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2,6-Bis[2,4-bis(heptyloxy)phenyl]pyridine

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Key indicators

Single-crystal X-ray study
T = 180 K
Mean σ(C–C) = 0.004 Å
Disorder in main residue
R factor = 0.060
wR factor = 0.168
Data-to-parameter ratio = 14.5

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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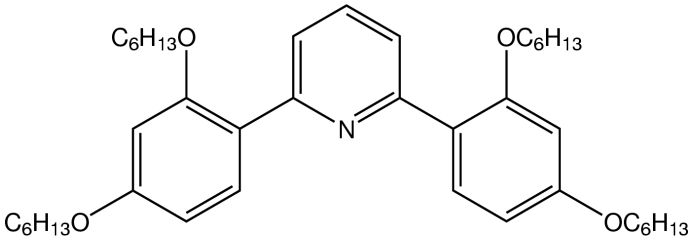
The title 2,6-disubstituted pyridine, $C_{41}H_{61}NO_4$, with a crystallographic twofold axis, has an arrangement of molecules well organized to undergo multiple cyclometallation reactions.

Comment

2,6-Disubstituted pyridines are ideally set up to undergo multiple cyclometallations, reactions of considerable interest to us (Cave *et al.*, 1999, 2000). In addition to their ability to undergo multiple cyclometallations, such compounds have also been shown to be activated by other reagents (Cave *et al.*, 1998).



(I)

The title molecule, (I) (Fig. 1), has crystallographic twofold symmetry and the aliphatic chains are each in an extended form. Within the unit cell, the molecules are aligned in an antiparallel fashion (Figs. 2 and 3).

Experimental

1-Chloro-2,4-bis(heptyloxy)benzene (15.0 g, 48.0 mmol) was added dropwise to a stirred solution of magnesium (1.22 g, 50.0 mmol) and methyl iodide (0.30 g, 2.11 mmol) in tetrahydrofuran (THF, 25 ml) under an inert atmosphere. The resulting Grignard reagent was transferred *via* a cannula to a stirred solution of 2,6-dichloropyridine (2.96 g, 20.0 mmol) and tetrakis(triphenylphosphine)palladium (0.45 g, 0.50 mmol) in THF (25 ml). The reaction mixture was then heated under reflux (24 h) under an inert atmosphere. Excess Grignard was destroyed with water (20 ml) and hydrochloric acid (5 ml, 2 *M*). The neutralized (aqueous NaOH) reaction mixture was extracted with diethyl ether (2 × 200 ml) and dried (saturated NaCl and magnesium sulfate). The solvent was removed under vacuum and the product crystallized out as white needle-like crystals (yield: 12.0 g, 19.0 mmol, 95%). ^{1}H NMR ($CDCl_3$, 250.13 MHz): δ 7.96 (2H, *d*, ^3J = 8.5 Hz), 7.75 (2H, *d*, ^3J = 7.3 Hz), 7.60 (1H, *t*, ^3J = 7.3 Hz), 6.59 (2H, *dd*, ^3J = 8.5, ^4J = 2.1 Hz), 6.53 (2H, *d*, ^4J = 2.1 Hz), 3.99 (8H, *t*, ^3J = 6.7 Hz), 1.79 (8H, *m*), 1.48 (24H, *m*), 0.89 (12H, *m*). ^{13}C NMR ($CDCl_3$, 250.13 MHz): δ 160.5, 157.7, 154.7, 134.8, 132.1, 131.5, 121.9, 105.6, 100.0, 68.2, 31.4, 25.7, 22.5. Elemental analysis found (expected): C 77.8 (77.9), H 9.6 (9.7), N 2.4% (2.2%).

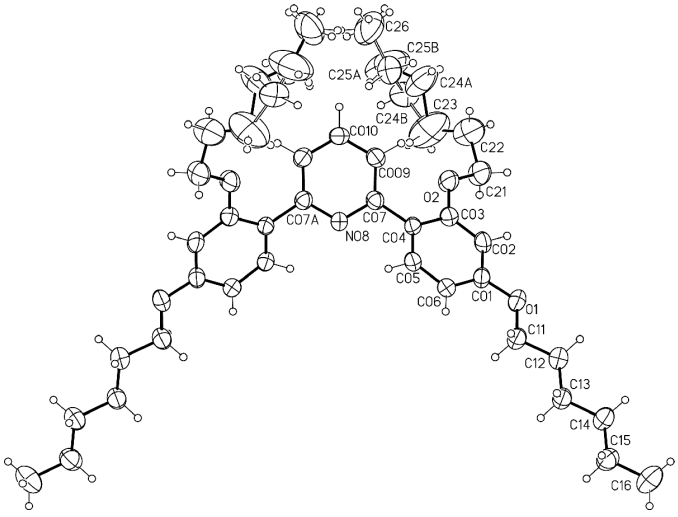


Figure 1
View of the title molecule, showing the atomic numbering. Displacement ellipsoids are drawn at the 50% probability level. Both disorder components are shown in all Figures.

Crystal data

$C_{41}H_{61}NO_4$	D_x = 1.117 Mg m^{-3}
M_r = 631.91	Mo $K\alpha$ radiation
Monoclinic, $P2/n$	Cell parameters from 2201 reflections
a = 11.2502 (10) Å	θ = 3–15°
b = 6.9682 (6) Å	μ = 0.07 mm^{-1}
c = 24.014 (2) Å	T = 180 (2) K
β = 93.963 (2)°	Block, colourless
V = 1878.0 (3) Å^3	0.45 × 0.25 × 0.20 mm
Z = 2	

Data collection

Bruker SMART diffractometer	1753 reflections with $I > 2\sigma(I)$
ω scans	R_{int} = 0.045
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	θ_{max} = 25.0°
T_{min} = 0.896, T_{max} = 0.989	$h = -13 \rightarrow 13$
8996 measured reflections	$k = -8 \rightarrow 7$
3318 independent reflections	$l = -18 \rightarrow 28$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.060	$w = 1/[\sigma^2(F_o^2) + (0.078P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.168	$(\Delta/\sigma)_{max}$ = 0.043
S = 1.04	$\Delta\rho_{max}$ = 0.21 e Å^{-3}
3318 reflections	$\Delta\rho_{min}$ = −0.22 e Å^{-3}
229 parameters	

H atoms were added at calculated positions (C—H = 0.95–0.99 Å) and refined using a riding model (including free rotation about C—C bonds for methyl groups), with U_{iso}(H) = 1.2 (or 1.5 for methyl H atoms) times U_{eq}(C). The terminal section of one of the heptane chains was found to be disordered between two positions [relative occupancies 0.43 (1):0.57 (1)]. This disorder is believed to be responsible for various anomalies in the displacement parameters of the atoms in this region of the molecule.

Data collection: *SMART* (Siemens, 1994); cell refinement: *SAINT* (Siemens, 1995); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

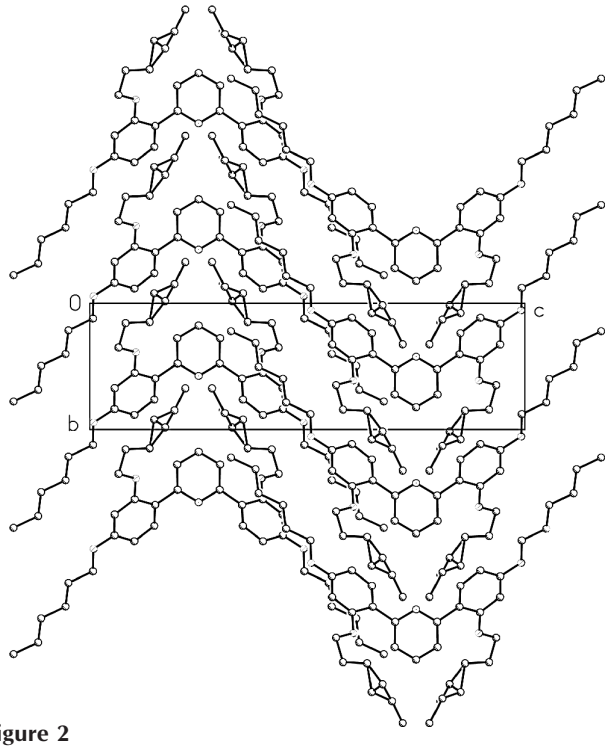


Figure 2
Packing diagram of (I), viewed down the *a* axis. H atoms have been omitted.

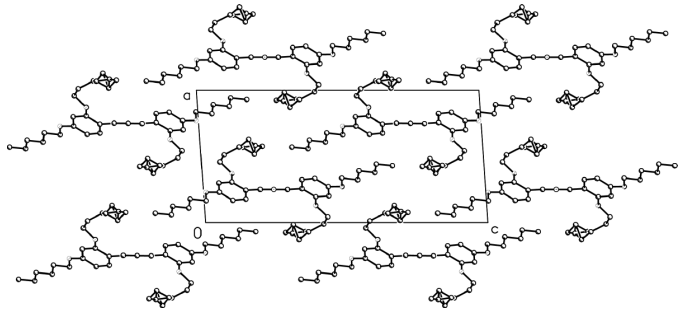


Figure 3
Packing diagram of (I), viewed down the *b* axis. H atoms have been omitted.

The EPSRC and Siemens generously supported the purchase of the SMART diffractometer.

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supporting information

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Cell parameters from 2201 reflections
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Block, colourless
0.45 × 0.25 × 0.2 mm

Data collection

Siemens SMART diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 8.192 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
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3318 independent reflections
1753 reflections with $I > 2\sigma(I)$
$R_{int} = 0.045$
$\theta_{max} = 25.0°$, $\theta_{min} = 1.7°$
$h = -13\rightarrow13$
$k = -8\rightarrow7$
$l = -18\rightarrow28$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.060$
$wR(F^2) = 0.168$
$S = 1.04$
3318 reflections
229 parameters
2 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
$w = 1/[\sigma^2(F_o^2) + (0.078P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.043$
$\Delta\rho_{max} = 0.21$ e Å^{-3}
$\Delta\rho_{min} = -0.22$ e Å^{-3}

Special details

Experimental. The temperature of the crystal was controlled using the Oxford Cryosystem Cryostream Cooler (Cosier & Glazer, 1986). The data collection nominally covered over a hemisphere of reciprocal space, by a combination of three sets of exposures with different φ angles for the crystal; each 10 s exposure covered 0.3° in ω. The crystal-to-detector distance was 5.0 cm. Coverage of the unique set is over 97% complete to at least 26° in θ. Crystal decay was found to be negligible by by repeating the initial frames at data collection and analyzing the duplicate reflections.
Hydrogen atoms were added at calculated positions and refined using a riding model. Anisotropic displacement parameters were used for all non-H atoms H-atoms were given isotropic displacement parameter equal to 1.2 (or 1.5 for methyl atoms) times the equivalent isotropic displacement parameter of the atom to which they are attached.

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}	Occ. (<1)
O1	0.27150 (17)	0.9445 (3)	0.49155 (7)	0.0557 (6)	
O2	0.12875 (16)	0.3876 (2)	0.39451 (7)	0.0541 (6)	
C01	0.2706 (2)	0.8380 (4)	0.44357 (10)	0.0443 (7)	
C02	0.2012 (2)	0.6730 (4)	0.44313 (10)	0.0451 (7)	
H02A	0.1582	0.6425	0.4746	0.054*	
C03	0.1942 (2)	0.5526 (4)	0.39711 (10)	0.0422 (7)	
C04	0.2560 (2)	0.5969 (3)	0.34979 (9)	0.0366 (6)	
C05	0.3235 (2)	0.7629 (4)	0.35173 (10)	0.0413 (7)	
H05A	0.3653	0.7958	0.3200	0.050*	
C06	0.3333 (2)	0.8842 (4)	0.39782 (10)	0.0437 (7)	
H06A	0.3818	0.9958	0.3979	0.052*	
C07	0.2497 (2)	0.4772 (4)	0.29833 (10)	0.0372 (6)	
N08	0.2500	0.5760 (4)	0.2500	0.0376 (7)	
C009	0.2482 (2)	0.2775 (4)	0.29932 (11)	0.0435 (7)	
H09A	0.2460	0.2110	0.3338	0.052*	
C010	0.2500	0.1771 (5)	0.2500	0.0430 (9)	
H01C	0.2500	0.0408	0.2500	0.052*	
C11	0.3361 (2)	1.1221 (4)	0.49299 (10)	0.0492 (7)	
H11A	0.3040	1.2079	0.4627	0.059*	
H11B	0.4214	1.0980	0.4877	0.059*	
C12	0.3225 (3)	1.2141 (4)	0.54911 (10)	0.0535 (8)	
H12A	0.3514	1.1239	0.5789	0.064*	
H12B	0.2371	1.2390	0.5535	0.064*	
C13	0.3912 (2)	1.4015 (4)	0.55598 (11)	0.0490 (7)	
H13A	0.4766	1.3763	0.5515	0.059*	
H13B	0.3623	1.4913	0.5261	0.059*	
C14	0.3784 (2)	1.4954 (4)	0.61216 (11)	0.0540 (8)	
H14A	0.2927	1.5150	0.6172	0.065*	

H14B	0.4102	1.4071	0.6419	0.065*	
C15	0.4417 (3)	1.6856 (4)	0.61915 (12)	0.0585 (8)	
H15A	0.4093	1.7744	0.5897	0.070*	
H15B	0.5273	1.6663	0.6136	0.070*	
C16	0.4301 (3)	1.7785 (5)	0.67574 (13)	0.0759 (10)	
H16A	0.4709	1.9028	0.6769	0.114*	
H16B	0.4663	1.6951	0.7051	0.114*	
H16C	0.3456	1.7975	0.6817	0.114*	
C21	0.0420 (3)	0.3509 (4)	0.43410 (13)	0.0642 (9)	
H21A	−0.0202	0.4517	0.4321	0.077*	
H21B	0.0800	0.3472	0.4725	0.077*	
C22	−0.0114 (4)	0.1576 (5)	0.41802 (17)	0.0954 (14)	
H22A	0.0528	0.0602	0.4208	0.114*	
H22B	−0.0697	0.1228	0.4454	0.114*	
C23	−0.0705 (4)	0.1487 (7)	0.3625 (2)	0.145 (2)	
H23A	−0.0256	0.2193	0.3350	0.174*	0.554 (17)
H23B	−0.1530	0.1988	0.3618	0.174*	0.554 (17)
H23C	−0.0142	0.2079	0.3376	0.174*	0.446 (17)
H23D	−0.1383	0.2389	0.3635	0.174*	0.446 (17)
C24A	−0.0681 (14)	−0.0784 (13)	0.3520 (6)	0.112 (6)	0.554 (17)
H24A	0.0098	−0.1248	0.3684	0.134*	0.554 (17)
H24B	−0.1295	−0.1346	0.3747	0.134*	0.554 (17)
C25A	−0.083 (2)	−0.152 (2)	0.3054 (8)	0.181 (8)	0.554 (17)
H25A	−0.0297	−0.0728	0.2833	0.218*	0.554 (17)
H25B	−0.1643	−0.1095	0.2931	0.218*	0.554 (17)
C24B	−0.1284 (9)	−0.0165 (13)	0.3271 (5)	0.070 (4)	0.446 (17)
H24C	−0.1757	0.0331	0.2939	0.084*	0.446 (17)
H24D	−0.1801	−0.0969	0.3494	0.084*	0.446 (17)
C25B	−0.0166 (9)	−0.130 (2)	0.3104 (5)	0.066 (4)	0.446 (17)
H25C	0.0368	−0.1626	0.3435	0.079*	0.446 (17)
H25D	0.0287	−0.0562	0.2837	0.079*	0.446 (17)
C26	−0.0762 (4)	−0.3254 (7)	0.28082 (17)	0.1204 (16)	
H26A	−0.1069	−0.3160	0.2417	0.181*	0.554 (17)
H26B	−0.1240	−0.4180	0.3003	0.181*	0.554 (17)
H26C	0.0070	−0.3682	0.2826	0.181*	0.554 (17)
H26D	−0.0117	−0.4042	0.2676	0.181*	0.446 (17)
H26E	−0.1300	−0.2868	0.2490	0.181*	0.446 (17)
H26F	−0.1206	−0.3997	0.3071	0.181*	0.446 (17)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0802 (15)	0.0520 (13)	0.0360 (11)	−0.0067 (10)	0.0114 (10)	−0.0088 (9)
O2	0.0646 (13)	0.0517 (12)	0.0484 (12)	−0.0118 (10)	0.0215 (9)	−0.0057 (10)
C01	0.0566 (18)	0.0463 (17)	0.0298 (15)	0.0079 (14)	0.0023 (13)	−0.0010 (13)
C02	0.0545 (18)	0.0496 (18)	0.0325 (16)	0.0021 (14)	0.0121 (12)	0.0044 (13)
C03	0.0490 (17)	0.0400 (16)	0.0381 (16)	0.0025 (13)	0.0069 (12)	0.0017 (13)
C04	0.0443 (15)	0.0355 (15)	0.0300 (14)	0.0073 (12)	0.0027 (11)	0.0010 (12)

C05	0.0516 (17)	0.0407 (16)	0.0320 (15)	0.0033 (13)	0.0068 (12)	0.0039 (12)
C06	0.0567 (18)	0.0376 (15)	0.0367 (16)	0.0009 (13)	0.0034 (13)	0.0012 (13)
C07	0.0373 (15)	0.0392 (16)	0.0355 (15)	0.0032 (12)	0.0062 (12)	0.0023 (12)
N08	0.0451 (18)	0.0372 (18)	0.0307 (17)	0.000	0.0040 (13)	0.000
C009	0.0495 (17)	0.0416 (17)	0.0400 (16)	0.0034 (13)	0.0071 (12)	0.0048 (13)
C010	0.051 (2)	0.032 (2)	0.046 (2)	0.000	0.0066 (18)	0.000
C11	0.0569 (18)	0.0506 (18)	0.0400 (16)	0.0015 (14)	0.0017 (13)	−0.0064 (14)
C12	0.066 (2)	0.0540 (19)	0.0406 (17)	−0.0002 (15)	0.0045 (14)	−0.0038 (14)
C13	0.0570 (18)	0.0502 (18)	0.0398 (16)	0.0056 (14)	0.0023 (13)	−0.0041 (14)
C14	0.0570 (19)	0.0567 (19)	0.0489 (18)	−0.0020 (15)	0.0077 (14)	−0.0110 (15)
C15	0.063 (2)	0.0550 (19)	0.057 (2)	0.0009 (15)	−0.0013 (15)	−0.0082 (15)
C16	0.072 (2)	0.080 (2)	0.076 (2)	−0.0088 (18)	0.0062 (18)	−0.0286 (19)
C21	0.067 (2)	0.066 (2)	0.063 (2)	−0.0104 (16)	0.0337 (16)	−0.0064 (17)
C22	0.095 (3)	0.082 (3)	0.118 (3)	−0.030 (2)	0.063 (3)	−0.014 (3)
C23	0.106 (4)	0.144 (5)	0.185 (6)	−0.057 (3)	0.012 (4)	−0.065 (4)
C24A	0.114 (10)	0.104 (9)	0.121 (11)	−0.043 (7)	0.042 (8)	−0.054 (7)
C25A	0.22 (2)	0.102 (10)	0.23 (2)	−0.045 (14)	0.080 (17)	−0.060 (10)
C24B	0.044 (6)	0.068 (6)	0.094 (8)	0.012 (4)	−0.018 (4)	0.002 (5)
C25B	0.049 (6)	0.086 (8)	0.064 (6)	0.004 (5)	0.011 (4)	0.003 (5)
C26	0.141 (4)	0.122 (4)	0.099 (3)	0.044 (3)	0.018 (3)	−0.030 (3)

Geometric parameters (Å, º)

O1—C01	1.370 (3)	C15—H15B	0.9900
O1—C11	1.434 (3)	C16—H16A	0.9800
O2—C03	1.364 (3)	C16—H16B	0.9800
O2—C21	1.432 (3)	C16—H16C	0.9800
C01—C06	1.384 (3)	C21—C22	1.514 (4)
C01—C02	1.390 (3)	C21—H21A	0.9900
C02—C03	1.385 (3)	C21—H21B	0.9900
C02—H02A	0.9500	C22—C23	1.450 (6)
C03—C04	1.407 (3)	C22—H22A	0.9900
C04—C05	1.382 (3)	C22—H22B	0.9900
C04—C07	1.489 (3)	C23—C24B	1.547 (8)
C05—C06	1.391 (3)	C23—C24A	1.603 (8)
C05—H05A	0.9500	C23—H23A	0.9900
C06—H06A	0.9500	C23—H23B	0.9900
C07—N08	1.350 (3)	C23—H23C	0.9900
C07—C009	1.392 (3)	C23—H23D	0.9899
N08—C07^{i}	1.350 (3)	C24A—C25A	1.23 (2)
C009—C010	1.377 (3)	C24A—H24A	0.9900
C009—H09A	0.9500	C24A—H24B	0.9900
C010—C009^{i}	1.377 (3)	C25A—C26	1.352 (16)
C010—H01C	0.9500	C25A—H25A	0.9900
C11—C12	1.509 (3)	C25A—H25B	0.9900
C11—H11A	0.9900	C24B—C25B	1.563 (18)
C11—H11B	0.9900	C24B—H24C	0.9900
C12—C13	1.520 (4)	C24B—H24D	0.9900

C12—H12A	0.9900	C25B—C26	1.654 (16)
C12—H12B	0.9900	C25B—H25C	0.9900
C13—C14	1.515 (3)	C25B—H25D	0.9900
C13—H13A	0.9900	C26—H26A	0.9800
C13—H13B	0.9900	C26—H26B	0.9800
C14—C15	1.508 (3)	C26—H26C	0.9800
C14—H14A	0.9900	C26—H26D	0.9800
C14—H14B	0.9900	C26—H26E	0.9799
C15—C16	1.519 (4)	C26—H26F	0.9800
C15—H15A	0.9900		

C01—O1—C11	117.5 (2)	H16B—C16—H16C	109.5
C03—O2—C21	120.7 (2)	O2—C21—C22	105.5 (2)
O1—C01—C06	124.5 (2)	O2—C21—H21A	110.7
O1—C01—C02	115.2 (2)	C22—C21—H21A	110.7
C06—C01—C02	120.2 (2)	O2—C21—H21B	110.7
C03—C02—C01	120.5 (2)	C22—C21—H21B	110.7
C03—C02—H02A	119.7	H21A—C21—H21B	108.8
C01—C02—H02A	119.7	C23—C22—C21	114.9 (4)
O2—C03—C02	123.2 (2)	C23—C22—H22A	108.5
O2—C03—C04	116.3 (2)	C21—C22—H22A	108.5
C02—C03—C04	120.5 (2)	C23—C22—H22B	108.5
C05—C04—C03	117.2 (2)	C21—C22—H22B	108.5
C05—C04—C07	119.4 (2)	H22A—C22—H22B	107.5
C03—C04—C07	123.3 (2)	C22—C23—C24B	133.3 (6)
C04—C05—C06	123.3 (2)	C22—C23—C24A	100.1 (7)
C04—C05—H05A	118.4	C22—C23—H23A	111.8
C06—C05—H05A	118.4	C24B—C23—H23A	102.6
C01—C06—C05	118.3 (2)	C24A—C23—H23A	111.8
C01—C06—H06A	120.9	C22—C23—H23B	111.8
C05—C06—H06A	120.9	C24B—C23—H23B	83.9
N08—C07—C009	121.7 (2)	C24A—C23—H23B	111.7
N08—C07—C04	115.1 (2)	H23A—C23—H23B	109.5
C009—C07—C04	123.1 (2)	C22—C23—H23C	105.4
C07^{i}—N08—C07	118.6 (3)	C24B—C23—H23C	104.0
C010—C009—C07	119.5 (3)	C24A—C23—H23C	107.3
C010—C009—H09A	120.3	H23B—C23—H23C	118.7
C07—C009—H09A	120.3	C22—C23—H23D	104.8
C009—C010—C009^{i}	119.0 (3)	C24B—C23—H23D	100.9
C009—C010—H01C	120.5	C24A—C23—H23D	130.7
C009^{i}—C010—H01C	120.5	H23C—C23—H23D	106.1
O1—C11—C12	107.8 (2)	C25A—C24A—C23	123.3 (15)
O1—C11—H11A	110.2	C25A—C24A—H24A	106.5
C12—C11—H11A	110.2	C23—C24A—H24A	106.5
O1—C11—H11B	110.2	C25A—C24A—H24B	106.5
C12—C11—H11B	110.2	C23—C24A—H24B	106.5
H11A—C11—H11B	108.5	H24A—C24A—H24B	106.5
C11—C12—C13	112.3 (2)	C24A—C25A—C26	139.6 (19)

C11—C12—H12A	109.1	C24A—C25A—H25A	102.2
C13—C12—H12A	109.1	C26—C25A—H25A	102.2
C11—C12—H12B	109.1	C24A—C25A—H25B	102.1
C13—C12—H12B	109.1	C26—C25A—H25B	102.2
H12A—C12—H12B	107.9	H25A—C25A—H25B	104.8
C14—C13—C12	112.9 (2)	C23—C24B—C25B	101.7 (9)
C14—C13—H13A	109.0	C23—C24B—H24C	111.4
C12—C13—H13A	109.0	C25B—C24B—H24C	111.4
C14—C13—H13B	109.0	C23—C24B—H24D	111.4
C12—C13—H13B	109.0	C25B—C24B—H24D	111.4
H13A—C13—H13B	107.8	C24B—C25B—C26	102.6 (7)
C15—C14—C13	113.9 (2)	C24B—C25B—H25D	111.3
C15—C14—H14A	108.8	C26—C25B—H25D	111.3
C13—C14—H14A	108.8	C25A—C26—H26A	109.5
C15—C14—H14B	108.8	C25B—C26—H26A	117.5
C13—C14—H14B	108.8	C25A—C26—H26B	109.5
H14A—C14—H14B	107.7	C25B—C26—H26B	123.8
C14—C15—C16	113.9 (2)	H26A—C26—H26B	109.5
C14—C15—H15A	108.8	C25A—C26—H26C	109.4
C16—C15—H15A	108.8	C25B—C26—H26C	82.7
C14—C15—H15B	108.8	H26A—C26—H26C	109.5
C16—C15—H15B	108.8	H26B—C26—H26C	109.5
H15A—C15—H15B	107.7	C25B—C26—H26D	108.2
C15—C16—H16A	109.5	C25B—C26—H26E	108.6
C15—C16—H16B	109.5	H26D—C26—H26E	109.5
H16A—C16—H16B	109.5	C25B—C26—H26F	111.6
C15—C16—H16C	109.5	H26D—C26—H26F	109.5
H16A—C16—H16C	109.5	H26E—C26—H26F	109.5

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