflections
 333 parameters

8 restraints
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.63$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.34$ e Å⁻³

Data collection: SMART (Bruker, 1998); cell refinement: SAINT (Bruker, 2003); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 1997); software used to prepare material for publication: SHELXTL.

This work is supported by the National Analytical Research Center of Electrochemistry and Spectroscopy, Changchun Institute of Applied Chemistry, China.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2238).

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supplementary materials

Acta Cryst. (2007). E63, m1437 [doi:10.1107/S1600536807018399]

[*meso*-Tetrakis(4-pentyloxyphenyl)porphyrinato]silver(II)

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Comment

Porphyrins and their metal complexes are used as catalysts (Ostovic & Bruice, 1989), photosensitizers (Milgrom, 1984; Davila & Harriman, 1990) or useful synthetic precursors to mono-oxygenase and allosteric enzyme model systems (Tabushi & Kugimiya, 1986). In this paper, the structure of silver(II) meso-tetrakis[*p*-(pentyloxy)phenyl]porphyrinate is reported.

The title complex, (I), (Fig. 1) crystallizes in the centrosymmetric space group P 21/c. The porphyrin moiety is essentially planar, the macrocyclic core 24-membered ring is planar with the mean deviation of 0.0428 Å. The four-coordinate Ag^{II} ion is located at its center with Ag—N distances of 2.0918 (18)–2.1024 (18) Å, from the surrounding pyrrole N atoms, which agrees with that found in a related compound (Scheidt *et al.*, 1986).

The *p*-pentyloxyphenyl groups are rotated at angles of 65.73 (9)° and 58.42 (8)° with respect to the porphyrin mean plane, due to steric hindrance with the pyrrole-H atoms of the macrocycle.

Experimental

Single crystals were recrystallization from a chloroform solution at room temperature.

Refinement

H atoms were placed in calculated positions with C—H = 0.95, 0.98 or 0.99 Å, and refined in riding mode, with $U_{iso}(H) = 1.2U_{eq}(C)$.

Figures

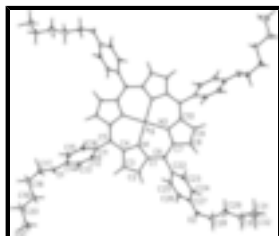


Fig. 1. A view of (I), with the atom-labeling scheme and 30% probability displacement ellipsoids.

meso-Tetrakis(4-pentyloxyphenyl)porphyrinato]silver(II)

Crystal data

[Ag(C₆₄H₆₈N₄O₄)]

$M_r = 1065.09$

$F_{000} = 1118$

$D_x = 1.293 \text{ Mg m}^{-3}$

supplementary materials

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 13.678$ (2) Å

$b = 16.164$ (3) Å

$c = 12.396$ (2) Å

$\beta = 93.788$ (2)°

$V = 2734.7$ (8) Å³

$Z = 2$

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 5101 reflections

$\theta = 2.3$ – 26.0 °

$\mu = 0.42$ mm⁻¹

$T = 187$ (2) K

Block, purple

$0.36 \times 0.30 \times 0.12$ mm

Data collection

Bruker SMART APEX CCD
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 187$ (2) K

φ and ω ' scans

Absorption correction: multi-scan
(SADABS; Sheldrick, 2002)

$T_{\min} = 0.864$, $T_{\max} = 0.952$

14680 measured reflections

5226 independent reflections

4753 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.015$

$\theta_{\max} = 25.9$ °

$\theta_{\min} = 1.9$ °

$h = -16 \rightarrow 16$

$k = -17 \rightarrow 19$

$l = -15 \rightarrow 14$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.027$

$wR(F^2) = 0.075$

$S = 1.05$

5226 reflections

333 parameters

8 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

$$w = 1/[\sigma^2(F_o^2) + (0.0429P)^2 + 1.2689P]$$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.63$ e Å⁻³

$\Delta\rho_{\min} = -0.34$ e Å⁻³

Extinction correction: none

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.

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 $F^2 > 2\sigma(F^2)$ is used only for calculat-

ing 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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Ag	0.0000	0.0000	0.5000	0.02183 (7)
N1	0.06302 (10)	0.11126 (8)	0.45039 (11)	0.0244 (3)
N2	-0.09288 (10)	0.06840 (8)	0.59370 (11)	0.0254 (3)
O1	0.47339 (9)	0.12144 (10)	0.03853 (11)	0.0449 (3)
O2	-0.11905 (11)	0.55140 (8)	0.62631 (11)	0.0423 (3)
C1	0.04189 (12)	0.18952 (10)	0.48553 (13)	0.0249 (3)
C2	0.11104 (12)	0.24725 (10)	0.44355 (13)	0.0281 (3)
H2	0.1135	0.3052	0.4559	0.034*
C3	0.17160 (12)	0.20282 (10)	0.38324 (14)	0.0282 (3)
H3	0.2243	0.2243	0.3455	0.034*
C4	0.14163 (12)	0.11674 (10)	0.38650 (13)	0.0253 (3)
C5	0.18590 (12)	0.05000 (10)	0.33525 (13)	0.0255 (3)
C6	-0.03328 (12)	0.21064 (10)	0.55457 (13)	0.0249 (3)
C7	-0.09475 (12)	0.15377 (10)	0.60421 (13)	0.0253 (3)
C8	-0.17030 (13)	0.17448 (11)	0.67589 (14)	0.0307 (4)
H8	-0.1886	0.2287	0.6964	0.037*
C9	-0.21041 (13)	0.10282 (11)	0.70860 (14)	0.0314 (4)
H9	-0.2607	0.0977	0.7575	0.038*
C10	-0.16286 (12)	0.03542 (11)	0.65556 (13)	0.0258 (3)
C11	0.26491 (12)	0.07098 (10)	0.26084 (13)	0.0269 (3)
C12	0.24079 (12)	0.11307 (11)	0.16326 (14)	0.0306 (4)
H12	0.1753	0.1306	0.1466	0.037*
C13	0.31194 (13)	0.12909 (12)	0.09132 (14)	0.0346 (4)
H13	0.2950	0.1577	0.0258	0.042*
C14	0.40901 (13)	0.10309 (12)	0.11521 (15)	0.0338 (4)
C15	0.43462 (13)	0.06145 (13)	0.21173 (16)	0.0398 (4)
H15	0.5002	0.0439	0.2281	0.048*
C16	0.36250 (13)	0.04596 (12)	0.28369 (15)	0.0361 (4)
H16	0.3797	0.0179	0.3495	0.043*
C17	0.57623 (14)	0.10189 (15)	0.06331 (19)	0.0498 (5)
H17A	0.5861	0.0412	0.0645	0.060*
H17B	0.5987	0.1245	0.1349	0.060*
C18	0.63274 (15)	0.14100 (15)	-0.02468 (19)	0.0523 (6)
H18A	0.6067	0.1198	-0.0958	0.063*
H18B	0.7023	0.1242	-0.0145	0.063*
C19	0.62680 (16)	0.23566 (15)	-0.02539 (19)	0.0521 (5)
H19A	0.5576	0.2524	-0.0399	0.062*
H19B	0.6491	0.2566	0.0471	0.062*
C20	0.68808 (18)	0.27573 (17)	-0.1092 (2)	0.0613 (6)
H20A	0.7568	0.2568	-0.0968	0.074*
H20B	0.6637	0.2567	-0.1820	0.074*
C21	0.6862 (2)	0.36948 (19)	-0.1068 (3)	0.0800 (9)

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H21A	0.6186	0.3889	-0.1208	0.120*
H21B	0.7268	0.3912	-0.1625	0.120*
H21C	0.7118	0.3890	-0.0356	0.120*
C22	-0.05032 (12)	0.30117 (10)	0.57551 (13)	0.0252 (3)
C23	-0.04484 (13)	0.33313 (10)	0.68103 (14)	0.0300 (4)
H23	-0.0250	0.2978	0.7398	0.036*
C24	-0.06782 (13)	0.41569 (10)	0.70177 (14)	0.0320 (4)
H24	-0.0638	0.4359	0.7739	0.038*
C25	-0.07693 (12)	0.35620 (10)	0.49028 (13)	0.0276 (3)
H25	-0.0793	0.3366	0.4179	0.033*
C26	-0.09982 (13)	0.43843 (10)	0.50961 (14)	0.0307 (4)
H26	-0.1176	0.4743	0.4508	0.037*
C27	-0.09674 (13)	0.46849 (11)	0.61594 (14)	0.0295 (4)
C28	-0.14184 (16)	0.58336 (12)	0.73057 (16)	0.0417 (5)
H28A	-0.1182	0.6411	0.7384	0.050*
H28B	-0.1081	0.5498	0.7886	0.050*
C29	-0.25253 (17)	0.58070 (15)	0.74160 (18)	0.0525 (5)
H29A	-0.2864	0.6106	0.6802	0.063*
H29B	-0.2752	0.5225	0.7390	0.063*
C30	-0.27887 (19)	0.61995 (19)	0.8472 (2)	0.0649 (7)
H30A	-0.2428	0.5907	0.9077	0.078*
H30B	-0.2562	0.6781	0.8484	0.078*
C31	-0.3873 (2)	0.6187 (2)	0.8663 (3)	0.0884 (10)
H31A	-0.4100	0.5605	0.8638	0.106*
H31B	-0.3959	0.6398	0.9400	0.106*
C32	-0.4512 (3)	0.6679 (3)	0.7878 (3)	0.0971 (15)
H32A	-0.4280	0.7253	0.7872	0.100*
H32B	-0.5188	0.6667	0.8095	0.100*
H32C	-0.4488	0.6441	0.7153	0.100*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag	0.02553 (11)	0.01700 (10)	0.02370 (11)	-0.00092 (6)	0.00718 (7)	0.00031 (5)
N1	0.0269 (7)	0.0202 (7)	0.0271 (7)	-0.0011 (5)	0.0084 (5)	0.0004 (5)
N2	0.0284 (7)	0.0189 (7)	0.0297 (7)	-0.0001 (5)	0.0088 (6)	0.0007 (5)
O1	0.0289 (7)	0.0654 (10)	0.0421 (7)	-0.0003 (6)	0.0146 (6)	0.0123 (7)
O2	0.0686 (9)	0.0216 (7)	0.0375 (7)	0.0085 (6)	0.0104 (6)	-0.0002 (5)
C1	0.0269 (8)	0.0207 (8)	0.0271 (8)	-0.0010 (6)	0.0029 (6)	0.0000 (6)
C2	0.0310 (8)	0.0206 (8)	0.0330 (9)	-0.0040 (7)	0.0050 (7)	0.0000 (6)
C3	0.0293 (8)	0.0231 (8)	0.0330 (9)	-0.0053 (7)	0.0075 (7)	0.0023 (7)
C4	0.0269 (8)	0.0232 (8)	0.0261 (8)	-0.0031 (6)	0.0051 (6)	0.0033 (6)
C5	0.0266 (8)	0.0243 (8)	0.0260 (8)	-0.0007 (6)	0.0053 (6)	0.0023 (6)
C6	0.0283 (8)	0.0205 (8)	0.0259 (8)	0.0009 (6)	0.0025 (6)	0.0004 (6)
C7	0.0287 (8)	0.0206 (8)	0.0269 (8)	0.0018 (6)	0.0049 (6)	-0.0014 (6)
C8	0.0354 (9)	0.0234 (8)	0.0345 (9)	0.0022 (7)	0.0117 (7)	-0.0032 (7)
C9	0.0351 (9)	0.0267 (9)	0.0340 (9)	0.0004 (7)	0.0133 (7)	-0.0010 (7)
C10	0.0286 (8)	0.0235 (8)	0.0258 (8)	-0.0003 (7)	0.0064 (6)	0.0014 (6)

C11	0.0290 (8)	0.0231 (8)	0.0295 (8)	-0.0017 (6)	0.0083 (7)	-0.0010 (6)
C12	0.0256 (8)	0.0331 (9)	0.0337 (9)	0.0014 (7)	0.0068 (7)	0.0029 (7)
C13	0.0322 (9)	0.0410 (10)	0.0313 (9)	0.0000 (8)	0.0068 (7)	0.0086 (7)
C14	0.0286 (9)	0.0383 (10)	0.0357 (9)	-0.0038 (7)	0.0120 (7)	0.0009 (8)
C15	0.0265 (9)	0.0477 (12)	0.0458 (11)	0.0038 (8)	0.0068 (8)	0.0112 (9)
C16	0.0327 (9)	0.0404 (11)	0.0357 (9)	0.0022 (8)	0.0062 (7)	0.0112 (8)
C17	0.0300 (10)	0.0624 (14)	0.0586 (13)	0.0052 (9)	0.0159 (9)	0.0135 (11)
C18	0.0349 (10)	0.0633 (15)	0.0614 (14)	0.0032 (10)	0.0227 (10)	0.0087 (11)
C19	0.0428 (11)	0.0645 (15)	0.0502 (12)	-0.0031 (10)	0.0126 (10)	0.0013 (11)
C20	0.0505 (13)	0.0733 (17)	0.0611 (15)	-0.0064 (12)	0.0117 (11)	0.0147 (13)
C21	0.088 (2)	0.0692 (19)	0.081 (2)	-0.0140 (16)	-0.0100 (16)	0.0218 (16)
C22	0.0259 (8)	0.0205 (8)	0.0297 (8)	-0.0024 (6)	0.0053 (6)	-0.0002 (6)
C23	0.0374 (9)	0.0240 (8)	0.0283 (8)	0.0018 (7)	0.0001 (7)	0.0016 (7)
C24	0.0437 (10)	0.0237 (8)	0.0285 (9)	0.0009 (7)	0.0028 (7)	-0.0028 (7)
C25	0.0323 (8)	0.0254 (8)	0.0257 (8)	-0.0014 (7)	0.0056 (6)	-0.0004 (6)
C26	0.0382 (9)	0.0238 (8)	0.0303 (9)	0.0025 (7)	0.0043 (7)	0.0052 (7)
C27	0.0338 (9)	0.0195 (8)	0.0356 (9)	0.0016 (7)	0.0049 (7)	-0.0012 (7)
C28	0.0623 (13)	0.0251 (9)	0.0377 (10)	0.0087 (9)	0.0027 (9)	-0.0051 (7)
C29	0.0605 (14)	0.0525 (13)	0.0444 (12)	-0.0082 (11)	0.0028 (10)	-0.0059 (10)
C30	0.0603 (15)	0.0806 (19)	0.0541 (14)	0.0028 (13)	0.0062 (12)	-0.0151 (13)
C31	0.0686 (19)	0.082 (3)	0.081 (2)	-0.0031 (19)	0.0154 (16)	-0.024 (2)
C32	0.077 (2)	0.086 (4)	0.089 (3)	0.028 (2)	-0.012 (2)	-0.056 (3)

Geometric parameters (Å, °)

Ag—N2	2.0930 (13)	C17—H17A	0.9900
Ag—N2 ⁱ	2.0930 (13)	C17—H17B	0.9900
Ag—N1	2.1037 (13)	C18—C19	1.532 (3)
Ag—N1 ⁱ	2.1037 (13)	C18—H18A	0.9900
N1—C1	1.375 (2)	C18—H18B	0.9900
N1—C4	1.380 (2)	C19—C20	1.522 (3)
N2—C10	1.373 (2)	C19—H19A	0.9900
N2—C7	1.386 (2)	C19—H19B	0.9900
O1—C14	1.370 (2)	C20—C21	1.516 (4)
O1—C17	1.455 (2)	C20—H20A	0.9900
O2—C27	1.382 (2)	C20—H20B	0.9900
O2—C28	1.445 (2)	C21—H21A	0.9800
C1—C6	1.422 (2)	C21—H21B	0.9800
C1—C2	1.450 (2)	C21—H21C	0.9800
C2—C3	1.357 (2)	C22—C23	1.404 (2)
C2—H2	0.9500	C22—C25	1.410 (2)
C3—C4	1.452 (2)	C23—C24	1.399 (2)
C3—H3	0.9500	C23—H23	0.9500
C4—C5	1.409 (2)	C24—C27	1.400 (2)
C5—C10 ⁱ	1.422 (3)	C24—H24	0.9500
C5—C11	1.505 (2)	C25—C26	1.390 (2)
C6—C7	1.414 (2)	C25—H25	0.9500
C6—C22	1.507 (2)	C26—C27	1.403 (2)

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C7—C8	1.446 (2)	C26—H26	0.9500
C8—C9	1.355 (2)	C28—C29	1.530 (3)
C8—H8	0.9500	C28—H28A	0.9900
C9—C10	1.449 (2)	C28—H28B	0.9900
C9—H9	0.9500	C29—C30	1.519 (3)
C10—C5 ⁱ	1.422 (3)	C29—H29A	0.9900
C11—C16	1.406 (2)	C29—H29B	0.9900
C11—C12	1.408 (2)	C30—C31	1.517 (4)
C12—C13	1.387 (2)	C30—H30A	0.9900
C12—H12	0.9500	C30—H30B	0.9900
C13—C14	1.405 (2)	C31—C32	1.494 (5)
C13—H13	0.9500	C31—H31A	0.9900
C14—C15	1.397 (3)	C31—H31B	0.9900
C15—C16	1.396 (2)	C32—H32A	0.9800
C15—H15	0.9500	C32—H32B	0.9800
C16—H16	0.9500	C32—H32C	0.9800
C17—C18	1.516 (3)		
N2—Ag—N2 ⁱ	180.0	C19—C18—H18A	109.0
N2—Ag—N1	89.20 (5)	C17—C18—H18B	109.0
N2 ⁱ —Ag—N1	90.80 (5)	C19—C18—H18B	109.0
N2—Ag—N1 ⁱ	90.80 (5)	H18A—C18—H18B	107.8
N2 ⁱ —Ag—N1 ⁱ	89.20 (5)	C20—C19—C18	113.43 (19)
N1—Ag—N1 ⁱ	180.00 (4)	C20—C19—H19A	108.9
C1—N1—C4	108.11 (13)	C18—C19—H19A	108.9
C1—N1—Ag	126.53 (11)	C20—C19—H19B	108.9
C4—N1—Ag	124.93 (11)	C18—C19—H19B	108.9
C10—N2—C7	108.43 (13)	H19A—C19—H19B	107.7
C10—N2—Ag	125.16 (11)	C21—C20—C19	113.7 (2)
C7—N2—Ag	126.41 (11)	C21—C20—H20A	108.8
C14—O1—C17	117.60 (15)	C19—C20—H20A	108.8
C27—O2—C28	119.46 (13)	C21—C20—H20B	108.8
N1—C1—C6	125.95 (15)	C19—C20—H20B	108.8
N1—C1—C2	108.83 (14)	H20A—C20—H20B	107.7
C6—C1—C2	125.19 (15)	C20—C21—H21A	109.5
C3—C2—C1	107.07 (15)	C20—C21—H21B	109.5
C3—C2—H2	126.5	H21A—C21—H21B	109.5
C1—C2—H2	126.5	C20—C21—H21C	109.5
C2—C3—C4	107.94 (14)	H21A—C21—H21C	109.5
C2—C3—H3	126.0	H21B—C21—H21C	109.5
C4—C3—H3	126.0	C23—C22—C25	117.46 (15)
N1—C4—C5	125.74 (15)	C23—C22—C6	121.23 (15)
N1—C4—C3	108.04 (14)	C25—C22—C6	121.24 (14)
C5—C4—C3	126.21 (15)	C24—C23—C22	121.57 (16)
C4—C5—C10 ⁱ	127.09 (15)	C24—C23—H23	119.2
C4—C5—C11	116.82 (14)	C22—C23—H23	119.2
C10 ⁱ —C5—C11	116.08 (14)	C23—C24—C27	119.83 (16)
C7—C6—C1	125.47 (15)	C23—C24—H24	120.1

C7—C6—C22	116.94 (14)	C27—C24—H24	120.1
C1—C6—C22	117.58 (14)	C26—C25—C22	121.60 (15)
N2—C7—C6	126.22 (14)	C26—C25—H25	119.2
N2—C7—C8	107.85 (14)	C22—C25—H25	119.2
C6—C7—C8	125.92 (15)	C25—C26—C27	120.00 (16)
C9—C8—C7	107.81 (15)	C25—C26—H26	120.0
C9—C8—H8	126.1	C27—C26—H26	120.0
C7—C8—H8	126.1	O2—C27—C24	124.98 (15)
C8—C9—C10	107.71 (15)	O2—C27—C26	115.47 (15)
C8—C9—H9	126.1	C24—C27—C26	119.48 (16)
C10—C9—H9	126.1	O2—C28—C29	110.07 (17)
N2—C10—C5 ⁱ	126.01 (15)	O2—C28—H28A	109.6
N2—C10—C9	108.17 (14)	C29—C28—H28A	109.6
C5 ⁱ —C10—C9	125.82 (14)	O2—C28—H28B	109.6
C16—C11—C12	118.54 (15)	C29—C28—H28B	109.6
C16—C11—C5	121.50 (15)	H28A—C28—H28B	108.2
C12—C11—C5	119.89 (15)	C30—C29—C28	110.96 (19)
C13—C12—C11	120.53 (16)	C30—C29—H29A	109.4
C13—C12—H12	119.7	C28—C29—H29A	109.4
C11—C12—H12	119.7	C30—C29—H29B	109.4
C12—C13—C14	120.13 (16)	C28—C29—H29B	109.4
C12—C13—H13	119.9	H29A—C29—H29B	108.0
C14—C13—H13	119.9	C31—C30—C29	114.8 (2)
O1—C14—C15	124.20 (16)	C31—C30—H30A	108.6
O1—C14—C13	115.51 (16)	C29—C30—H30A	108.6
C15—C14—C13	120.30 (16)	C31—C30—H30B	108.6
C16—C15—C14	119.07 (16)	C29—C30—H30B	108.6
C16—C15—H15	120.5	H30A—C30—H30B	107.6
C14—C15—H15	120.5	C32—C31—C30	115.3 (3)
C15—C16—C11	121.44 (16)	C32—C31—H31A	108.5
C15—C16—H16	119.3	C30—C31—H31A	108.5
C11—C16—H16	119.3	C32—C31—H31B	108.5
O1—C17—C18	106.82 (17)	C30—C31—H31B	108.5
O1—C17—H17A	110.4	H31A—C31—H31B	107.5
C18—C17—H17A	110.4	C31—C32—H32A	109.5
O1—C17—H17B	110.4	C31—C32—H32B	109.5
C18—C17—H17B	110.4	H32A—C32—H32B	109.5
H17A—C17—H17B	108.6	C31—C32—H32C	109.5
C17—C18—C19	113.03 (19)	H32A—C32—H32C	109.5
C17—C18—H18A	109.0	H32B—C32—H32C	109.5

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

Fig. 1

