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N,*N*,*N*′,*N*′-Tetraphenylnaphthalene-1,4-dicarboxamide

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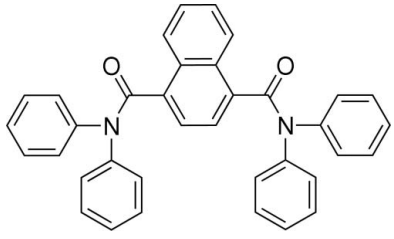
Key indicators: single-crystal X-ray study; T = 153 K; mean σ(C–C) = 0.005 Å; R factor = 0.066; wR factor = 0.192; data-to-parameter ratio = 13.4.

The title compound, $C_{36}H_{26}N_2O_2$, crystallizes with two molecules in the asymmetric unit. The two molecules differ slightly in the orientations of the phenyl rings; the dihedral angles between the two phenyl rings attached to each N atom are 68.77 (1)/83.28 (1) and 74.05 (1)/64.84 (1)°. The crystal packing is stabilized by C—H···O and C—H···π interactions.

Related literature

For related structures, see: Jing, Qin, Gu, Zhang & Lei (2006); Jing, Qin, Gu, Zhang & Mao (2006). For applications of 1,4-naphthalenedicarboxylic acid derivatives, see: Fukuzumi *et al.* (1994); Tsukada *et al.* (1994).



Experimental

Crystal data

$C_{36}H_{26}N_2O_2$
M_r = 518.59
Triclinic, $P\overline{1}$
a = 10.0276 (8) Å
b = 13.4211 (11) Å
c = 20.2414 (13) Å
α = 88.560 (2)°
β = 89.279 (2)°
γ = 74.523 (3)°
V = 2624.5 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 153 (2) K
0.49 × 0.28 × 0.21 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: none
20350 measured reflections
9674 independent reflections
5904 reflections with $I > 2\sigma(I)$
R_{int} = 0.055

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.066
$wR(F^2)$ = 0.192
S = 1.00
9674 reflections
722 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.69 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C14—H14···O1^{i}	0.95	2.41	3.342 (4)	166
C30—H30···O1^{ii}	0.95	2.48	3.413 (4)	168
C65—H65···O3^{iii}	0.95	2.59	3.420 (4)	146
C42—H42···O4^{iv}	0.95	2.51	3.105 (4)	120
C68—H68···O4^{v}	0.95	2.35	3.209 (4)	150
C16—H16···*Cg*2^{vi}	0.95	2.85	3.443 (1)	122
C21—H21···*Cg*4	0.95	2.90	3.643 (1)	135
C39—H39···*Cg*4^{vii}	0.95	2.86	3.430 (1)	119
C44—H44···*Cg*3^{vi}	0.95	2.90	3.600 (1)	132
C69—H69···*Cg*2^{viii}	0.95	2.87	3.711 (4)	148
C71—H71···*Cg*1	0.95	2.91	3.670 (1)	138

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $-x+1, -y+2, -z+1$; (iii) $x-1, y+1, z$; (iv) $-x+2, -y+1, -z+2$; (v) $-x+1, -y+1, -z+2$; (vi) $x+1, y-1, z$; (vii) $-x+1, -y+2, -z+2$; (viii) $x, y-1, z$.

Data collection: *RAPID-AUTO* (Rigaku/MSC, 2004); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2483).

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supplementary materials

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N,*N*,*N*',*N*'-Tetraphenylnaphthalene-1,4-dicarboxamide

L.-H. Jing and D.-B. Qin

Comment

1,4-Naphthalenedicarboxylic acid derivatives are a class of intermediates important for applications as monomers in the preparation of polymers (Fukuzumi *et al.*, 1994; Tsukada *et al.*, 1994). Previously, we have reported the crystal structures of *N*,*N*'-bis(4-nitrophenyl)naphthalene-1,4-dicarboxamide dimethylsulfoxide disolvate (Jing, Qin, Gu, Zhang & Mao, 2006) and *N*,*N*'-bis(2-methoxyphenyl)naphthalene-1,4-dicarboxamide (Jing, Qin, Gu, Zhang & Lei, 2006). We now report the crystal structure of the title compound, (I).

The asymmetric unit of (I) consists of two crystallographically independent molecules which differ in the orientations of the phenyl groups (Fig. 1). Bond lengths and angles of these two molecules agree with each other and are normal. In both independent molecules, the naphthalene ring systems are planar, with maximum deviation of 0.039 (4) Å for atom C6 and 0.032 (3) Å for atom C45. As a result of steric effects, the substituent groups are twisted away from the planes of the naphthalene ring systems (Fig. 1). The dihedral angles formed between various planes are as follows: C1—C10 and O1/N1/C1/C11 66.7 (2)°, C1—C10 and O2/N2/C4/C24 61.1 (2)°, C37—C46 and O3/N3/C37/C47 59.4 (2)°, C37—C46 and O4/N4/C40/C60 89.5 (2)°, O1/N1/C1/C11 and C12—C17 69.4 (2)°, O1/N1/C1/C11 and C18—C23 65.4 (2)°, O2/N2/C4/C24 and C25—C30 68.3 (2)°, O2/N2/C4/C24 and C31—C36 52.8 (2)°, O3/N3/C37/C47 and C48—C53 63.3 (2)°, O3/N3/C37/C47 and C54—C59 54.8 (2)°, O4/N4/C40/C60 and C61—C66 58.0 (2)°, O4/N4/C40/C60 and C67—C72 82.1 (2)°, C12—C17 and C18—C23 68.8 (2)°, C25—C30 and C31—C36 83.3 (2)°, C48—C53 and C54—C59 74.0 (2)° and C61—C66 and C67—C72 64.8 (2)°. The crystal packing is stabilized by C—H···O hydrogen bonds and C—H···π interactions (Table 1; *Cg*1, *Cg*2, *Cg*3 and *Cg*4 are the centroids of the C12—C17, C25—C30, C31—C36 and C61—C66 rings, respectively)

Experimental

Naphthalene-1,4-dicarboxylic acid (2 mmol) and an excess of thionyl chloride (6 mmol) in dioxane (20 ml) were boiled under reflux for 6 h. The solution was distilled under reduced pressure and a yellow solid was formed. Diphenylamine (4 mmol) in tetrahydrofuran (20 ml) was added to the yellow solid and boiled under reflux for 1 d. The solution was then cooled to ambient temperature and filtered to remove the tetrahydrofuran. The precipitate was dissolved in dimethylsulfoxide and allowed to stand for one month at ambient temperature, after which time white single crystals of (I) suitable for X-ray diffraction were obtained.

Refinement

All H atoms were placed in calculated positions, with C—H = 0.95 Å, and refined using a riding model, with U_{iso}(H) = 1.2U_{eq}(C).

Figures

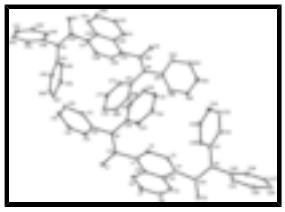


Fig. 1. The molecular structure of (I), showing 30% probability displacement ellipsoids.

N,*N*,*N*',*N*'-Tetraphenylnaphthalene-1,4-dicarboxamide

Crystal data

$C_{36}H_{26}N_2O_2$	$Z = 4$
$M_r = 518.59$	$F_{000} = 1088$
Triclinic, $P\overline{1}$	$D_x = 1.312$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 10.0276$ (8) Å	Cell parameters from 13361 reflections
$b = 13.4211$ (11) Å	$\theta = 3.0$–27.5°
$c = 20.2414$ (13) Å	$\mu = 0.08$ mm^{-1}
$\alpha = 88.560$ (2)°	$T = 153$ (2) K
$\beta = 89.279$ (2)°	Block, white
$\gamma = 74.523$ (3)°	0.49 × 0.28 × 0.21 mm
$V = 2624.5$ (3) Å^3	

Data collection

Rigaku R-AXIS RAPID diffractometer	5904 reflections with $I > 2\sigma(I)$
Radiation source: Rotating anode	$R_{int} = 0.055$
Monochromator: graphite	$\theta_{max} = 25.5^\circ$
$T = 153$(2) K	$\theta_{min} = 3.0^\circ$
ω scans	$h = -12 \rightarrow 12$
Absorption correction: none	$k = -16 \rightarrow 16$
20350 measured reflections	$l = -24 \rightarrow 23$
9674 independent reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.066$	$w = 1/[\sigma^2(F_o^2) + (0.061P)^2 + 5P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.192$	$(\Delta/\sigma)_{max} = 0.001$
$S = 1.00$	$\Delta\rho_{max} = 0.69$ e Å^{-3}

9674 reflections

722 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

$\Delta\rho_{min} = -0.40$ e Å^{-3}

Extinction correction: SHELXL97 (Sheldrick, 1997), $Fc^{*}=kFc[1+0.001xFc^{2}\lambda^{3}/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.0062 (8)

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 $F^2 > 2\text{sigma}(F^2)$ 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}
O1	0.5048 (2)	0.74330 (18)	0.48167 (10)	0.0295 (5)
O2	0.1292 (3)	1.2351 (2)	0.56123 (12)	0.0428 (7)
O3	1.0879 (3)	0.0431 (2)	0.93001 (12)	0.0415 (7)
O4	0.6618 (3)	0.5119 (2)	1.01899 (11)	0.0357 (6)
N1	0.6095 (3)	0.7125 (2)	0.58195 (12)	0.0269 (6)
N2	0.2346 (3)	1.2341 (2)	0.65984 (13)	0.0303 (7)
N3	0.9590 (3)	0.0321 (2)	0.84020 (13)	0.0325 (7)
N4	0.6043 (3)	0.5654 (2)	0.91324 (12)	0.0273 (6)
C1	0.4381 (3)	0.8770 (3)	0.55987 (14)	0.0264 (7)
C2	0.5034 (3)	0.9527 (2)	0.57279 (14)	0.0241 (7)
H2	0.6015	0.9368	0.5703	0.029*
C3	0.4280 (3)	1.0518 (3)	0.58946 (14)	0.0281 (8)
H3	0.4751	1.1029	0.5979	0.034*
C4	0.2851 (3)	1.0769 (3)	0.59392 (15)	0.0283 (8)
C5	0.0682 (4)	1.0197 (3)	0.59077 (17)	0.0382 (9)
H5	0.0153	1.0866	0.6031	0.046*
C6	0.0036 (4)	0.9439 (3)	0.58117 (18)	0.0402 (9)
H6	−0.0936	0.9581	0.5877	0.048*
C7	0.0786 (4)	0.8459 (3)	0.56193 (18)	0.0411 (9)
H7	0.0317	0.7945	0.5541	0.049*
C8	0.2189 (4)	0.8230 (3)	0.55423 (16)	0.0334 (8)
H8	0.2690	0.7555	0.5417	0.040*
C9	0.2905 (3)	0.8995 (3)	0.56481 (14)	0.0258 (7)
C10	0.2151 (3)	0.9997 (3)	0.58244 (15)	0.0276 (7)
C11	0.5192 (3)	0.7723 (3)	0.53754 (15)	0.0251 (7)
C12	0.6774 (3)	0.6061 (3)	0.56730 (14)	0.0247 (7)
C13	0.5991 (3)	0.5355 (3)	0.56387 (15)	0.0276 (7)

H13	0.5011	0.5587	0.5667	0.033*
C14	0.6627 (4)	0.4318 (3)	0.55629 (15)	0.0318 (8)
H14	0.6084	0.3840	0.5529	0.038*
C15	0.8050 (4)	0.3975 (3)	0.55365 (15)	0.0310 (8)
H15	0.8493	0.3258	0.5501	0.037*
C16	0.8833 (4)	0.4686 (3)	0.55627 (16)	0.0316 (8)
H16	0.9813	0.4453	0.5541	0.038*
C17	0.8197 (3)	0.5728 (3)	0.56202 (15)	0.0302 (8)
H17	0.8736	0.6212	0.5624	0.036*
C18	0.6154 (4)	0.7416 (3)	0.64971 (15)	0.0287 (8)
C19	0.7372 (4)	0.7577 (3)	0.67385 (18)	0.0357 (9)
H19	0.8157	0.7515	0.6459	0.043*
C20	0.7414 (4)	0.7832 (3)	0.73996 (19)	0.0457 (11)
H20	0.8248	0.7917	0.7577	0.055*
C21	0.6258 (5)	0.7962 (3)	0.77997 (18)	0.0459 (11)
H21	0.6288	0.8162	0.8245	0.055*
C22	0.5064 (4)	0.7801 (3)	0.75530 (17)	0.0407 (9)
H22	0.4271	0.7883	0.7829	0.049*
C23	0.5018 (4)	0.7522 (3)	0.69054 (16)	0.0357 (9)
H23	0.4194	0.7402	0.6739	0.043*
C24	0.2087 (4)	1.1875 (3)	0.60324 (16)	0.0311 (8)
C25	0.1900 (3)	1.3461 (3)	0.66238 (15)	0.0271 (7)
C26	0.0965 (3)	1.3928 (3)	0.71010 (16)	0.0313 (8)
H26	0.0604	1.3519	0.7408	0.038*
C27	0.0553 (4)	1.5001 (3)	0.71307 (17)	0.0360 (9)
H27	−0.0087	1.5328	0.7460	0.043*
C28	0.1079 (4)	1.5592 (3)	0.66786 (17)	0.0359 (9)
H28	0.0790	1.6326	0.6692	0.043*
C29	0.2031 (4)	1.5105 (3)	0.62054 (16)	0.0331 (8)
H29	0.2401	1.5510	0.5899	0.040*
C30	0.2449 (4)	1.4037 (3)	0.61751 (16)	0.0318 (8)
H30	0.3100	1.3706	0.5851	0.038*
C31	0.3036 (4)	1.1801 (3)	0.71727 (15)	0.0296 (8)
C32	0.3998 (4)	1.2187 (3)	0.74882 (17)	0.0341 (8)
H32	0.4226	1.2784	0.7314	0.041*
C33	0.4629 (4)	1.1706 (3)	0.80566 (18)	0.0413 (10)
H33	0.5270	1.1986	0.8279	0.050*
C34	0.4336 (4)	1.0820 (3)	0.83032 (17)	0.0442 (10)
H34	0.4789	1.0482	0.8688	0.053*
C35	0.3383 (4)	1.0429 (3)	0.79884 (17)	0.0401 (9)
H35	0.3183	0.9817	0.8156	0.048*
C36	0.2712 (4)	1.0926 (3)	0.74273 (16)	0.0350 (8)
H36	0.2033	1.0667	0.7219	0.042*
C37	0.9085 (4)	0.1931 (3)	0.90240 (15)	0.0282 (8)
C38	0.7680 (4)	0.2105 (3)	0.91349 (16)	0.0319 (8)
H38	0.7259	0.1554	0.9096	0.038*
C39	0.6872 (4)	0.3090 (3)	0.93039 (15)	0.0286 (7)
H39	0.5908	0.3196	0.9381	0.034*
C40	0.7443 (4)	0.3892 (3)	0.93589 (15)	0.0284 (8)

C41	0.9507 (4)	0.4578 (3)	0.92473 (16)	0.0333 (8)
H41	0.8961	0.5245	0.9363	0.040*
C42	1.0879 (4)	0.4434 (3)	0.91044 (17)	0.0382 (9)
H42	1.1277	0.5001	0.9119	0.046*
C43	1.1698 (4)	0.3458 (3)	0.89371 (17)	0.0368 (9)
H43	1.2651	0.3366	0.8836	0.044*
C44	1.1141 (4)	0.2630 (3)	0.89171 (17)	0.0358 (9)
H44	1.1711	0.1968	0.8806	0.043*
C45	0.9712 (3)	0.2758 (3)	0.90621 (15)	0.0293 (8)
C46	0.8887 (3)	0.3748 (3)	0.92251 (15)	0.0263 (7)
C47	0.9939 (4)	0.0847 (3)	0.89241 (16)	0.0318 (8)
C48	1.0115 (4)	−0.0788 (3)	0.83908 (17)	0.0320 (8)
C49	0.9870 (4)	−0.1382 (3)	0.89221 (19)	0.0435 (10)
H49	0.9387	−0.1063	0.9301	0.052*
C50	1.0338 (5)	−0.2450 (3)	0.8895 (2)	0.0502 (11)
H50	1.0174	−0.2865	0.9258	0.060*
C51	1.1044 (4)	−0.2920 (3)	0.8341 (2)	0.0471 (11)
H51	1.1355	−0.3652	0.8324	0.057*
C52	1.1289 (4)	−0.2318 (3)	0.7823 (2)	0.0428 (10)
H52	1.1780	−0.2636	0.7445	0.051*
C53	1.0827 (4)	−0.1246 (3)	0.78424 (18)	0.0366 (9)
H53	1.1000	−0.0832	0.7480	0.044*
C54	0.8826 (4)	0.0821 (3)	0.78338 (16)	0.0306 (8)
C55	0.7856 (4)	0.0398 (3)	0.75558 (18)	0.0390 (9)
H55	0.7654	−0.0193	0.7756	0.047*
C56	0.7179 (4)	0.0837 (3)	0.69838 (19)	0.0449 (10)
H56	0.6536	0.0529	0.6786	0.054*
C57	0.7423 (4)	0.1711 (3)	0.66984 (18)	0.0440 (10)
H57	0.6943	0.2013	0.6310	0.053*
C58	0.8375 (4)	0.2149 (3)	0.69816 (17)	0.0422 (10)
H58	0.8539	0.2760	0.6791	0.051*
C59	0.9090 (4)	0.1698 (3)	0.75415 (16)	0.0354 (8)
H59	0.9763	0.1990	0.7726	0.042*
C60	0.6635 (3)	0.4933 (3)	0.95938 (15)	0.0264 (7)
C61	0.5503 (4)	0.6726 (3)	0.93096 (15)	0.0303 (8)
C62	0.6368 (4)	0.7212 (3)	0.96301 (18)	0.0401 (9)
H62	0.7298	0.6845	0.9724	0.048*
C63	0.5869 (4)	0.8231 (3)	0.98110 (19)	0.0466 (10)
H63	0.6442	0.8559	1.0045	0.056*
C64	0.4523 (5)	0.8772 (3)	0.96485 (19)	0.0473 (10)
H64	0.4196	0.9481	0.9757	0.057*
C65	0.3659 (4)	0.8300 (3)	0.93334 (17)	0.0396 (9)
H65	0.2735	0.8671	0.9233	0.048*
C66	0.4166 (4)	0.7262 (3)	0.91635 (16)	0.0367 (9)
H66	0.3580	0.6926	0.8945	0.044*
C67	0.5813 (3)	0.5334 (3)	0.84756 (15)	0.0287 (8)
C68	0.4591 (4)	0.5074 (3)	0.83508 (16)	0.0312 (8)
H68	0.3919	0.5108	0.8691	0.037*
C69	0.4365 (4)	0.4764 (3)	0.77233 (16)	0.0366 (9)

H69	0.3522	0.4603	0.7627	0.044*
C70	0.5365 (4)	0.4691 (3)	0.72372 (16)	0.0344 (8)
H70	0.5215	0.4465	0.6810	0.041*
C71	0.6583 (4)	0.4945 (3)	0.73674 (16)	0.0339 (8)
H71	0.7271	0.4890	0.7033	0.041*
C72	0.6790 (3)	0.5279 (3)	0.79878 (15)	0.0305 (8)
H72	0.7613	0.5473	0.8077	0.037*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0352 (13)	0.0278 (14)	0.0258 (11)	−0.0084 (11)	−0.0037 (10)	−0.0024 (9)
O2	0.0499 (16)	0.0291 (15)	0.0441 (14)	0.0003 (12)	−0.0239 (12)	−0.0042 (11)
O3	0.0469 (16)	0.0324 (15)	0.0421 (14)	−0.0042 (12)	−0.0173 (12)	−0.0016 (11)
O4	0.0434 (15)	0.0360 (15)	0.0267 (12)	−0.0084 (12)	−0.0033 (10)	−0.0026 (10)
N1	0.0333 (15)	0.0216 (15)	0.0247 (13)	−0.0053 (12)	−0.0043 (11)	−0.0032 (11)
N2	0.0355 (16)	0.0246 (16)	0.0263 (14)	0.0006 (13)	−0.0073 (12)	−0.0042 (11)
N3	0.0390 (17)	0.0250 (16)	0.0315 (15)	−0.0045 (13)	−0.0083 (12)	−0.0021 (12)
N4	0.0310 (15)	0.0230 (15)	0.0252 (13)	−0.0021 (12)	−0.0020 (11)	−0.0026 (11)
C1	0.0306 (17)	0.0285 (19)	0.0188 (14)	−0.0054 (15)	−0.0056 (13)	−0.0014 (13)
C2	0.0245 (16)	0.0235 (18)	0.0255 (15)	−0.0083 (14)	−0.0033 (12)	−0.0004 (13)
C3	0.0350 (19)	0.0269 (19)	0.0218 (15)	−0.0066 (15)	−0.0063 (13)	−0.0017 (13)
C4	0.0318 (18)	0.0265 (19)	0.0241 (15)	−0.0030 (15)	−0.0042 (13)	−0.0049 (13)
C5	0.034 (2)	0.039 (2)	0.0400 (19)	−0.0044 (17)	−0.0075 (16)	−0.0097 (16)
C6	0.0259 (18)	0.049 (3)	0.048 (2)	−0.0133 (18)	0.0043 (16)	−0.0138 (18)
C7	0.037 (2)	0.043 (2)	0.046 (2)	−0.0137 (18)	−0.0043 (17)	−0.0109 (18)
C8	0.036 (2)	0.030 (2)	0.0363 (18)	−0.0128 (16)	−0.0035 (15)	−0.0061 (15)
C9	0.0298 (17)	0.0253 (18)	0.0228 (15)	−0.0077 (14)	−0.0010 (13)	−0.0035 (13)
C10	0.0332 (18)	0.0242 (18)	0.0263 (16)	−0.0086 (15)	−0.0064 (13)	−0.0034 (13)
C11	0.0266 (17)	0.0245 (18)	0.0265 (16)	−0.0108 (14)	−0.0024 (13)	0.0002 (13)
C12	0.0261 (17)	0.0267 (18)	0.0212 (14)	−0.0066 (14)	−0.0021 (12)	−0.0012 (13)
C13	0.0286 (17)	0.0280 (19)	0.0289 (16)	−0.0120 (15)	−0.0036 (13)	−0.0004 (13)
C14	0.040 (2)	0.029 (2)	0.0279 (16)	−0.0100 (16)	−0.0066 (15)	−0.0020 (14)
C15	0.043 (2)	0.0256 (19)	0.0234 (16)	−0.0065 (16)	−0.0067 (14)	0.0008 (13)
C16	0.0263 (17)	0.035 (2)	0.0328 (17)	−0.0057 (15)	−0.0033 (14)	−0.0063 (15)
C17	0.0285 (18)	0.032 (2)	0.0308 (17)	−0.0091 (15)	−0.0029 (14)	−0.0033 (14)
C18	0.0342 (19)	0.0230 (18)	0.0269 (16)	−0.0039 (15)	−0.0034 (14)	−0.0021 (13)
C19	0.0339 (19)	0.033 (2)	0.0414 (19)	−0.0101 (17)	−0.0071 (16)	−0.0037 (16)
C20	0.052 (3)	0.037 (2)	0.048 (2)	−0.0094 (19)	−0.023 (2)	−0.0064 (18)
C21	0.075 (3)	0.033 (2)	0.0285 (18)	−0.011 (2)	−0.0094 (19)	−0.0004 (15)
C22	0.056 (2)	0.036 (2)	0.0288 (18)	−0.0096 (19)	0.0009 (17)	0.0021 (15)
C23	0.043 (2)	0.034 (2)	0.0298 (17)	−0.0101 (17)	−0.0028 (15)	0.0023 (15)
C24	0.0311 (18)	0.028 (2)	0.0314 (17)	−0.0037 (15)	−0.0038 (14)	−0.0038 (14)
C25	0.0287 (17)	0.0221 (18)	0.0261 (16)	0.0012 (14)	−0.0042 (13)	−0.0062 (13)
C26	0.0310 (18)	0.032 (2)	0.0320 (17)	−0.0108 (16)	0.0018 (14)	−0.0030 (14)
C27	0.035 (2)	0.032 (2)	0.0389 (19)	−0.0050 (17)	−0.0033 (15)	−0.0088 (16)
C28	0.039 (2)	0.029 (2)	0.0383 (19)	−0.0045 (16)	−0.0128 (16)	−0.0024 (15)
C29	0.038 (2)	0.034 (2)	0.0297 (17)	−0.0129 (16)	−0.0082 (15)	0.0013 (14)

C30	0.0341 (19)	0.034 (2)	0.0250 (16)	−0.0043 (16)	−0.0048 (14)	−0.0046 (14)
C31	0.0354 (19)	0.0242 (19)	0.0258 (16)	−0.0018 (15)	−0.0034 (14)	−0.0036 (13)
C32	0.0349 (19)	0.032 (2)	0.0360 (18)	−0.0098 (16)	−0.0055 (15)	−0.0032 (15)
C33	0.039 (2)	0.043 (2)	0.040 (2)	−0.0054 (18)	−0.0110 (17)	−0.0056 (17)
C34	0.045 (2)	0.050 (3)	0.0291 (18)	0.001 (2)	−0.0053 (16)	0.0009 (17)
C35	0.051 (2)	0.032 (2)	0.0330 (18)	−0.0039 (18)	0.0045 (17)	0.0033 (15)
C36	0.042 (2)	0.032 (2)	0.0305 (17)	−0.0085 (17)	0.0020 (15)	−0.0042 (15)
C37	0.0358 (19)	0.0222 (18)	0.0270 (16)	−0.0080 (15)	−0.0070 (14)	−0.0008 (13)
C38	0.0339 (19)	0.031 (2)	0.0316 (17)	−0.0104 (16)	−0.0059 (14)	−0.0012 (14)
C39	0.0284 (17)	0.0279 (19)	0.0290 (16)	−0.0064 (15)	−0.0015 (13)	−0.0026 (14)
C40	0.0363 (19)	0.0254 (19)	0.0231 (15)	−0.0071 (15)	−0.0046 (13)	−0.0002 (13)
C41	0.036 (2)	0.030 (2)	0.0344 (18)	−0.0100 (16)	0.0013 (15)	−0.0049 (15)
C42	0.040 (2)	0.038 (2)	0.0386 (19)	−0.0127 (18)	−0.0020 (16)	−0.0054 (16)
C43	0.0300 (19)	0.040 (2)	0.0419 (19)	−0.0118 (17)	0.0018 (15)	−0.0087 (16)
C44	0.0335 (19)	0.038 (2)	0.0343 (18)	−0.0063 (17)	−0.0005 (15)	−0.0094 (15)
C45	0.0319 (18)	0.032 (2)	0.0236 (15)	−0.0080 (15)	−0.0061 (13)	−0.0008 (13)
C46	0.0300 (17)	0.0250 (18)	0.0246 (15)	−0.0084 (14)	−0.0002 (13)	−0.0035 (13)
C47	0.0348 (19)	0.031 (2)	0.0303 (17)	−0.0088 (16)	−0.0030 (15)	0.0001 (14)
C48	0.0331 (19)	0.0235 (19)	0.0377 (18)	−0.0039 (15)	−0.0095 (15)	−0.0041 (14)
C49	0.049 (2)	0.033 (2)	0.047 (2)	−0.0103 (19)	−0.0019 (18)	0.0002 (17)
C50	0.060 (3)	0.028 (2)	0.062 (3)	−0.012 (2)	−0.007 (2)	0.0086 (19)
C51	0.044 (2)	0.030 (2)	0.066 (3)	−0.0063 (18)	−0.018 (2)	−0.0011 (19)
C52	0.037 (2)	0.033 (2)	0.057 (2)	−0.0049 (18)	−0.0097 (18)	−0.0138 (18)
C53	0.040 (2)	0.031 (2)	0.0402 (19)	−0.0112 (17)	−0.0022 (16)	−0.0057 (16)
C54	0.0345 (19)	0.0255 (19)	0.0291 (16)	−0.0032 (15)	−0.0034 (14)	−0.0027 (14)
C55	0.0325 (19)	0.040 (2)	0.047 (2)	−0.0126 (17)	−0.0077 (16)	−0.0055 (17)
C56	0.038 (2)	0.050 (3)	0.043 (2)	−0.0035 (19)	−0.0108 (17)	−0.0074 (19)
C57	0.043 (2)	0.046 (3)	0.0327 (19)	0.0059 (19)	−0.0048 (16)	−0.0017 (17)
C58	0.051 (2)	0.038 (2)	0.0342 (19)	−0.0066 (19)	−0.0038 (17)	0.0020 (16)
C59	0.045 (2)	0.029 (2)	0.0321 (18)	−0.0085 (17)	−0.0023 (15)	−0.0024 (15)
C60	0.0279 (17)	0.0234 (18)	0.0289 (16)	−0.0085 (14)	−0.0027 (13)	−0.0014 (13)
C61	0.0332 (18)	0.033 (2)	0.0229 (15)	−0.0055 (16)	−0.0010 (13)	−0.0026 (14)
C62	0.040 (2)	0.032 (2)	0.046 (2)	−0.0035 (17)	−0.0046 (17)	−0.0073 (16)
C63	0.053 (3)	0.040 (2)	0.047 (2)	−0.011 (2)	−0.0046 (19)	−0.0082 (18)
C64	0.066 (3)	0.031 (2)	0.044 (2)	−0.012 (2)	0.002 (2)	0.0001 (17)
C65	0.046 (2)	0.033 (2)	0.0309 (18)	0.0055 (18)	−0.0064 (16)	0.0007 (15)
C66	0.042 (2)	0.033 (2)	0.0320 (18)	−0.0041 (17)	−0.0082 (16)	−0.0052 (15)
C67	0.0323 (18)	0.0285 (19)	0.0219 (15)	−0.0019 (15)	−0.0055 (13)	−0.0012 (13)
C68	0.0327 (18)	0.032 (2)	0.0294 (17)	−0.0097 (16)	0.0000 (14)	−0.0015 (14)
C69	0.039 (2)	0.040 (2)	0.0314 (17)	−0.0109 (18)	−0.0065 (15)	−0.0031 (16)
C70	0.045 (2)	0.037 (2)	0.0238 (16)	−0.0161 (17)	−0.0034 (15)	−0.0032 (14)
C71	0.039 (2)	0.034 (2)	0.0275 (17)	−0.0089 (17)	0.0013 (15)	−0.0001 (14)
C72	0.0271 (17)	0.036 (2)	0.0286 (16)	−0.0086 (16)	0.0008 (13)	−0.0012 (14)

Geometric parameters (Å, °)

O1—C11	1.228 (4)	C32—H32	0.95
O2—C24	1.219 (4)	C33—C34	1.379 (6)
O3—C47	1.223 (4)	C33—H33	0.95

O4—C60	1.237 (4)	C34—C35	1.376 (6)
N1—C11	1.366 (4)	C34—H34	0.95
N1—C18	1.442 (4)	C35—C36	1.389 (5)
N1—C12	1.446 (4)	C35—H35	0.95
N2—C24	1.379 (4)	C36—H36	0.95
N2—C31	1.437 (4)	C37—C38	1.382 (5)
N2—C25	1.452 (4)	C37—C45	1.418 (5)
N3—C47	1.384 (4)	C37—C47	1.495 (5)
N3—C54	1.438 (4)	C38—C39	1.401 (5)
N3—C48	1.441 (4)	C38—H38	0.95
N4—C60	1.350 (4)	C39—C40	1.356 (5)
N4—C67	1.447 (4)	C39—H39	0.95
N4—C61	1.449 (4)	C40—C46	1.432 (5)
C1—C2	1.379 (5)	C40—C60	1.501 (5)
C1—C9	1.433 (5)	C41—C42	1.365 (5)
C1—C11	1.501 (4)	C41—C46	1.415 (5)
C2—C3	1.391 (4)	C41—H41	0.95
C2—H2	0.95	C42—C43	1.395 (5)
C3—C4	1.384 (5)	C42—H42	0.95
C3—H3	0.95	C43—C44	1.373 (5)
C4—C10	1.423 (5)	C43—H43	0.95
C4—C24	1.493 (5)	C44—C45	1.425 (5)
C5—C6	1.363 (5)	C44—H44	0.95
C5—C10	1.433 (5)	C45—C46	1.410 (5)
C5—H5	0.95	C48—C53	1.378 (5)
C6—C7	1.392 (5)	C48—C49	1.381 (5)
C6—H6	0.95	C49—C50	1.387 (6)
C7—C8	1.365 (5)	C49—H49	0.95
C7—H7	0.95	C50—C51	1.389 (6)
C8—C9	1.422 (5)	C50—H50	0.95
C8—H8	0.95	C51—C52	1.368 (6)
C9—C10	1.408 (4)	C51—H51	0.95
C12—C17	1.381 (5)	C52—C53	1.390 (5)
C12—C13	1.385 (5)	C52—H52	0.95
C13—C14	1.378 (5)	C53—H53	0.95
C13—H13	0.95	C54—C55	1.382 (5)
C14—C15	1.379 (5)	C54—C59	1.391 (5)
C14—H14	0.95	C55—C56	1.386 (5)
C15—C16	1.390 (5)	C55—H55	0.95
C15—H15	0.95	C56—C57	1.373 (6)
C16—C17	1.380 (5)	C56—H56	0.95
C16—H16	0.95	C57—C58	1.384 (6)
C17—H17	0.95	C57—H57	0.95
C18—C23	1.378 (5)	C58—C59	1.385 (5)
C18—C19	1.392 (5)	C58—H58	0.95
C19—C20	1.393 (5)	C59—H59	0.95
C19—H19	0.95	C61—C66	1.374 (5)
C20—C21	1.381 (6)	C61—C62	1.391 (5)
C20—H20	0.95	C62—C63	1.381 (5)

C21—C22	1.374 (6)	C62—H62	0.95
C21—H21	0.95	C63—C64	1.391 (6)
C22—C23	1.377 (5)	C63—H63	0.95
C22—H22	0.95	C64—C65	1.374 (6)
C23—H23	0.95	C64—H64	0.95
C25—C26	1.378 (5)	C65—C66	1.399 (5)
C25—C30	1.380 (5)	C65—H65	0.95
C26—C27	1.392 (5)	C66—H66	0.95
C26—H26	0.95	C67—C72	1.371 (5)
C27—C28	1.385 (5)	C67—C68	1.389 (5)
C27—H27	0.95	C68—C69	1.386 (5)
C28—C29	1.390 (5)	C68—H68	0.95
C28—H28	0.95	C69—C70	1.383 (5)
C29—C30	1.385 (5)	C69—H69	0.95
C29—H29	0.95	C70—C71	1.383 (5)
C30—H30	0.95	C70—H70	0.95
C31—C32	1.381 (5)	C71—C72	1.380 (5)
C31—C36	1.385 (5)	C71—H71	0.95
C32—C33	1.380 (5)	C72—H72	0.95
C11—N1—C18	122.3 (3)	C34—C35—C36	120.3 (4)
C11—N1—C12	119.8 (2)	C34—C35—H35	119.8
C18—N1—C12	116.1 (2)	C36—C35—H35	119.8
C24—N2—C31	124.9 (3)	C31—C36—C35	119.7 (4)
C24—N2—C25	118.4 (3)	C31—C36—H36	120.1
C31—N2—C25	116.7 (2)	C35—C36—H36	120.1
C47—N3—C54	123.9 (3)	C38—C37—C45	120.0 (3)
C47—N3—C48	118.9 (3)	C38—C37—C47	118.8 (3)
C54—N3—C48	117.0 (3)	C45—C37—C47	121.0 (3)
C60—N4—C67	119.5 (3)	C37—C38—C39	120.5 (3)
C60—N4—C61	120.4 (3)	C37—C38—H38	119.7
C67—N4—C61	119.7 (2)	C39—C38—H38	119.7
C2—C1—C9	119.9 (3)	C40—C39—C38	121.0 (3)
C2—C1—C11	120.8 (3)	C40—C39—H39	119.5
C9—C1—C11	119.2 (3)	C38—C39—H39	119.5
C1—C2—C3	121.0 (3)	C39—C40—C46	120.0 (3)
C1—C2—H2	119.5	C39—C40—C60	122.5 (3)
C3—C2—H2	119.5	C46—C40—C60	117.5 (3)
C4—C3—C2	120.8 (3)	C42—C41—C46	120.9 (3)
C4—C3—H3	119.6	C42—C41—H41	119.5
C2—C3—H3	119.6	C46—C41—H41	119.5
C3—C4—C10	119.5 (3)	C41—C42—C43	120.3 (4)
C3—C4—C24	118.3 (3)	C41—C42—H42	119.8
C10—C4—C24	121.9 (3)	C43—C42—H42	119.8
C6—C5—C10	120.7 (3)	C44—C43—C42	120.6 (4)
C6—C5—H5	119.6	C44—C43—H43	119.7
C10—C5—H5	119.6	C42—C43—H43	119.7
C5—C6—C7	120.7 (3)	C43—C44—C45	120.3 (3)
C5—C6—H6	119.7	C43—C44—H44	119.8
C7—C6—H6	119.7	C45—C44—H44	119.8

C8—C7—C6	120.6 (4)	C46—C45—C37	119.1 (3)
C8—C7—H7	119.7	C46—C45—C44	118.8 (3)
C6—C7—H7	119.7	C37—C45—C44	122.1 (3)
C7—C8—C9	120.4 (3)	C45—C46—C41	119.0 (3)
C7—C8—H8	119.8	C45—C46—C40	119.4 (3)
C9—C8—H8	119.8	C41—C46—C40	121.6 (3)
C10—C9—C8	119.4 (3)	O3—C47—N3	121.3 (3)
C10—C9—C1	118.6 (3)	O3—C47—C37	121.4 (3)
C8—C9—C1	122.0 (3)	N3—C47—C37	117.2 (3)
C9—C10—C4	120.2 (3)	C53—C48—C49	120.7 (4)
C9—C10—C5	118.2 (3)	C53—C48—N3	119.6 (3)
C4—C10—C5	121.7 (3)	C49—C48—N3	119.7 (3)
O1—C11—N1	122.4 (3)	C48—C49—C50	119.1 (4)
O1—C11—C1	120.8 (3)	C48—C49—H49	120.5
N1—C11—C1	116.8 (3)	C50—C49—H49	120.5
C17—C12—C13	119.9 (3)	C49—C50—C51	120.6 (4)
C17—C12—N1	120.6 (3)	C49—C50—H50	119.7
C13—C12—N1	119.3 (3)	C51—C50—H50	119.7
C14—C13—C12	120.4 (3)	C52—C51—C50	119.4 (4)
C14—C13—H13	119.8	C52—C51—H51	120.3
C12—C13—H13	119.8	C50—C51—H51	120.3
C13—C14—C15	120.0 (3)	C51—C52—C53	120.6 (4)
C13—C14—H14	120.0	C51—C52—H52	119.7
C15—C14—H14	120.0	C53—C52—H52	119.7
C14—C15—C16	119.4 (3)	C48—C53—C52	119.5 (4)
C14—C15—H15	120.3	C48—C53—H53	120.2
C16—C15—H15	120.3	C52—C53—H53	120.2
C17—C16—C15	120.6 (3)	C55—C54—C59	119.3 (3)
C17—C16—H16	119.7	C55—C54—N3	119.5 (3)
C15—C16—H16	119.7	C59—C54—N3	121.1 (3)
C16—C17—C12	119.6 (3)	C54—C55—C56	119.9 (4)
C16—C17—H17	120.2	C54—C55—H55	120.1
C12—C17—H17	120.2	C56—C55—H55	120.1
C23—C18—C19	120.2 (3)	C57—C56—C55	120.9 (4)
C23—C18—N1	120.2 (3)	C57—C56—H56	119.5
C19—C18—N1	119.6 (3)	C55—C56—H56	119.5
C18—C19—C20	118.5 (4)	C56—C57—C58	119.4 (4)
C18—C19—H19	120.8	C56—C57—H57	120.3
C20—C19—H19	120.8	C58—C57—H57	120.3
C21—C20—C19	120.8 (4)	C57—C58—C59	120.2 (4)
C21—C20—H20	119.6	C57—C58—H58	119.9
C19—C20—H20	119.6	C59—C58—H58	119.9
C22—C21—C20	119.9 (3)	C58—C59—C54	120.2 (4)
C22—C21—H21	120.1	C58—C59—H59	119.9
C20—C21—H21	120.1	C54—C59—H59	119.9
C21—C22—C23	120.0 (4)	O4—C60—N4	122.8 (3)
C21—C22—H22	120.0	O4—C60—C40	119.3 (3)
C23—C22—H22	120.0	N4—C60—C40	117.7 (3)
C22—C23—C18	120.6 (4)	C66—C61—C62	120.1 (3)

C22—C23—H23	119.7	C66—C61—N4	121.1 (3)
C18—C23—H23	119.7	C62—C61—N4	118.7 (3)
O2—C24—N2	121.5 (3)	C63—C62—C61	119.7 (4)
O2—C24—C4	120.8 (3)	C63—C62—H62	120.2
N2—C24—C4	117.7 (3)	C61—C62—H62	120.2
C26—C25—C30	121.3 (3)	C62—C63—C64	119.7 (4)
C26—C25—N2	119.7 (3)	C62—C63—H63	120.2
C30—C25—N2	119.0 (3)	C64—C63—H63	120.2
C25—C26—C27	119.7 (4)	C65—C64—C63	121.1 (4)
C25—C26—H26	120.2	C65—C64—H64	119.5
C27—C26—H26	120.2	C63—C64—H64	119.5
C28—C27—C26	119.8 (3)	C64—C65—C66	118.8 (4)
C28—C27—H27	120.1	C64—C65—H65	120.6
C26—C27—H27	120.1	C66—C65—H65	120.6
C27—C28—C29	119.6 (4)	C61—C66—C65	120.6 (4)
C27—C28—H28	120.2	C61—C66—H66	119.7
C29—C28—H28	120.2	C65—C66—H66	119.7
C30—C29—C28	120.8 (4)	C72—C67—C68	120.7 (3)
C30—C29—H29	119.6	C72—C67—N4	120.6 (3)
C28—C29—H29	119.6	C68—C67—N4	118.7 (3)
C25—C30—C29	118.8 (3)	C69—C68—C67	119.1 (3)
C25—C30—H30	120.6	C69—C68—H68	120.5
C29—C30—H30	120.6	C67—C68—H68	120.5
C32—C31—C36	119.7 (3)	C70—C69—C68	120.0 (3)
C32—C31—N2	119.2 (3)	C70—C69—H69	120.0
C36—C31—N2	121.1 (3)	C68—C69—H69	120.0
C33—C32—C31	120.1 (4)	C69—C70—C71	120.5 (3)
C33—C32—H32	119.9	C69—C70—H70	119.7
C31—C32—H32	119.9	C71—C70—H70	119.7
C34—C33—C32	120.4 (4)	C72—C71—C70	119.3 (3)
C34—C33—H33	119.8	C72—C71—H71	120.3
C32—C33—H33	119.8	C70—C71—H71	120.3
C35—C34—C33	119.7 (3)	C67—C72—C71	120.4 (3)
C35—C34—H34	120.2	C67—C72—H72	119.8
C33—C34—H34	120.2	C71—C72—H72	119.8
C9—C1—C2—C3	−1.2 (4)	C45—C37—C38—C39	−1.8 (5)
C11—C1—C2—C3	175.9 (3)	C47—C37—C38—C39	172.8 (3)
C1—C2—C3—C4	0.4 (5)	C37—C38—C39—C40	0.4 (5)
C2—C3—C4—C10	1.1 (5)	C38—C39—C40—C46	1.8 (5)
C2—C3—C4—C24	−172.1 (3)	C38—C39—C40—C60	−174.7 (3)
C10—C5—C6—C7	−1.1 (6)	C46—C41—C42—C43	−0.4 (5)
C5—C6—C7—C8	2.0 (6)	C41—C42—C43—C44	−0.4 (5)
C6—C7—C8—C9	−0.9 (5)	C42—C43—C44—C45	0.5 (5)
C7—C8—C9—C10	−0.9 (5)	C38—C37—C45—C46	1.1 (4)
C7—C8—C9—C1	177.4 (3)	C47—C37—C45—C46	−173.4 (3)
C2—C1—C9—C10	0.5 (4)	C38—C37—C45—C44	−176.6 (3)
C11—C1—C9—C10	−176.7 (3)	C47—C37—C45—C44	8.9 (5)
C2—C1—C9—C8	−177.7 (3)	C43—C44—C45—C46	0.0 (5)
C11—C1—C9—C8	5.1 (4)	C43—C44—C45—C37	177.7 (3)

C8—C9—C10—C4	179.3 (3)	C37—C45—C46—C41	−178.5 (3)
C1—C9—C10—C4	1.0 (4)	C44—C45—C46—C41	−0.8 (4)
C8—C9—C10—C5	1.6 (4)	C37—C45—C46—C40	1.0 (4)
C1—C9—C10—C5	−176.6 (3)	C44—C45—C46—C40	178.8 (3)
C3—C4—C10—C9	−1.8 (4)	C42—C41—C46—C45	0.9 (5)
C24—C4—C10—C9	171.2 (3)	C42—C41—C46—C40	−178.6 (3)
C3—C4—C10—C5	175.8 (3)	C39—C40—C46—C45	−2.5 (4)
C24—C4—C10—C5	−11.2 (5)	C60—C40—C46—C45	174.2 (3)
C6—C5—C10—C9	−0.7 (5)	C39—C40—C46—C41	177.0 (3)
C6—C5—C10—C4	−178.3 (3)	C60—C40—C46—C41	−6.3 (4)
C18—N1—C11—O1	−173.0 (3)	C54—N3—C47—O3	−159.9 (4)
C12—N1—C11—O1	−8.8 (5)	C48—N3—C47—O3	14.4 (5)
C18—N1—C11—C1	7.6 (5)	C54—N3—C47—C37	22.4 (5)
C12—N1—C11—C1	171.8 (3)	C48—N3—C47—C37	−163.3 (3)
C2—C1—C11—O1	−113.1 (4)	C38—C37—C47—O3	−118.5 (4)
C9—C1—C11—O1	64.1 (4)	C45—C37—C47—O3	56.1 (5)
C2—C1—C11—N1	66.3 (4)	C38—C37—C47—N3	59.2 (4)
C9—C1—C11—N1	−116.6 (3)	C45—C37—C47—N3	−126.2 (3)
C11—N1—C12—C17	118.4 (3)	C47—N3—C48—C53	−126.1 (4)
C18—N1—C12—C17	−76.5 (4)	C54—N3—C48—C53	48.5 (5)
C11—N1—C12—C13	−66.8 (4)	C47—N3—C48—C49	55.6 (5)
C18—N1—C12—C13	98.3 (3)	C54—N3—C48—C49	−129.8 (4)
C17—C12—C13—C14	1.1 (5)	C53—C48—C49—C50	−0.6 (6)
N1—C12—C13—C14	−173.8 (3)	N3—C48—C49—C50	177.7 (3)
C12—C13—C14—C15	1.5 (5)	C48—C49—C50—C51	0.0 (6)
C13—C14—C15—C16	−2.3 (5)	C49—C50—C51—C52	0.6 (6)
C14—C15—C16—C17	0.5 (5)	C50—C51—C52—C53	−0.6 (6)
C15—C16—C17—C12	2.0 (5)	C49—C48—C53—C52	0.6 (5)
C13—C12—C17—C16	−2.8 (5)	N3—C48—C53—C52	−177.7 (3)
N1—C12—C17—C16	171.9 (3)	C51—C52—C53—C48	0.0 (5)
C11—N1—C18—C23	61.9 (5)	C47—N3—C54—C55	−141.9 (4)
C12—N1—C18—C23	−102.8 (4)	C48—N3—C54—C55	43.7 (5)
C11—N1—C18—C19	−118.8 (4)	C47—N3—C54—C59	40.9 (5)
C12—N1—C18—C19	76.4 (4)	C48—N3—C54—C59	−133.5 (4)
C23—C18—C19—C20	0.9 (5)	C59—C54—C55—C56	1.3 (5)
N1—C18—C19—C20	−178.4 (3)	N3—C54—C55—C56	−175.9 (3)
C18—C19—C20—C21	−2.5 (6)	C54—C55—C56—C57	−2.2 (6)
C19—C20—C21—C22	2.5 (6)	C55—C56—C57—C58	1.0 (6)
C20—C21—C22—C23	−0.7 (6)	C56—C57—C58—C59	1.0 (6)
C21—C22—C23—C18	−1.0 (6)	C57—C58—C59—C54	−1.9 (6)
C19—C18—C23—C22	0.9 (6)	C55—C54—C59—C58	0.7 (5)
N1—C18—C23—C22	−179.9 (3)	N3—C54—C59—C58	177.9 (3)
C31—N2—C24—O2	166.9 (3)	C67—N4—C60—O4	−165.4 (3)
C25—N2—C24—O2	−13.4 (5)	C61—N4—C60—O4	7.8 (5)
C31—N2—C24—C4	−15.2 (5)	C67—N4—C60—C40	19.8 (5)
C25—N2—C24—C4	164.6 (3)	C61—N4—C60—C40	−167.0 (3)
C3—C4—C24—O2	116.2 (4)	C39—C40—C60—O4	91.3 (4)
C10—C4—C24—O2	−56.9 (5)	C46—C40—C60—O4	−85.3 (4)
C3—C4—C24—N2	−61.8 (4)	C39—C40—C60—N4	−93.7 (4)

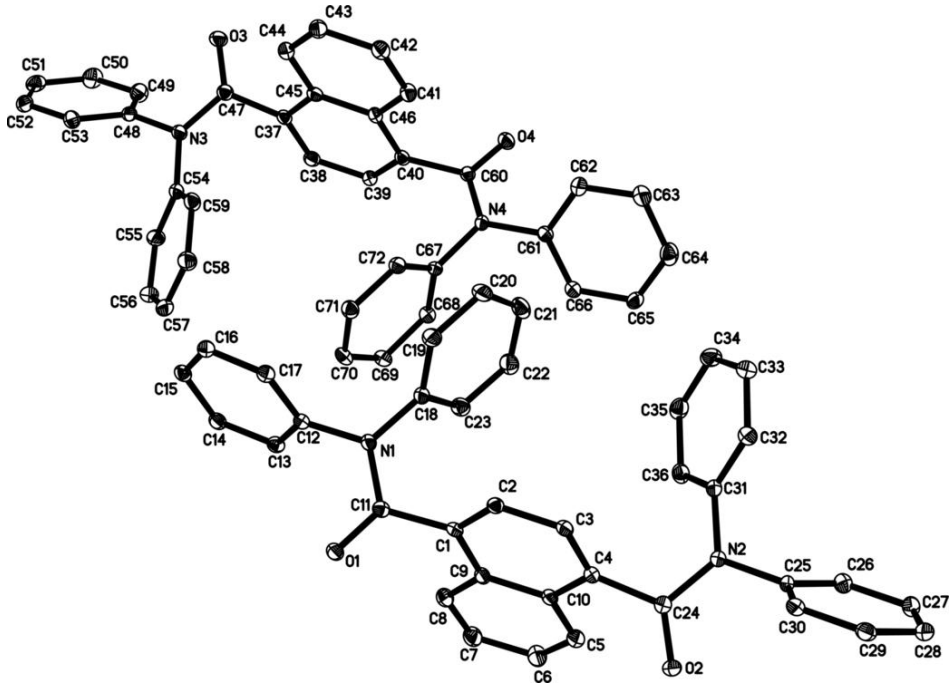
C10—C4—C24—N2	125.1 (4)	C46—C40—C60—N4	89.7 (4)
C24—N2—C25—C26	119.6 (4)	C60—N4—C61—C66	−126.6 (4)
C31—N2—C25—C26	−60.6 (4)	C67—N4—C61—C66	46.6 (5)
C24—N2—C25—C30	−61.7 (4)	C60—N4—C61—C62	53.7 (5)
C31—N2—C25—C30	118.0 (3)	C67—N4—C61—C62	−133.1 (4)
C30—C25—C26—C27	0.5 (5)	C66—C61—C62—C63	1.1 (6)
N2—C25—C26—C27	179.1 (3)	N4—C61—C62—C63	−179.2 (3)
C25—C26—C27—C28	0.4 (5)	C61—C62—C63—C64	−2.5 (6)
C26—C27—C28—C29	−1.0 (5)	C62—C63—C64—C65	2.6 (6)
C27—C28—C29—C30	0.8 (5)	C63—C64—C65—C66	−1.4 (6)
C26—C25—C30—C29	−0.7 (5)	C62—C61—C66—C65	0.1 (6)
N2—C25—C30—C29	−179.3 (3)	N4—C61—C66—C65	−179.6 (3)
C28—C29—C30—C25	0.1 (5)	C64—C65—C66—C61	0.0 (6)
C24—N2—C31—C32	138.0 (4)	C60—N4—C67—C72	−91.8 (4)
C25—N2—C31—C32	−41.7 (4)	C61—N4—C67—C72	94.9 (4)
C24—N2—C31—C36	−44.5 (5)	C60—N4—C67—C68	87.6 (4)
C25—N2—C31—C36	135.8 (3)	C61—N4—C67—C68	−85.7 (4)
C36—C31—C32—C33	−0.3 (5)	C72—C67—C68—C69	−0.4 (5)
N2—C31—C32—C33	177.2 (3)	N4—C67—C68—C69	−179.9 (3)
C31—C32—C33—C34	1.9 (6)	C67—C68—C69—C70	1.7 (5)
C32—C33—C34—C35	−1.5 (6)	C68—C69—C70—C71	−1.4 (6)
C33—C34—C35—C36	−0.4 (6)	C69—C70—C71—C72	−0.4 (6)
C32—C31—C36—C35	−1.6 (5)	C68—C67—C72—C71	−1.3 (5)
N2—C31—C36—C35	−179.1 (3)	N4—C67—C72—C71	178.1 (3)
C34—C35—C36—C31	2.0 (5)	C70—C71—C72—C67	1.7 (5)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C14—H14···O1^{i}	0.95	2.41	3.342 (4)	166
C30—H30···O1^{ii}	0.95	2.48	3.413 (4)	168
C65—H65···O3^{iii}	0.95	2.59	3.420 (4)	146
C42—H42···O4^{iv}	0.95	2.51	3.105 (4)	120
C68—H68···O4^{v}	0.95	2.35	3.209 (4)	150
C16—H16···Cg2^{vi}	0.95	2.85	3.443 (1)	122
C21—H21···Cg4	0.95	2.90	3.643 (1)	135
C39—H39···Cg4^{vii}	0.95	2.86	3.430 (1)	119
C44—H44···Cg3^{vi}	0.95	2.90	3.600 (1)	132
C69—H69···Cg2^{viii}	0.95	2.87	3.711 (4)	148
C71—H71···Cg1	0.95	2.91	3.670 (1)	138

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1; (ii) −*x*+1, −*y*+2, −*z*+1; (iii) *x*−1, *y*+1, *z*; (iv) −*x*+2, −*y*+1, −*z*+2; (v) −*x*+1, −*y*+1, −*z*+2; (vi) *x*+1, *y*−1, *z*; (vii) −*x*+1, −*y*+2, −*z*+2; (viii) *x*, *y*−1, *z*.

Fig. 1


C43
C44
O3
C42
C51
C50
C49
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C46
O4
C38
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C30
C5
C29
C28
C7
O2
C6