Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

N,*N*′-(Pyrene-1,8-diyl)bis(2,3-dimethoxybenzaldehyde)

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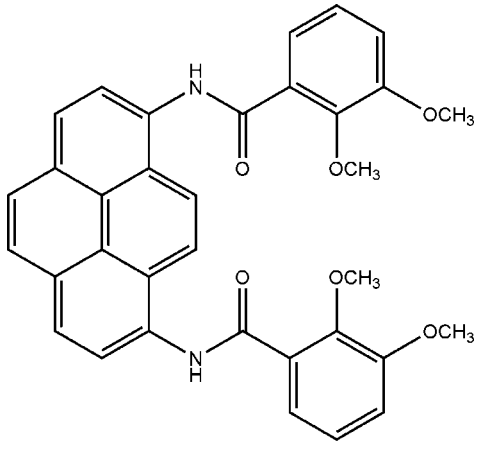
Received 6 July 2007; accepted 22 July 2007

Key indicators: single-crystal X-ray study; T = 141 K; mean σ(C–C) = 0.007 Å; R factor = 0.049; wR factor = 0.053; data-to-parameter ratio = 7.4.

The title compound, $C_{34}H_{28}N_2O_6$, crystallizes with two molecules per asymmetric unit, both stabilized by intramolecular N—H···O interactions. In the crystal structure, weak intermolecular π–π interactions occur at distances ranging from 3.383 (7) to 3.533 (7) Å at closest contact.

Related literature

For related literature, see: Janiak (2000); Vollman *et al.* (1937).



Experimental

Crystal data

$C_{34}H_{28}N_2O_6$
M_r = 560.60
Orthorhombic, $P2_12_12_1$
a = 12.5065 (9) Å
b = 15.074 (1) Å
c = 28.223 (2) Å
V = 5320.8 (6) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 141.2 K
0.24 × 0.18 × 0.07 mm

Data collection

Bruker SMART 1000 diffractometer
Absorption correction: multi-scan (Blessing, 1995)
T_{min} = 0.914, T_{max} = 0.993
23940 measured reflections
5011 independent reflections
3491 reflections with $F^2 > 3\sigma(F^2)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.053
S = 2.16
3491 reflections
473 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H53···O11	0.96 (6)	1.95 (5)	2.700 (6)	134 (4)
N2—H54···O8	0.95 (4)	2.00 (4)	2.746 (5)	134 (4)
N3—H55···O5	0.95 (6)	1.96 (6)	2.723 (5)	136 (5)
N4—H56···O2	0.94 (6)	2.03 (5)	2.727 (5)	130 (4)

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *TEXSAN* (Molecular Structure Corporation, 1999); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *TEXSAN*.

The authors thank Professor Kenneth N. Raymond and Dr Frederick Hollander, Department of Chemistry, UC Berkeley, for valuable instruction in the theory and practice of X-ray crystallography.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2475).

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 doi:10.1107/S1600536807035751

supplementary materials

Acta Cryst. (2007). E**63**, o3621 [**doi:10.1107/S1600536807035751**]

N,*N*'-(Pyrene-1,8-diyl)bis(2,3-dimethoxybenzaldehyde)

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Comment

The title compound, (I), cyrstallizes in space group $P2_12_12_1$ with a pseudo-inversion center that lies between the two molecules of the asymmetric unit. The pseudo-inversion center is not located at coordinates appropriate to generate a centrosymmetric space group. The structure exhibits C—N, C—C, and C—O bond lengths and angles typical for common organic molecules. There are intramolecular hydrogen bonds located between the amide NH groups and the methoxy oxygen atoms for both molecules (Table 1).

Intermolecular distances between pyrene and catechol-derived rings range between 3.753 (7) Å and 3.800 (7) Å. These can be attributed to weak π–π interactions (Janiak, 2000). Such intermolecular contacts are not unexpected in a molecule with many aromatic rings. The aromatic rings do not stack closer to one another because the methoxy groups are positioned between the ring systems. Interplanar angles between the pyrene and a catechol-derivative ring range from 7.85–12.25 degrees. The angle between the two pyrene rings in the asymmetric unit is 3.38 degrees. The angle between catechol-derivative rings of the same molecule ranges from 5.93 to 11.24 degrees. Deviations from planarity between rings within the same molecule are most likely a result of the molecule accomodating favorable π–π interactions.

Experimental

The title compound was prepared by condensation of 1,8-diaminopyrene with the appropriate acid chloride according to the method described by Vollman *et al.* (1937). X-ray quality crystals of (I) were obtained by vapor diffusion of petroleum ether into chloroform at room temperature.

Refinement

Due to negligible anomalous dispersion, Friedel pairs were merged before refinement. Only the oxygen, nitrogen and methoxy carbon atoms were refined anisotropically due to the low data to parameter ratio. The C-bound H atoms were geometrically placed and refined as riding. The N-bound H atoms were located in difference maps and their positions were refined.

Figures

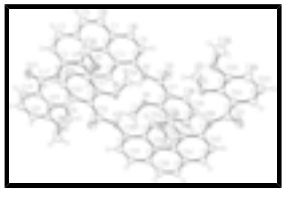
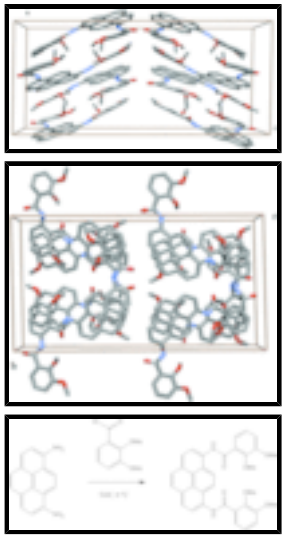


Fig. 1. The molecular structure of (I) showing 50% displacement ellipsoids/spheres (arbitrary spheres for the H atoms).
Fig. 2. View of the unit cell of (I) along the *b* axis.
Fig. 3. View of the unit cell of (I) along the *a* axis.



N,N'-(Pyrene-1,8-diyl)bis(2,3-dimethoxybenzaldehyde)

Crystal data

$C_{34}H_{28}N_2O_6$	D_x = 1.400 Mg m^{-3}
M_r = 560.60	Mo $K\alpha$ radiation λ = 0.7107 Å
Orthorhombic, $P2_12_12_1$	Cell parameters from 4595 reflections
a = 12.5065 (9) Å	θ = 3.3–23.5º
b = 15.074 (1) Å	μ = 0.10 mm^{-1}
c = 28.223 (2) Å	T = 141.2 K
V = 5320.8 (6) Å^3	Slab, green
Z = 8	0.24 × 0.18 × 0.07 mm
F_{000} = 2352.00	

Data collection

Bruker SMART 1000 diffractometer	3491 reflections with $F^2 > 3\sigma(F^2)$
ω scans	R_{int} = 0.025
Absorption correction: multi-scan (Blessing, 1995)	θ_{max} = 24.7º
T_{min} = 0.914, T_{max} = 0.993	h = 0→14
23940 measured reflections	k = 0→17
5011 independent reflections	l = 0→33

Refinement

Refinement on F	$(\Delta/\sigma)_{max}$ = 0.001
$R[F^2 > 2\sigma(F^2)]$ = 0.049	$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$wR(F^2)$ = 0.053	$\Delta\rho_{min}$ = −0.30 e Å^{-3}

S = 2.16
3491 reflections
473 parameters
H atoms treated by a mixture of
independent and constrained refinement
$w = 1/[\sigma^2(F_o) + 0.00022|F_o|^2]$

Extinction correction: none

Special details

Refinement. Refinement using reflections with $F^2 > 3.0$ sigma(F^2). The weighted *R*-factor (*wR*), goodness of fit (S) and *R*-factor (gt) are based on F, with F set to zero for negative F. The threshold expression of $F^2 > 3.0$ sigma(F^2) is used only for calculating *R*-factor (gt).

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.1497 (3)	−0.3210 (2)	0.1913 (1)	0.051 (1)
O2	0.1194 (3)	−0.1567 (2)	0.1632 (1)	0.0335 (10)
O3	0.0472 (4)	−0.1003 (3)	0.0231 (1)	0.077 (2)
O4	0.1354 (3)	0.3934 (2)	0.3115 (1)	0.057 (1)
O5	0.1516 (3)	0.1158 (2)	0.3304 (1)	0.0324 (9)
O6	0.2436 (3)	0.0517 (2)	0.4074 (1)	0.043 (1)
O7	0.2627 (3)	0.3786 (2)	0.0847 (1)	0.050 (1)
O8	0.3468 (3)	0.3176 (2)	0.1643 (1)	0.0333 (10)
O9	0.3531 (3)	0.0418 (2)	0.1885 (1)	0.059 (1)
O10	0.4824 (4)	0.5331 (3)	0.4771 (1)	0.066 (1)
O11	0.3775 (3)	0.5875 (2)	0.3402 (1)	0.037 (1)
O12	0.3409 (3)	0.7512 (2)	0.3127 (1)	0.051 (1)
N1	0.4875 (3)	0.4834 (3)	0.4009 (2)	0.034 (1)
N2	0.4193 (3)	0.1729 (3)	0.2139 (1)	0.033 (1)
N3	0.0788 (3)	0.2612 (3)	0.2831 (1)	0.030 (1)
N4	0.0194 (4)	−0.0517 (3)	0.0982 (1)	0.035 (1)
C1	0.5229 (4)	0.3959 (3)	0.4064 (2)	0.032 (1)*
C2	0.5754 (4)	0.3684 (3)	0.4475 (2)	0.037 (1)*
C3	0.6079 (4)	0.2809 (3)	0.4523 (2)	0.044 (1)*
C4	0.5879 (4)	0.2174 (3)	0.4179 (2)	0.035 (1)*
C5	0.6150 (4)	0.1261 (4)	0.4237 (2)	0.045 (1)*
C6	0.5947 (4)	0.0663 (4)	0.3903 (2)	0.046 (1)*
C7	0.5499 (4)	0.0913 (3)	0.3452 (2)	0.035 (1)*
C8	0.5340 (4)	0.0315 (3)	0.3082 (2)	0.040 (1)*
C9	0.4940 (4)	0.0579 (3)	0.2656 (2)	0.037 (1)*
C10	0.4659 (4)	0.1460 (3)	0.2572 (2)	0.030 (1)*
C11	0.4792 (4)	0.2093 (3)	0.2933 (2)	0.029 (1)*
C12	0.4477 (4)	0.3005 (3)	0.2889 (2)	0.035 (1)*
C13	0.4592 (4)	0.3589 (3)	0.3248 (2)	0.033 (1)*
C14	0.5073 (4)	0.3355 (3)	0.3689 (2)	0.028 (1)*
C15	0.5397 (4)	0.2457 (3)	0.3748 (2)	0.031 (1)*
C16	0.5231 (4)	0.1836 (3)	0.3376 (2)	0.032 (1)*

C17	0.4704 (4)	0.5460 (3)	0.4347 (2)	0.035 (1)*
C18	0.4411 (4)	0.6363 (3)	0.4165 (2)	0.033 (1)*
C19	0.4602 (4)	0.7072 (3)	0.4470 (2)	0.044 (1)*
C20	0.4406 (5)	0.7924 (4)	0.4327 (2)	0.051 (2)*
C21	0.4011 (4)	0.8114 (4)	0.3881 (2)	0.045 (1)*
C22	0.3791 (4)	0.7425 (4)	0.3574 (2)	0.039 (1)*
C23	0.3985 (4)	0.6547 (3)	0.3718 (2)	0.031 (1)*
C24	0.2656 (5)	0.5666 (4)	0.3378 (2)	0.054 (2)
C25	0.3139 (5)	0.8375 (4)	0.2961 (2)	0.065 (2)
C26	0.3647 (4)	0.1219 (3)	0.1828 (2)	0.034 (1)*
C27	0.3196 (4)	0.1662 (3)	0.1390 (2)	0.032 (1)*
C28	0.2814 (4)	0.1075 (3)	0.1042 (2)	0.038 (1)*
C29	0.2360 (4)	0.1399 (3)	0.0634 (2)	0.042 (1)*
C30	0.2268 (4)	0.2297 (3)	0.0551 (2)	0.042 (1)*
C31	0.2651 (4)	0.2891 (3)	0.0890 (2)	0.040 (1)*
C32	0.3103 (4)	0.2562 (3)	0.1311 (2)	0.032 (1)*
C33	0.2590 (4)	0.3556 (3)	0.1908 (2)	0.047 (2)
C34	0.1973 (4)	0.4145 (4)	0.0483 (2)	0.052 (2)
C35	0.0323 (4)	0.2886 (3)	0.2398 (2)	0.031 (1)*
C36	0.0046 (4)	0.3761 (3)	0.2310 (2)	0.036 (1)*
C37	−0.0330 (4)	0.4011 (3)	0.1870 (2)	0.037 (1)*
C38	−0.0470 (4)	0.3411 (3)	0.1501 (2)	0.034 (1)*
C39	−0.0869 (4)	0.3666 (3)	0.1044 (2)	0.040 (1)*
C40	−0.1005 (4)	0.3069 (3)	0.0701 (2)	0.038 (1)*
C41	−0.0720 (4)	0.2155 (3)	0.0767 (2)	0.036 (1)*
C42	−0.0829 (4)	0.1524 (3)	0.0411 (2)	0.040 (1)*
C43	−0.0519 (4)	0.0656 (3)	0.0468 (2)	0.039 (1)*
C44	−0.0105 (4)	0.0371 (3)	0.0901 (2)	0.032 (1)*
C45	−0.0010 (4)	0.0974 (3)	0.1281 (2)	0.028 (1)*
C46	0.0395 (4)	0.0738 (3)	0.1738 (2)	0.034 (1)*
C47	0.0487 (4)	0.1326 (3)	0.2093 (2)	0.034 (1)*
C48	0.0189 (4)	0.2238 (3)	0.2037 (2)	0.029 (1)*
C49	−0.0200 (4)	0.2510 (3)	0.1587 (2)	0.028 (1)*
C50	−0.0306 (4)	0.1878 (3)	0.1212 (2)	0.028 (1)*
C51	0.1290 (4)	0.3131 (3)	0.3153 (2)	0.034 (1)*
C52	0.1779 (4)	0.2675 (3)	0.3578 (2)	0.031 (1)*
C53	0.2180 (4)	0.3227 (3)	0.3934 (2)	0.039 (1)*
C54	0.2678 (4)	0.2896 (3)	0.4324 (2)	0.038 (1)*
C55	0.2798 (4)	0.1990 (3)	0.4387 (2)	0.040 (1)*
C56	0.2395 (4)	0.1418 (3)	0.4049 (2)	0.036 (1)*
C57	0.1883 (4)	0.1765 (3)	0.3639 (2)	0.031 (1)*
C58	0.2379 (4)	0.0788 (3)	0.3031 (2)	0.044 (2)
C59	0.2925 (5)	0.0143 (4)	0.4484 (2)	0.056 (2)
C60	0.0461 (4)	−0.1147 (4)	0.0659 (2)	0.040 (1)*
C61	0.0686 (4)	−0.2063 (3)	0.0849 (2)	0.035 (1)*
C62	0.0519 (4)	−0.2768 (3)	0.0538 (2)	0.042 (1)*
C63	0.0648 (5)	−0.3622 (4)	0.0687 (2)	0.049 (2)*
C64	0.0973 (4)	−0.3808 (3)	0.1144 (2)	0.045 (1)*
C65	0.1173 (4)	−0.3115 (3)	0.1455 (2)	0.036 (1)*

C66	0.1015 (4)	−0.2243 (3)	0.1306 (2)	0.032 (1)*
C67	0.2306 (5)	−0.1351 (4)	0.1675 (2)	0.050 (2)
C68	0.1803 (5)	−0.4063 (4)	0.2073 (2)	0.064 (2)
H1	0.3892	0.8711	0.3787	0.0543*
H2	0.4870	0.6963	0.4779	0.0529*
H3	0.4545	0.8398	0.4540	0.0615*
H4	0.5890	0.4096	0.4722	0.0440*
H5	0.6451	0.2639	0.4801	0.0524*
H6	0.6484	0.1076	0.4523	0.0542*
H7	0.6101	0.0056	0.3963	0.0552*
H8	0.5515	−0.0293	0.3129	0.0483*
H9	0.4850	0.0154	0.2410	0.0439*
H10	0.4179	0.3204	0.2598	0.0420*
H11	0.4344	0.4179	0.3206	0.0400*
H12	0.2870	0.0453	0.1090	0.0456*
H13	0.2104	0.0993	0.0402	0.0501*
H14	0.1947	0.2508	0.0268	0.0505*
H15	0.0115	0.4191	0.2554	0.0433*
H16	−0.0500	0.4618	0.1817	0.0438*
H17	−0.1039	0.4271	0.0985	0.0476*
H18	−0.1297	0.3253	0.0406	0.0459*
H19	−0.1131	0.1699	0.0116	0.0476*
H20	−0.0585	0.0250	0.0212	0.0469*
H21	0.0606	0.0141	0.1792	0.0407*
H22	0.0758	0.1131	0.2390	0.0408*
H23	0.0314	−0.2653	0.0220	0.0503*
H24	0.0512	−0.4096	0.0473	0.0586*
H25	0.1060	−0.4405	0.1244	0.0546*
H26	0.2103	0.3851	0.3902	0.0463*
H27	0.2947	0.3292	0.4557	0.0455*
H28	0.3152	0.1765	0.4659	0.0477*
H29	0.2269	0.6177	0.3280	0.0652*
H30	0.2547	0.5201	0.3156	0.0652*
H31	0.2412	0.5484	0.3681	0.0652*
H32	0.3755	0.8744	0.2972	0.0782*
H33	0.2886	0.8338	0.2645	0.0782*
H34	0.2597	0.8620	0.3158	0.0782*
H35	0.2691	−0.1860	0.1777	0.0594*
H36	0.2573	−0.1162	0.1376	0.0594*
H37	0.2393	−0.0888	0.1900	0.0594*
H38	0.1216	−0.4460	0.2041	0.0765*
H39	0.2387	−0.4272	0.1889	0.0765*
H40	0.2009	−0.4031	0.2397	0.0765*
H41	0.2861	0.3967	0.2133	0.0560*
H42	0.2120	0.3854	0.1696	0.0560*
H43	0.2213	0.3098	0.2067	0.0560*
H44	0.2855	0.0480	0.3236	0.0527*
H45	0.2100	0.0388	0.2803	0.0527*
H46	0.2754	0.1252	0.2875	0.0527*

H47	0.2023	0.4774	0.0488	0.0620*
H48	0.2207	0.3930	0.0184	0.0620*
H49	0.1252	0.3973	0.0534	0.0620*
H50	0.2535	0.0315	0.4758	0.0668*
H51	0.2926	−0.0486	0.4459	0.0668*
H52	0.3640	0.0350	0.4509	0.0668*
H53	0.473 (4)	0.501 (3)	0.369 (2)	0.04 (1)*
H54	0.427 (4)	0.234 (3)	0.206 (1)	0.04 (1)*
H55	0.074 (5)	0.200 (4)	0.290 (2)	0.04 (2)*
H56	0.021 (4)	−0.070 (3)	0.130 (2)	0.04 (1)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.071 (3)	0.038 (2)	0.042 (2)	0.014 (2)	0.003 (2)	0.005 (2)
O2	0.036 (2)	0.030 (2)	0.034 (2)	−0.002 (2)	−0.002 (2)	−0.004 (2)
O3	0.134 (4)	0.066 (3)	0.031 (2)	0.042 (3)	0.016 (2)	0.004 (2)
O4	0.075 (3)	0.028 (2)	0.066 (3)	−0.006 (2)	−0.024 (2)	0.002 (2)
O5	0.037 (2)	0.029 (2)	0.031 (2)	−0.001 (2)	0.002 (2)	−0.005 (1)
O6	0.060 (3)	0.032 (2)	0.039 (2)	−0.001 (2)	−0.009 (2)	0.005 (2)
O7	0.057 (3)	0.037 (2)	0.056 (2)	−0.001 (2)	−0.019 (2)	0.007 (2)
O8	0.029 (2)	0.031 (2)	0.039 (2)	−0.003 (2)	0.000 (2)	−0.009 (2)
O9	0.081 (3)	0.031 (2)	0.065 (3)	−0.014 (2)	−0.025 (2)	0.004 (2)
O10	0.109 (4)	0.060 (2)	0.028 (2)	0.023 (3)	0.004 (2)	−0.002 (2)
O11	0.038 (2)	0.035 (2)	0.036 (2)	−0.003 (2)	−0.003 (2)	−0.005 (2)
O12	0.069 (3)	0.042 (2)	0.043 (2)	0.014 (2)	−0.004 (2)	0.006 (2)
N1	0.045 (3)	0.029 (2)	0.028 (2)	0.002 (2)	0.000 (2)	−0.005 (2)
N2	0.040 (3)	0.024 (3)	0.035 (3)	−0.004 (2)	0.001 (2)	−0.002 (2)
N3	0.038 (3)	0.025 (2)	0.028 (2)	−0.001 (2)	0.002 (2)	−0.002 (2)
N4	0.051 (3)	0.029 (2)	0.026 (2)	−0.003 (2)	0.002 (2)	−0.001 (2)
C24	0.053 (4)	0.045 (3)	0.065 (4)	−0.008 (3)	−0.017 (3)	−0.003 (3)
C25	0.081 (5)	0.057 (4)	0.058 (4)	0.025 (4)	0.007 (4)	0.015 (3)
C33	0.039 (3)	0.040 (3)	0.060 (4)	0.001 (3)	0.005 (3)	−0.011 (3)
C34	0.052 (4)	0.050 (4)	0.053 (4)	0.011 (3)	−0.002 (3)	0.004 (3)
C58	0.037 (3)	0.041 (3)	0.054 (3)	0.005 (3)	0.011 (3)	−0.010 (3)
C59	0.073 (5)	0.044 (4)	0.050 (3)	0.005 (3)	−0.007 (3)	0.005 (3)
C67	0.044 (4)	0.048 (3)	0.056 (4)	−0.007 (3)	−0.008 (3)	−0.009 (3)
C68	0.078 (5)	0.046 (4)	0.067 (4)	0.019 (4)	0.009 (4)	0.017 (3)

Geometric parameters (Å, °)

O1—C65	1.363 (5)	C45—C50	1.425 (6)
O1—C68	1.417 (6)	C46—C47	1.344 (6)
O2—C66	1.391 (6)	C47—C48	1.434 (7)
O2—C67	1.434 (6)	C48—C49	1.420 (6)
O3—C60	1.228 (6)	C49—C50	1.430 (6)
O4—C51	1.217 (6)	C51—C52	1.514 (6)
O5—C57	1.393 (5)	C52—C53	1.396 (7)
O5—C58	1.438 (5)	C52—C57	1.388 (7)

O6—C56	1.361 (6)	C53—C54	1.361 (7)
O6—C59	1.426 (6)	C54—C55	1.384 (7)
O7—C31	1.355 (6)	C55—C56	1.382 (7)
O7—C34	1.419 (6)	C56—C57	1.421 (6)
O8—C32	1.393 (5)	C60—C61	1.506 (7)
O8—C33	1.446 (6)	C61—C62	1.394 (6)
O9—C26	1.225 (6)	C61—C66	1.382 (6)
O10—C17	1.222 (5)	C62—C63	1.364 (7)
O11—C23	1.375 (5)	C63—C64	1.380 (7)
O11—C24	1.436 (6)	C64—C65	1.387 (7)
O12—C22	1.357 (6)	C65—C66	1.394 (7)
O12—C25	1.422 (6)	N1—H53	0.93 (5)
N1—C1	1.401 (6)	N2—H54	0.87 (4)
N1—C17	1.358 (6)	N3—H55	0.91 (6)
N2—C10	1.413 (6)	N4—H56	0.95 (5)
N2—C26	1.354 (6)	C2—H4	0.950
N3—C35	1.413 (6)	C3—H5	0.950
N3—C51	1.354 (6)	C5—H6	0.950
N4—C44	1.408 (6)	C6—H7	0.950
N4—C60	1.359 (6)	C8—H8	0.950
C1—C2	1.396 (6)	C9—H9	0.950
C1—C14	1.409 (6)	C12—H10	0.950
C2—C3	1.385 (7)	C13—H11	0.950
C3—C4	1.386 (7)	C19—H2	0.950
C4—C5	1.427 (7)	C20—H3	0.950
C4—C15	1.422 (6)	C21—H1	0.950
C5—C6	1.330 (7)	C24—H29	0.950
C6—C7	1.441 (7)	C24—H30	0.950
C7—C8	1.392 (6)	C24—H31	0.950
C7—C16	1.447 (7)	C25—H32	0.950
C8—C9	1.364 (6)	C25—H33	0.950
C9—C10	1.395 (7)	C25—H34	0.950
C10—C11	1.405 (6)	C28—H12	0.950
C11—C12	1.436 (7)	C29—H13	0.950
C11—C16	1.420 (6)	C30—H14	0.950
C12—C13	1.351 (6)	C33—H41	0.950
C13—C14	1.427 (6)	C33—H42	0.950
C14—C15	1.422 (7)	C33—H43	0.950
C15—C16	1.423 (6)	C34—H47	0.950
C17—C18	1.500 (6)	C34—H48	0.950
C18—C19	1.393 (7)	C34—H49	0.950
C18—C23	1.398 (6)	C36—H15	0.950
C19—C20	1.368 (7)	C37—H16	0.950
C20—C21	1.383 (7)	C39—H17	0.950
C21—C22	1.380 (7)	C40—H18	0.950
C22—C23	1.404 (7)	C42—H19	0.950
C26—C27	1.514 (6)	C43—H20	0.950
C27—C28	1.405 (6)	C46—H21	0.950
C27—C32	1.380 (6)	C47—H22	0.950

C28—C29	1.375 (7)	C53—H26	0.950
C29—C30	1.379 (7)	C54—H27	0.950
C30—C31	1.394 (7)	C55—H28	0.950
C31—C32	1.407 (7)	C58—H44	0.950
C35—C36	1.386 (7)	C58—H45	0.950
C35—C48	1.423 (6)	C58—H46	0.950
C36—C37	1.380 (6)	C59—H50	0.950
C37—C38	1.391 (6)	C59—H51	0.950
C38—C39	1.435 (6)	C59—H52	0.950
C38—C49	1.421 (6)	C62—H23	0.950
C39—C40	1.334 (7)	C63—H24	0.950
C40—C41	1.435 (7)	C64—H25	0.950
C41—C42	1.391 (7)	C67—H35	0.950
C41—C50	1.423 (6)	C67—H36	0.950
C42—C43	1.374 (7)	C67—H37	0.950
C43—C44	1.397 (6)	C68—H38	0.950
C44—C45	1.410 (6)	C68—H39	0.950
C45—C46	1.431 (6)	C68—H40	0.950
O1···N3^{i}	3.198 (6)	O12···C10^{iv}	3.499 (6)
O1···C35^{i}	3.419 (6)	N1···C28^{iv}	3.446 (7)
O2···N3^{i}	3.159 (5)	N2···C23^{v}	3.335 (6)
O2···C51^{i}	3.198 (6)	N2···C22^{v}	3.393 (7)
O2···O4^{i}	3.351 (5)	N3···C66^{iii}	3.328 (6)
O2···C36^{i}	3.401 (6)	N3···C65^{iii}	3.360 (6)
O2···C35^{i}	3.431 (6)	N4···C53^{i}	3.529 (7)
O3···C59^{ii}	3.185 (7)	C3···C62^{vii}	3.494 (7)
O3···C5^{ii}	3.483 (7)	C9···C58	3.388 (7)
O3···C55^{ii}	3.546 (6)	C10···C58	3.291 (7)
O4···C24	3.166 (7)	C14···C67^{iv}	3.463 (7)
O4···N4^{iii}	3.305 (6)	C14···C54	3.559 (7)
O4···C46^{iii}	3.514 (6)	C15···C67^{iv}	3.591 (7)
O5···C64^{iii}	3.482 (6)	C17···C28^{iv}	3.420 (7)
O5···C37^{i}	3.593 (6)	C18···C27^{iv}	3.408 (7)
O6···C39^{i}	3.425 (6)	C18···C28^{iv}	3.546 (7)
O7···C6^{iv}	3.419 (6)	C23···C26^{iv}	3.375 (7)
O8···C21^{v}	3.484 (6)	C23···C27^{iv}	3.542 (7)
O9···C67	3.132 (6)	C24···C45^{iii}	3.478 (8)
O9···N1^{v}	3.334 (6)	C28···C45	3.599 (7)
O9···O11^{v}	3.533 (6)	C29···C44	3.533 (7)
O9···C58	3.586 (6)	C29···C45	3.540 (7)
O10···C34^{vi}	3.118 (7)	C33···C35	3.313 (7)
O11···N2^{iv}	3.233 (5)	C33···C36	3.393 (7)
O11···C26^{iv}	3.330 (6)	C51···C66^{iii}	3.311 (7)
O11···C9^{iv}	3.420 (6)	C52···C61^{iii}	3.505 (7)

O11···C10^{iv}	3.490 (6)	C52···C66^{iii}	3.512 (7)
O12···N2^{iv}	3.310 (6)		
C65—O1—C68	118.6 (4)	C60—C61—C62	116.6 (4)
C66—O2—C67	112.2 (4)	C60—C61—C66	124.6 (5)
C57—O5—C58	111.7 (4)	C62—C61—C66	118.8 (5)
C56—O6—C59	116.9 (4)	C61—C62—C63	120.6 (5)
C31—O7—C34	117.3 (4)	C62—C63—C64	121.0 (5)
C32—O8—C33	111.2 (4)	C63—C64—C65	119.4 (5)
C23—O11—C24	112.2 (4)	O1—C65—C64	125.1 (5)
C22—O12—C25	118.5 (4)	O1—C65—C66	115.2 (4)
C1—N1—C17	128.8 (4)	C64—C65—C66	119.6 (5)
C10—N2—C26	127.3 (4)	O2—C66—C61	121.4 (4)
C35—N3—C51	127.0 (4)	O2—C66—C65	118.0 (4)
C44—N4—C60	128.4 (4)	C61—C66—C65	120.6 (5)
N1—C1—C2	121.4 (4)	C1—N1—H53	119 (2)
N1—C1—C14	118.8 (4)	C17—N1—H53	111 (2)
C2—C1—C14	119.8 (4)	C10—N2—H54	117 (2)
C1—C2—C3	120.1 (5)	C26—N2—H54	114 (2)
C2—C3—C4	122.4 (5)	C35—N3—H55	114 (3)
C3—C4—C5	122.9 (5)	C51—N3—H55	119 (3)
C3—C4—C15	117.9 (5)	C44—N4—H56	116 (2)
C5—C4—C15	119.3 (4)	C60—N4—H56	115 (3)
C4—C5—C6	121.8 (5)	C1—C2—H4	119.949
C5—C6—C7	121.6 (5)	C3—C2—H4	119.940
C6—C7—C8	123.2 (5)	C2—C3—H5	118.796
C6—C7—C16	118.1 (4)	C4—C3—H5	118.790
C8—C7—C16	118.7 (4)	C4—C5—H6	119.115
C7—C8—C9	121.6 (5)	C6—C5—H6	119.117
C8—C9—C10	121.3 (5)	C5—C6—H7	119.191
N2—C10—C9	121.6 (4)	C7—C6—H7	119.187
N2—C10—C11	118.7 (4)	C7—C8—H8	119.189
C9—C10—C11	119.6 (4)	C9—C8—H8	119.193
C10—C11—C12	123.6 (4)	C8—C9—H9	119.327
C10—C11—C16	119.9 (4)	C10—C9—H9	119.330
C12—C11—C16	116.4 (4)	C11—C12—H10	119.031
C11—C12—C13	121.9 (4)	C13—C12—H10	119.040
C12—C13—C14	122.6 (4)	C12—C13—H11	118.676
C1—C14—C13	123.6 (4)	C14—C13—H11	118.679
C1—C14—C15	119.2 (4)	C18—C19—H2	119.750
C13—C14—C15	117.2 (4)	C20—C19—H2	119.755
C4—C15—C14	120.4 (4)	C19—C20—H3	119.120
C4—C15—C16	119.6 (4)	C21—C20—H3	119.112
C14—C15—C16	120.0 (4)	C20—C21—H1	120.424
C7—C16—C11	118.8 (4)	C22—C21—H1	120.419
C7—C16—C15	119.4 (4)	O11—C24—H29	109.457
C11—C16—C15	121.7 (4)	O11—C24—H30	109.465
O10—C17—N1	123.9 (5)	O11—C24—H31	109.467
O10—C17—C18	120.7 (5)	H29—C24—H30	109.476

N1—C17—C18	115.4 (4)	H29—C24—H31	109.477
C17—C18—C19	116.3 (4)	H30—C24—H31	109.486
C17—C18—C23	125.6 (4)	O12—C25—H32	109.478
C19—C18—C23	118.1 (5)	O12—C25—H33	109.478
C18—C19—C20	120.5 (5)	O12—C25—H34	109.472
C19—C20—C21	121.8 (5)	H32—C25—H33	109.475
C20—C21—C22	119.2 (5)	H32—C25—H34	109.465
O12—C22—C21	125.5 (5)	H33—C25—H34	109.460
O12—C22—C23	114.9 (5)	C27—C28—H12	119.915
C21—C22—C23	119.5 (5)	C29—C28—H12	119.924
O11—C23—C18	120.7 (4)	C28—C29—H13	119.199
O11—C23—C22	118.3 (4)	C30—C29—H13	119.191
C18—C23—C22	120.9 (5)	C29—C30—H14	120.437
O9—C26—N2	122.3 (5)	C31—C30—H14	120.427
O9—C26—C27	119.9 (5)	O8—C33—H41	109.476
N2—C26—C27	117.8 (4)	O8—C33—H42	109.466
C26—C27—C28	114.7 (4)	O8—C33—H43	109.470
C26—C27—C32	126.7 (5)	H41—C33—H42	109.473
C28—C27—C32	118.6 (5)	H41—C33—H43	109.479
C27—C28—C29	120.2 (5)	H42—C33—H43	109.464
C28—C29—C30	121.6 (5)	O7—C34—H47	109.474
C29—C30—C31	119.1 (5)	O7—C34—H48	109.468
O7—C31—C30	124.8 (5)	O7—C34—H49	109.471
O7—C31—C32	115.8 (5)	H47—C34—H48	109.472
C30—C31—C32	119.4 (5)	H47—C34—H49	109.474
O8—C32—C27	121.1 (4)	H48—C34—H49	109.468
O8—C32—C31	117.8 (4)	C35—C36—H15	119.766
C27—C32—C31	121.1 (5)	C37—C36—H15	119.759
N3—C35—C36	122.4 (4)	C36—C37—H16	118.701
N3—C35—C48	117.8 (4)	C38—C37—H16	118.703
C36—C35—C48	119.7 (4)	C38—C39—H17	119.453
C35—C36—C37	120.5 (5)	C40—C39—H17	119.455
C36—C37—C38	122.6 (5)	C39—C40—H18	119.272
C37—C38—C39	122.9 (4)	C41—C40—H18	119.285
C37—C38—C49	117.6 (4)	C41—C42—H19	118.690
C39—C38—C49	119.5 (4)	C43—C42—H19	118.680
C38—C39—C40	121.1 (5)	C42—C43—H20	119.993
C39—C40—C41	121.4 (5)	C44—C43—H20	119.988
C40—C41—C42	122.6 (5)	C45—C46—H21	118.664
C40—C41—C50	119.2 (4)	C47—C46—H21	118.660
C42—C41—C50	118.2 (4)	C46—C47—H22	119.110
C41—C42—C43	122.6 (5)	C48—C47—H22	119.111
C42—C43—C44	120.0 (5)	C52—C53—H26	119.085
N4—C44—C43	122.2 (4)	C54—C53—H26	119.065
N4—C44—C45	117.9 (4)	C53—C54—H27	119.532
C43—C44—C45	119.9 (4)	C55—C54—H27	119.532
C44—C45—C46	123.7 (4)	C54—C55—H28	120.381
C44—C45—C50	119.4 (4)	C56—C55—H28	120.392
C46—C45—C50	116.9 (4)	O5—C58—H44	109.471

C45—C46—C47	122.7 (4)	O5—C58—H45	109.473
C46—C47—C48	121.8 (4)	O5—C58—H46	109.466
C35—C48—C47	123.2 (4)	H44—C58—H45	109.476
C35—C48—C49	118.9 (4)	H44—C58—H46	109.469
C47—C48—C49	117.8 (4)	H45—C58—H46	109.472
C38—C49—C48	120.7 (4)	O6—C59—H50	109.474
C38—C49—C50	119.2 (4)	O6—C59—H51	109.470
C48—C49—C50	120.0 (4)	O6—C59—H52	109.470
C41—C50—C45	119.7 (4)	H50—C59—H51	109.471
C41—C50—C49	119.5 (4)	H50—C59—H52	109.472
C45—C50—C49	120.8 (4)	H51—C59—H52	109.469
O4—C51—N3	123.2 (5)	C61—C62—H23	119.719
O4—C51—C52	119.6 (5)	C63—C62—H23	119.715
N3—C51—C52	117.2 (4)	C62—C63—H24	119.521
C51—C52—C53	116.4 (4)	C64—C63—H24	119.516
C51—C52—C57	125.8 (5)	C63—C64—H25	120.297
C53—C52—C57	117.8 (4)	C65—C64—H25	120.306
C52—C53—C54	121.8 (5)	O2—C67—H35	109.469
C53—C54—C55	120.9 (5)	O2—C67—H36	109.468
C54—C55—C56	119.2 (5)	O2—C67—H37	109.468
O6—C56—C55	125.0 (5)	H35—C67—H36	109.475
O6—C56—C57	115.3 (4)	H35—C67—H37	109.474
C55—C56—C57	119.7 (5)	H36—C67—H37	109.474
O5—C57—C52	122.3 (4)	O1—C68—H38	109.465
O5—C57—C56	117.3 (4)	O1—C68—H39	109.467
C52—C57—C56	120.5 (4)	O1—C68—H40	109.473
O3—C60—N4	122.6 (5)	H38—C68—H39	109.468
O3—C60—C61	120.6 (5)	H38—C68—H40	109.475
N4—C60—C61	116.7 (4)	H39—C68—H40	109.479
O1—C65—C64—C63	−180.0 (5)	C12—C13—C14—C15	−2.5 (7)
O1—C65—C66—O2	−0.3 (7)	C13—C12—C11—C16	0.1 (7)
O1—C65—C66—C61	180.0 (4)	C13—C14—C15—C16	−0.3 (7)
O2—C66—C61—C60	−1.7 (8)	C14—C1—N1—C17	162.7 (5)
O2—C66—C61—C62	−180.0 (4)	C17—C18—C19—C20	177.0 (5)
O2—C66—C65—C64	178.2 (4)	C17—C18—C23—C22	−176.6 (5)
O3—C60—N4—C44	−0.1 (9)	C18—C19—C20—C21	0.3 (9)
O3—C60—C61—C62	−22.6 (8)	C18—C23—O11—C24	102.9 (5)
O3—C60—C61—C66	159.1 (6)	C18—C23—C22—C21	−0.8 (8)
O4—C51—N3—C35	3.8 (8)	C19—C18—C23—C22	2.2 (7)
O4—C51—C52—C53	6.9 (7)	C19—C20—C21—C22	1.1 (9)
O4—C51—C52—C57	−171.6 (5)	C20—C19—C18—C23	−1.9 (8)
O5—C57—C52—C51	−1.1 (7)	C20—C21—C22—C23	−0.9 (8)
O5—C57—C52—C53	−179.6 (4)	C21—C22—O12—C25	−4.4 (8)
O5—C57—C56—O6	−2.1 (6)	C22—C23—O11—C24	−79.0 (5)
O5—C57—C56—C55	178.4 (4)	C23—C22—O12—C25	176.9 (5)
O6—C56—C55—C54	−178.3 (5)	C26—C27—C28—C29	178.3 (4)
O6—C56—C57—C52	179.1 (4)	C26—C27—C32—C31	−178.9 (5)
O7—C31—C30—C29	178.6 (5)	C27—C28—C29—C30	0.1 (8)
O7—C31—C32—O8	0.8 (7)	C27—C32—O8—C33	−103.3 (5)

O7—C31—C32—C27	−178.3 (4)	C27—C32—C31—C30	1.5 (8)
O8—C32—C27—C26	2.1 (8)	C28—C27—C32—C31	−0.9 (7)
O8—C32—C27—C28	−180.0 (4)	C28—C29—C30—C31	0.5 (8)
O8—C32—C31—C30	−179.4 (4)	C29—C28—C27—C32	0.1 (8)
O9—C26—N2—C10	−3.0 (8)	C29—C30—C31—C32	−1.3 (8)
O9—C26—C27—C28	−9.5 (7)	C30—C31—O7—C34	13.9 (7)
O9—C26—C27—C32	168.5 (5)	C31—C32—O8—C33	77.6 (5)
O10—C17—N1—C1	−1.6 (9)	C32—C31—O7—C34	−166.3 (4)
O10—C17—C18—C19	18.9 (7)	C35—N3—C51—C52	−176.7 (4)
O10—C17—C18—C23	−162.2 (5)	C35—C36—C37—C38	1.3 (8)
O11—C23—C18—C17	1.5 (7)	C35—C48—C47—C46	−177.0 (5)
O11—C23—C18—C19	−179.7 (4)	C35—C48—C49—C38	−1.1 (7)
O11—C23—C22—O12	−0.2 (7)	C35—C48—C49—C50	177.8 (4)
O11—C23—C22—C21	−178.9 (5)	C36—C35—N3—C51	−19.4 (8)
O12—C22—C21—C20	−179.5 (5)	C36—C35—C48—C47	177.9 (5)
O12—C22—C23—C18	178.0 (4)	C36—C35—C48—C49	1.7 (7)
N1—C1—C2—C3	178.8 (5)	C36—C37—C38—C39	179.5 (5)
N1—C1—C14—C13	1.5 (8)	C36—C37—C38—C49	−0.6 (8)
N1—C1—C14—C15	−177.9 (4)	C37—C36—C35—C48	−1.9 (7)
N1—C17—C18—C19	−157.8 (5)	C37—C38—C39—C40	−179.1 (5)
N1—C17—C18—C23	21.0 (7)	C37—C38—C49—C48	0.5 (7)
N2—C10—C9—C8	−176.7 (5)	C37—C38—C49—C50	−178.3 (5)
N2—C10—C11—C12	0.2 (7)	C38—C39—C40—C41	−2.5 (8)
N2—C10—C11—C16	178.3 (4)	C38—C49—C48—C47	−177.5 (4)
N2—C26—C27—C28	168.9 (4)	C38—C49—C50—C41	−2.5 (7)
N2—C26—C27—C32	−13.1 (7)	C38—C49—C50—C45	177.9 (4)
N3—C35—C36—C37	175.0 (5)	C39—C38—C49—C48	−179.6 (5)
N3—C35—C48—C47	1.0 (7)	C39—C38—C49—C50	1.6 (7)
N3—C35—C48—C49	−175.2 (4)	C39—C40—C41—C42	−178.4 (5)
N3—C51—C52—C53	−172.6 (4)	C39—C40—C41—C50	1.4 (8)
N3—C51—C52—C57	8.9 (7)	C40—C39—C38—C49	1.0 (8)
N4—C44—C43—C42	178.0 (5)	C40—C41—C42—C43	177.4 (5)
N4—C44—C45—C46	1.4 (7)	C40—C41—C50—C45	−179.3 (5)
N4—C44—C45—C50	−179.9 (4)	C40—C41—C50—C49	1.1 (7)
N4—C60—C61—C62	153.9 (5)	C41—C42—C43—C44	2.1 (8)
N4—C60—C61—C66	−24.4 (8)	C41—C50—C45—C44	1.6 (7)
C1—N1—C17—C18	175.0 (5)	C41—C50—C45—C46	−179.6 (4)
C1—C2—C3—C4	−1.6 (8)	C41—C50—C49—C48	178.6 (4)
C1—C14—C13—C12	178.1 (5)	C42—C41—C50—C45	0.5 (7)
C1—C14—C15—C4	−0.4 (7)	C42—C41—C50—C49	−179.1 (5)
C1—C14—C15—C16	179.1 (4)	C42—C43—C44—C45	0.1 (8)
C2—C1—N1—C17	−19.0 (8)	C43—C42—C41—C50	−2.4 (8)
C2—C1—C14—C13	−176.8 (4)	C43—C44—N4—C60	22.4 (8)
C2—C1—C14—C15	3.8 (7)	C43—C44—C45—C46	179.4 (5)
C2—C3—C4—C5	−176.0 (5)	C43—C44—C45—C50	−2.0 (7)
C2—C3—C4—C15	5.0 (8)	C44—N4—C60—C61	−176.5 (5)
C3—C2—C1—C14	−2.9 (7)	C44—C45—C46—C47	179.4 (5)
C3—C4—C5—C6	179.8 (5)	C44—C45—C50—C49	−178.8 (5)
C3—C4—C15—C14	−3.9 (7)	C45—C44—N4—C60	−159.6 (5)

C3—C4—C15—C16	176.6 (5)	C45—C46—C47—C48	−0.3 (8)
C4—C5—C6—C7	3.7 (9)	C45—C50—C49—C48	−1.0 (7)
C4—C15—C14—C13	−179.8 (4)	C46—C45—C50—C49	−0.1 (7)
C4—C15—C16—C7	3.5 (7)	C46—C47—C48—C49	−0.7 (7)
C4—C15—C16—C11	−177.5 (4)	C47—C46—C45—C50	0.7 (7)
C5—C4—C15—C14	177.0 (5)	C47—C48—C49—C50	1.4 (7)
C5—C4—C15—C16	−2.4 (7)	C48—C35—N3—C51	157.5 (5)
C5—C6—C7—C8	175.7 (5)	C51—C52—C53—C54	−177.3 (5)
C5—C6—C7—C16	−2.5 (8)	C51—C52—C57—C56	177.6 (5)
C6—C5—C4—C15	−1.2 (8)	C52—C53—C54—C55	−0.7 (8)
C6—C7—C8—C9	−178.3 (5)	C52—C57—O5—C58	103.9 (5)
C6—C7—C16—C11	179.8 (5)	C52—C57—C56—C55	−0.4 (7)
C6—C7—C16—C15	−1.2 (7)	C53—C52—C57—C56	−0.8 (7)
C7—C8—C9—C10	−0.8 (8)	C53—C54—C55—C56	−0.6 (8)
C7—C16—C11—C10	−2.1 (7)	C54—C53—C52—C57	1.4 (8)
C7—C16—C11—C12	176.1 (4)	C54—C55—C56—C57	1.1 (8)
C7—C16—C15—C14	−175.9 (4)	C55—C56—O6—C59	0.6 (7)
C8—C7—C16—C11	1.5 (7)	C56—C57—O5—C58	−74.9 (5)
C8—C7—C16—C15	−179.5 (5)	C57—C56—O6—C59	−178.8 (4)
C8—C9—C10—C11	0.2 (8)	C60—C61—C62—C63	−176.5 (5)
C9—C8—C7—C16	−0.1 (8)	C60—C61—C66—C65	178.0 (5)
C9—C10—N2—C26	23.2 (7)	C61—C62—C63—C64	−1.7 (9)
C9—C10—C11—C12	−176.8 (5)	C61—C66—O2—C67	−99.2 (5)
C9—C10—C11—C16	1.3 (7)	C61—C66—C65—C64	−1.6 (8)
C10—N2—C26—C27	178.6 (4)	C62—C61—C66—C65	−0.2 (8)
C10—C11—C12—C13	178.2 (5)	C62—C63—C64—C65	−0.1 (9)
C10—C11—C16—C15	178.9 (4)	C63—C62—C61—C66	1.9 (8)
C11—C10—N2—C26	−153.7 (5)	C63—C64—C65—C66	1.7 (8)
C11—C12—C13—C14	2.7 (8)	C64—C65—O1—C68	9.4 (8)
C11—C16—C15—C14	3.1 (7)	C65—C66—O2—C67	81.1 (5)
C12—C11—C16—C15	−2.9 (7)	C66—C65—O1—C68	−172.3 (5)

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H53···O11	0.96 (6)	1.95 (5)	2.700 (6)	134 (4)
N2—H54···O8	0.95 (4)	2.00 (4)	2.746 (5)	134 (4)
N3—H55···O5	0.95 (6)	1.96 (6)	2.723 (5)	136 (5)
N4—H56···O2	0.94 (6)	2.03 (5)	2.727 (5)	130 (4)

Fig. 1

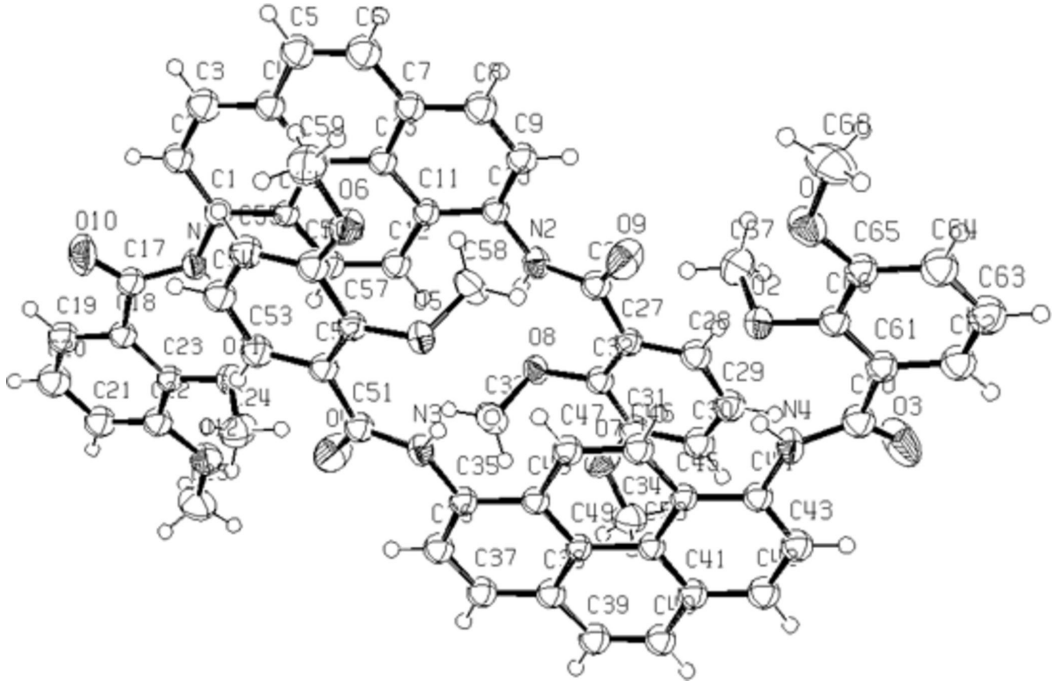

C5
C6
C3
C7
C8
C59
C9
C68
C1
O6
C11
O10
N1
C17
C58
N2
O9
C37
C65
C64
C63
C19
C18
C57
O5
C27
C28
C61
C62
C23
O7
C53
O8
C29
C21
C22
C24
C51
C31
N3
C47
N4
O3
C35
C34
C49
C43
C37
C41
C39

Fig. 2

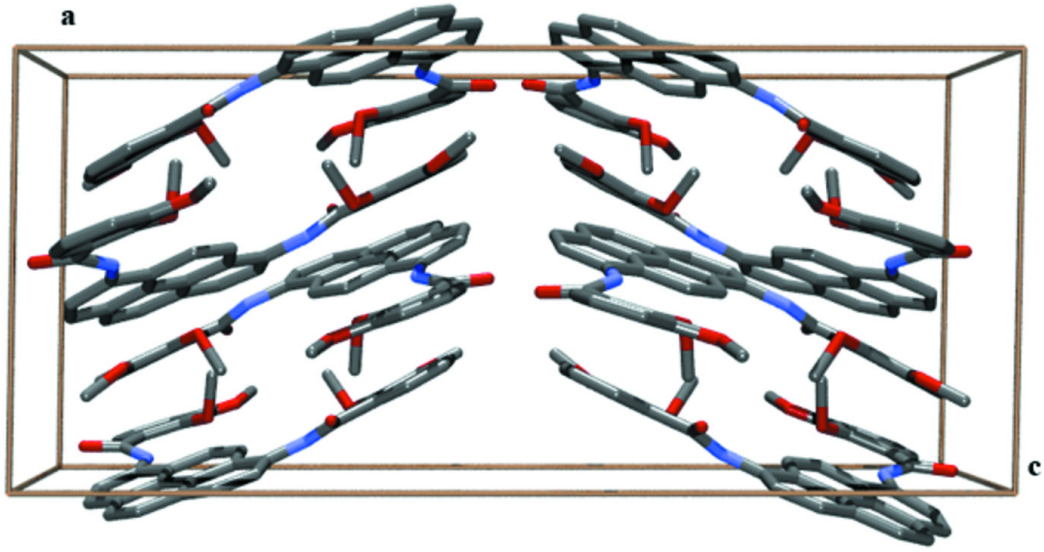


Fig. 3

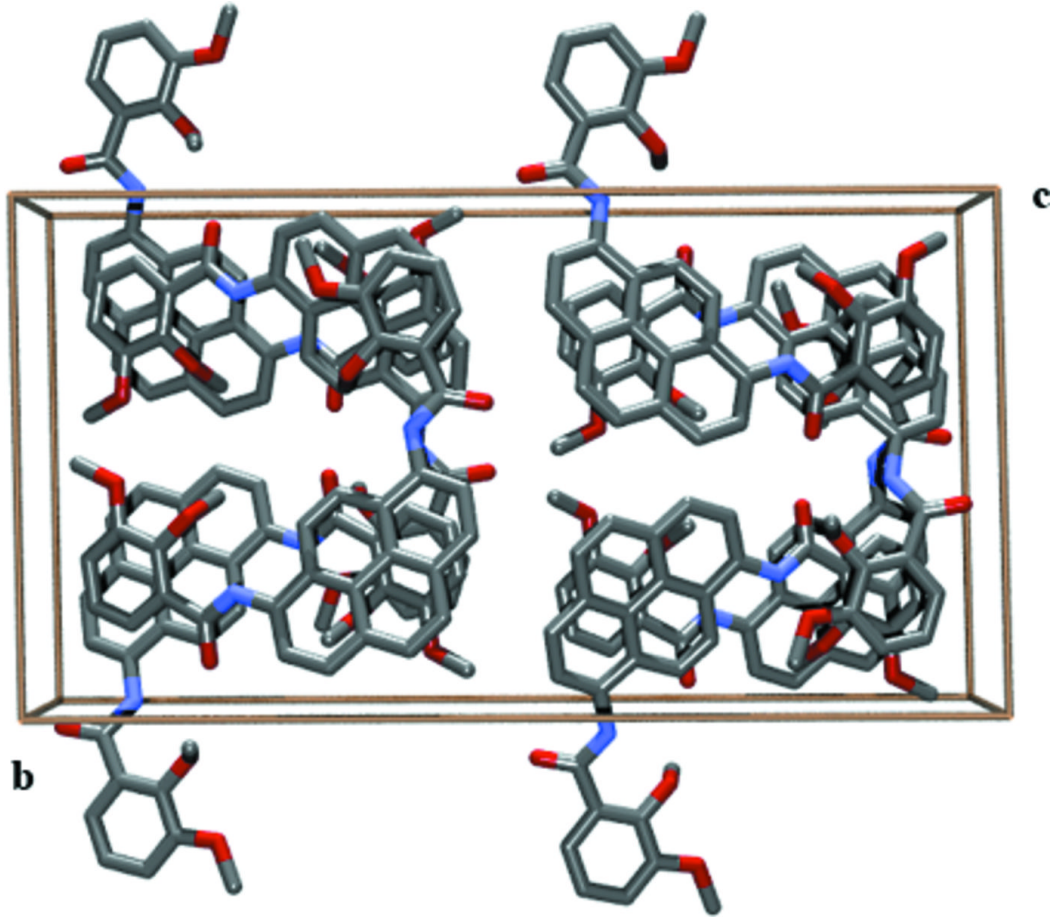


Fig. 4