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Syntheses and structures of two anthracene–benzoic acid derivatives as potential MOF linkers

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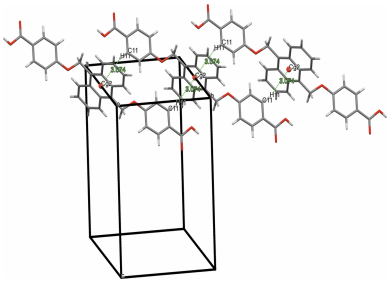
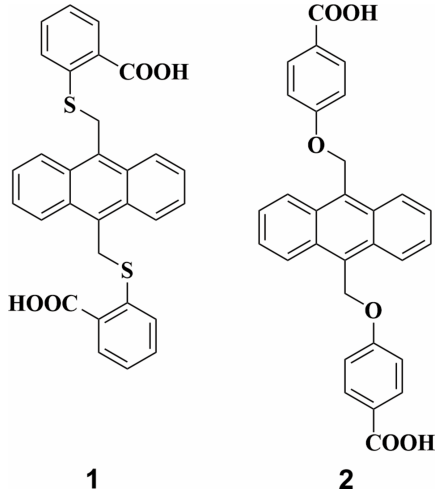
In the title compounds, 2,2′-{[anthracene-9,10-diylbis(methylene)]bis(sulfanediyl)}dibenzoic acid dimethylacetamide tetrasolvate, $C_{30}H_{22}O_4S_2\cdot4C_4H_9NO$ **1** and 4,4′-{[anthracene-9,10-diylbis(methylene)]bis(oxy)}dibenzoic acid dimethylformamide disolvate, $C_{30}H_{22}O_6\cdot2C_3H_7NO$ **2**, the complete anthracene–benzoic acid molecule is generated by a crystallographic centre of symmetry. The dihedral angle between the anthracene ring system and the pendant ring is 71.43 (7) in **1** and 75.27 (12)° in **2**. In the extended structures of **1** and **2**, O—H···O hydrogen bonds link the main molecules into pairs of solvent molecules to generate trimers. Weak C—H···O and C—H···π interactions further consolidate both structures.

1. Chemical context

Anthracene is a rigid and planar tricyclic aromatic hydrocarbon, has extensive π-conjugation, high photoluminescence efficiency and good thermal stability (Klosterman *et al.*, 2009; Hunter *et al.*, 2001). The anthracene core serves as a light-harvesting chromophore and a versatile structural unit for designing functional materials such as organic semiconductors, photoresponsive switches, fluorescent sensors and supramolecular hosts (Desiraju & Gavezzotti, 1989). In coordination chemistry, the incorporation of anthracene into ligands can significantly influence both the structural and electronic characteristics of the resulting complexes as reported by our group (*e.g.*, Verma *et al.*, 2022) and others (*e.g.*, Jindal *et al.*, 2021).





1 **2**

Herein we report the syntheses and crystal structures of the title compounds, **1** and **2**, with a thioether and ether linkage

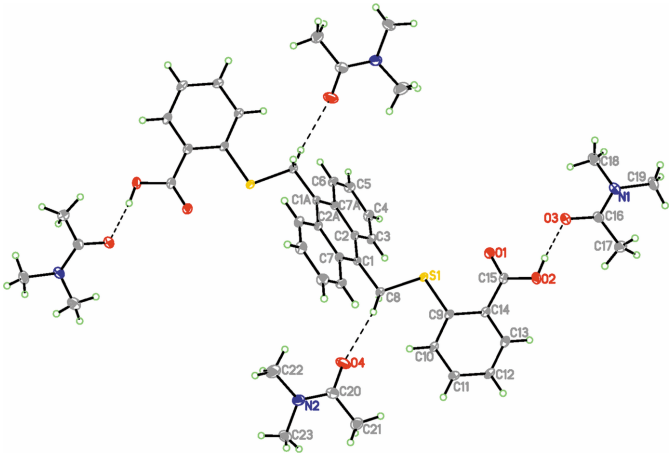


Figure 1
The molecular structure of **1** showing displacement ellipsoids drawn at the 50% level. Symmetry code: $1-x, 1-y, 1-z$.

between the anthracene ring system and benzoic acid moiety, respectively. These compounds could act as potential linkers in metal–organic frameworks (MOFs) after deprotonation of the carboxylic acid.

2. Structural commentary

Compound **1** (Fig. 1) crystallizes in the monoclinic space group $P2_1/c$ with half of the main molecule and two dimethylacetamide (DMA) solvent molecules in the asymmetric unit. The dihedral angle between the anthracene ring system and the phenyl ring of the 2-mercaptobenzoic acid moiety is 71.43 (7)°. The torsion angle between the anthracene ring and phenyl group (C1—C8—S1—C9) is 178.13 (9)° indicating an *anti* conformation for this grouping and the C8—S1—C9 bond angle is 103.13 (7)°. Compound **2** (Fig. 2) crystallizes in space group $P2_1/n$ with half of the main molecule and one dimethylformamide (DMF) molecule in the asymmetric unit. The C8—O1—C9 bond angle is 117.8 (2)° and the C1—C8—O1—C9 torsion angle is −178.3 (2)°, indicating an *anti* conformation. The dihedral angle between the plane of anthracene ring system and the phenyl ring of the 4-hydroxybenzoic acid moiety is 75.27 (12)°.

3. Supramolecular features

In the extended structure of **1**, the carboxylic acid group of the ligand forms an O2—H2···O3*A* hydrogen bond with the DMA molecule with an H···O bond length of 1.94 Å. The

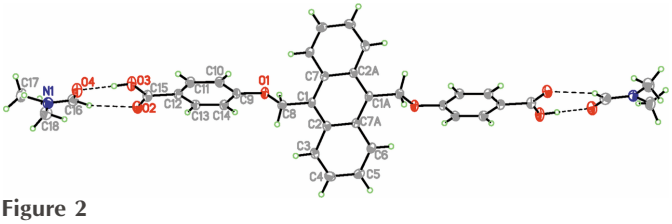


Figure 2
The molecular structure of **2** showing displacement ellipsoids drawn at the 50% level. Symmetry code: $1-x, -y, -z$.

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

*Cg*1 is the centroid of the C9–C14 ring of **1**.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···O3*A*^{i}	0.84	1.94	2.770 (14)	169
C8—H8*B*···O4*A*^{ii}	0.99	2.48	3.126 (8)	122
C17—H17*A*···O4^{iii}	0.98	2.62	3.518 (8)	152
C18*A*—H18*D*···S1^{iii}	0.98	3.02	3.83 (3)	142
C19*A*—H19*E*···O4*A*^{iii}	0.98	2.43	3.40 (4)	168
C21—H21*C*···O1	0.98	2.49	3.422 (7)	158
C22*A*—H22*F*···O1	0.98	2.54	3.51 (3)	168
C4—H4···*Cg*1	0.95	2.76	3.49	135

Symmetry codes: (i) $x-1, y, z$; (ii) $x+1, y, z$; (iii) $-x+1, y+\frac{1}{2}, -z+\frac{1}{2}$.

Table 2
Hydrogen-bond geometry (Å, °) for **2**.

*Cg*2 is the centroid of the C9–C14 ring of **2**.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3···O4	0.84	1.74	2.575 (3)	175
C8—H8*A*···O2^{i}	0.99	2.54	3.429 (4)	149
C16—H16···O2	0.95	2.31	3.080 (4)	138
C4—H4···*Cg*2	0.95	3.07	3.96	157

Symmetry code: (i) $-x+\frac{1}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$.

structure of **1** is further consolidated by a number of C—H···O, C—H···S and C—H···π weak interactions (Table 1). Among these, consecutive C—H···π interactions occur between the C4—H4 group of the anthracene ring and the centroid (*Cg*1) of the adjacent benzene ring with an H···π separation of 2.76 Å (Fig. 3). The packing also features a weak hydrogen bond between the methylene hydrogen atoms of the anthracene ring and oxygen atom of DMF molecule

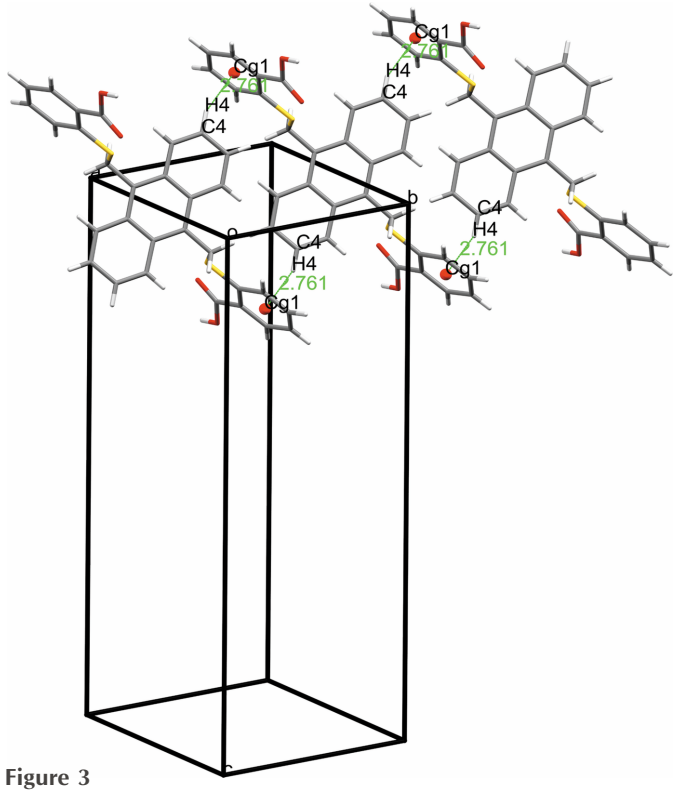


Figure 3
The packing of **1** showing C—H···π interactions.

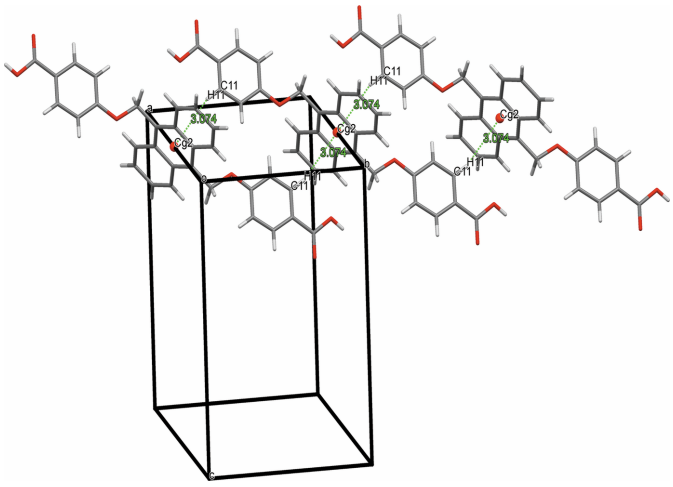


Figure 4
The packing of **2** showing C—H···π interactions.

(C8—H8B···O4*A*) at a distance of 2.48 Å, forming infinite chains running parallel to each other.

A similar strong hydrogen bond occurs in **2**, between the carboxylic acid group of the ligand and oxygen atom of the DMF molecule (O3—H3···O4) at a distance of 1.74 Å and the packing is supported by various weak interactions (Table 2), including consecutive C—H···π interactions involving the aromatic C11—H11 group of the phenyl ring and the centroid (*Cg2*) of the adjacent anthracene ring at an H···π distance of 3.07 Å, resulting in an array of chains running parallel to each other (Fig. 4). Additionally, the packing of **2** is reinforced by the hydrogen-bond interactions between the aromatic H atom of the benzene ring of one molecule and the oxygen atom of the ether bond in the adjacent molecule (C10—H10···O1) at a distance of 2.67 Å.

4. Database survey

A simple name search in the Cambridge Structural Database (CSD version 5.46, November 2024; Groom *et al.*, 2016) of both compounds **1** and **2** resulted in no hits. However, searching for the fragment anthracene-9,10-diylbis(methylene) resulted in more than thirty similar structures, for example including CSD refcode BIHNIR (Suresh *et al.*, 2013), XUTHAZ (Verma *et al.*, 2025), TAPYEQ (Chen *et al.*, 2010), WUTGUO01 (Kan *et al.*, 2011), YIGCEA (Li *et al.*, 2023) and ZIHFEF (Verma *et al.*, 2023). These structures are either ligand molecules or metal-organic structures having different substituents on the anthracene-9,10-diylbis(methylene) moiety.

5. Synthesis and crystallization

As outlined in Figs. 5 and 6, 2-mercaptobenzoic acid (2.0 mmol) and potassium carbonate (4.0 mmol) were dissolved in an acetone:water (1:1) mixture and refluxed for 1 h. After an hour, 9,10-bis(bromomethyl)anthracene (1.0 mmol) was added to the reaction mixture and it was refluxed overnight. After the completion of reaction, mixture was neutralized with 1 *N* HCl solution and the yellow precipitate was filtered, washed with water and dried to yield a yellow solid (yield: 92%). ^{1}H-NMR (500MHz, DMSO-d_6): δ 5.17 (*s*, 4H), 7.27–7.31 (*m*, 2H), 7.58–7.60 (*m*, 4H), 7.64–7.67 (*m*, 2H), 7.90–7.93 (*m*, 4H), 8.37–8.39 (*m*, 4H), 13.05 (*s*, 2H). The crystals of **1** were obtained by a solvothermal method using DMA solvent at 363 K for 96 h.

To prepare **2**, methyl-4-hydroxybenzoate was synthesized by following the previously reported procedure (Mondal *et al.*, 2023). Methyl-4-hydroxybenzoate (2.0 mmol) and potassium carbonate (2.2 mmol) were dissolved in acetonitrile (20 ml) and refluxed for 1 h. After an hour, 9,10-bis(bromomethyl)-anthracene (1.0 mmol) was added to the reaction mixture and refluxed overnight. After the completion of reaction, it was neutralized with 1 *N* HCl solution and the solid product was filtered, washed with water and dried in a hot air oven (yield: 92%). ^{1}H-NMR (500MHz, DMSO-d_6): δ 3.81 (*s*, 6H), 6.17 (*s*, 4H), 7.27–7.29 (*d*, 4H), 7.59–7.61 (*m*, 4H), 7.95–7.96 (*d*, 4H), 8.39–8.41 (*m*, 4H). The methyl ester derivative was taken in a 100 ml round-bottom flask and dissolved in mixed solvents of THF:MeOH (1:1). 4 *M* NaOH was added into the reaction mixture and stirred for 24 h at RT. After the completion of reaction, it was neutralized with 1 *N* HCl solution and precipitate was filtered, washed with water and dried (yield: 85%). Crystals of **2** were obtained by a solvothermal method using DMF solvent at 373 K for 72 h.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. The H atoms attached to carbon

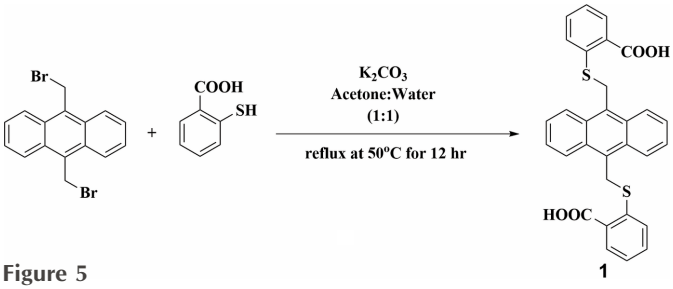


Figure 5
Synthesis schemes for compound **1**.

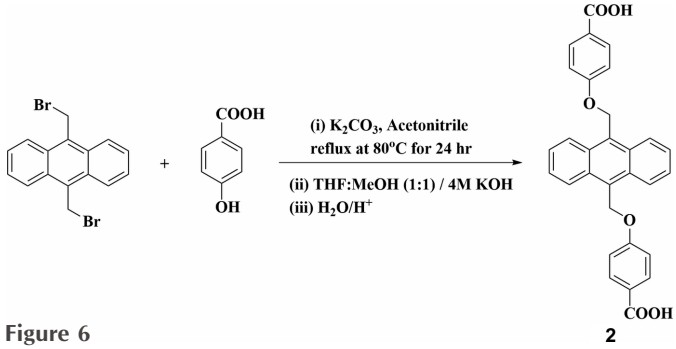


Figure 6
Synthesis schemes for compound **2**.

Table 3
Experimental details.

	1	**2**
Crystal data		
Chemical formula	$C_{30}H_{22}O_4S_2{\cdot}4C_4H_9NO$	$C_{30}H_{22}O_6{\cdot}2C_3H_7NO$
M_r	859.08	624.67
Crystal system, space group	Monoclinic, $P2_1/c$	Monoclinic, $P2_1/n$
Temperature (K)	104	104
a, b, c (Å)	9.9818 (3), 9.2026 (2), 24.1998 (7)	10.8761 (10), 9.6711 (9), 14.8968 (14)
β (°)	91.016 (1)	100.519 (3)
V (Å^3)	2222.61 (10)	1540.6 (2)
Z	2	2
Radiation type	Mo $K\alpha$	Mo $K\alpha$
μ (mm^{-1})	0.18	0.10
Crystal size (mm)	0.35 × 0.15 × 0.12	0.26 × 0.19 × 0.16
Data collection		
Diffractometer	Bruker APEXII CCD	Bruker APEXII CCD
Absorption correction	Multi-scan (*OLEX2*; Dolomanov *et al.*, 2009)	Multi-scan (*OLEX2*; Dolomanov *et al.*, 2009)
T_{min}, T_{max}	0.706, 0.746	0.666, 0.745
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	84923, 5544, 4374	49734, 3169, 1669
R_{int}	0.076	0.179
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.668	0.627
Refinement		
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.045, 0.112, 1.03	0.069, 0.182, 1.02
No. of reflections	5544	3169
No. of parameters	394	211
No. of restraints	422	0
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.41, −0.27	0.31, −0.24

Computer programs: *APEX4*, *APEX2* and *SAINT* (Bruker, 2016), *SHELXT2018/2* (Sheldrick, 2015*a*), *SHELXL-2019/2* (Sheldrick, 2015*b*) and *OLEX2* (Dolomanov *et al.*, 2009).

atoms were refined using a riding model with U_{iso}(H) = 1.2U_{eq}(C). In **1**, both DMA molecules were found to be disordered in a similar manner. This was modeled using SAME instructions in *SHELXL* for each component and resulted in occupancies of 0.799 (3)/0.201 (3) and 0.804 (3)/0.196 (3), respectively.

Acknowledgements

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Computing details

2,2′-{[Anthracene-9,10-diylbis(methylene)]bis(sulfanediyl)}dibenzoic acid dimethylacetamide tetrasolvate (1)

Crystal data

$C_{30}H_{22}O_4S_2·4C_4H_9NO$
M_r = 859.08
Monoclinic, $P2_1/c$
a = 9.9818 (3) Å
b = 9.2026 (2) Å
c = 24.1998 (7) Å
β = 91.016 (1)°
V = 2222.61 (10) Å^3
Z = 2
$F(000)$ = 916
D_x = 1.284 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9910 reflections
θ = 2.4–25.7°
μ = 0.18 mm^{-1}
T = 104 K
Block, clear yellowish yellow
0.35 × 0.15 × 0.12 mm

Data collection

Bruker APEXII CCD diffractometer
ω and φ scans
Absorption correction: multi-scan (Olex2; Dolomanov *et al.*, 2009)
T_{min} = 0.706, T_{max} = 0.746
84923 measured reflections
5544 independent reflections
4374 reflections with $I > 2\sigma(I)$
R_{int} = 0.076
θ_{max} = 28.3°, θ_{min} = 1.7°
h = −13→13
k = −12→12
l = −32→32

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.112
S = 1.03
5544 reflections
394 parameters
422 restraints
Primary atom site location: dual
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0474P)^2 + 1.119P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.41 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
S1	0.49737 (4)	0.76829 (4)	0.38089 (2)	0.01827 (10)	
O1	0.29231 (11)	0.87413 (12)	0.31863 (4)	0.0263 (3)	
O2	0.31257 (12)	0.96903 (14)	0.23437 (5)	0.0310 (3)	
H2	0.230729	0.948146	0.232140	0.047*	
C1	0.56861 (14)	0.58987 (15)	0.46196 (6)	0.0167 (3)	
C2	0.52491 (14)	0.45046 (15)	0.44587 (6)	0.0173 (3)	
C3	0.54843 (16)	0.39496 (16)	0.39171 (6)	0.0224 (3)	
H3	0.593487	0.454054	0.365752	0.027*	
C4	0.50773 (17)	0.25944 (17)	0.37653 (6)	0.0267 (4)	
H4	0.525167	0.224961	0.340360	0.032*	
C5	0.43976 (17)	0.16965 (17)	0.41413 (7)	0.0273 (4)	
H5	0.411335	0.075326	0.403109	0.033*	
C6	0.41483 (16)	0.21774 (16)	0.46609 (6)	0.0228 (3)	
H6	0.369268	0.155798	0.490923	0.027*	
C7	0.54455 (14)	0.64077 (15)	0.51567 (6)	0.0171 (3)	
C8	0.63542 (15)	0.68688 (16)	0.42042 (6)	0.0192 (3)	
H8A	0.694092	0.629672	0.396056	0.023*	
H8B	0.689817	0.762652	0.439262	0.023*	
C9	0.57997 (15)	0.88537 (15)	0.33438 (6)	0.0177 (3)	
C10	0.71660 (16)	0.91600 (16)	0.34057 (6)	0.0217 (3)	
H10	0.766922	0.871749	0.369702	0.026*	
C11	0.77937 (17)	1.01029 (17)	0.30463 (7)	0.0251 (3)	
H11	0.871972	1.031090	0.309790	0.030*	
C12	0.70906 (17)	1.07443 (16)	0.26140 (6)	0.0247 (3)	
H12	0.752673	1.139489	0.237117	0.030*	
C13	0.57494 (16)	1.04298 (16)	0.25390 (6)	0.0223 (3)	
H13	0.526989	1.085006	0.223637	0.027*	
C14	0.50800 (15)	0.95009 (15)	0.29011 (6)	0.0195 (3)	
C15	0.36146 (16)	0.92700 (16)	0.28293 (6)	0.0211 (3)	
O3	1.0671 (4)	0.9058 (3)	0.2180 (2)	0.0353 (7)	0.799 (3)
N1	0.88738 (18)	0.9245 (2)	0.16135 (7)	0.0285 (5)	0.799 (3)
C16	0.9981 (2)	0.9800 (2)	0.18493 (9)	0.0274 (5)	0.799 (3)
C17	1.0361 (8)	1.1340 (7)	0.1719 (4)	0.0353 (10)	0.799 (3)
H17A	1.050112	1.143580	0.132038	0.053*	0.799 (3)
H17B	1.118931	1.159241	0.191974	0.053*	0.799 (3)
H17C	0.964103	1.199522	0.183008	0.053*	0.799 (3)
C18	0.8425 (6)	0.7782 (5)	0.1765 (3)	0.0369 (10)	0.799 (3)
H18A	0.816616	0.724555	0.142961	0.055*	0.799 (3)
H18B	0.765414	0.785502	0.200811	0.055*	0.799 (3)
H18C	0.915606	0.726820	0.195702	0.055*	0.799 (3)
C19	0.7988 (6)	1.0049 (7)	0.1234 (3)	0.0360 (11)	0.799 (3)
H19A	0.781855	0.946712	0.090114	0.054*	0.799 (3)
H19B	0.841408	1.096737	0.113248	0.054*	0.799 (3)
H19C	0.713733	1.024955	0.141564	0.054*	0.799 (3)
O3A	1.0538 (16)	0.8659 (15)	0.2192 (8)	0.036 (2)	0.201 (3)

N1A	0.9312 (8)	1.0021 (9)	0.1604 (3)	0.0294 (12)	0.201 (3)
C16A	0.9542 (8)	0.8815 (9)	0.1884 (3)	0.0296 (12)	0.201 (3)
C17A	0.858 (2)	0.757 (2)	0.1825 (13)	0.035 (3)	0.201 (3)
H17D	0.766243	0.793275	0.184933	0.052*	0.201 (3)
H17E	0.875504	0.686684	0.212185	0.052*	0.201 (3)
H17F	0.870396	0.709975	0.146647	0.052*	0.201 (3)
C18A	0.815 (2)	1.025 (3)	0.1230 (13)	0.034 (3)	0.201 (3)
H18D	0.767338	1.113996	0.133881	0.051*	0.201 (3)
H18E	0.753673	0.942141	0.125383	0.051*	0.201 (3)
H18F	0.845163	1.035463	0.084941	0.051*	0.201 (3)
C19A	1.022 (3)	1.128 (3)	0.1644 (16)	0.033 (3)	0.201 (3)
H19D	0.983823	1.201294	0.188723	0.050*	0.201 (3)
H19E	1.034642	1.169307	0.127565	0.050*	0.201 (3)
H19F	1.109197	1.096129	0.179621	0.050*	0.201 (3)
O4	−0.0836 (2)	0.7997 (3)	0.45732 (9)	0.0501 (6)	0.804 (3)
N2	0.1140 (2)	0.7946 (2)	0.50291 (9)	0.0326 (5)	0.804 (3)
C20	0.0317 (2)	0.8450 (2)	0.46303 (9)	0.0317 (5)	0.804 (3)
C21	0.0868 (7)	0.9608 (6)	0.4254 (2)	0.0367 (8)	0.804 (3)
H21A	0.123902	1.040534	0.447754	0.055*	0.804 (3)
H21B	0.014736	0.997995	0.401298	0.055*	0.804 (3)
H21C	0.157583	0.918999	0.402787	0.055*	0.804 (3)
C22	0.0711 (7)	0.6745 (7)	0.53909 (16)	0.0553 (13)	0.804 (3)
H22A	0.083561	0.703059	0.577852	0.083*	0.804 (3)
H22B	0.125009	0.587919	0.531637	0.083*	0.804 (3)
H22C	−0.023695	0.652905	0.531759	0.083*	0.804 (3)
C23	0.2478 (4)	0.8572 (5)	0.51334 (18)	0.0365 (9)	0.804 (3)
H23A	0.300280	0.791520	0.537132	0.055*	0.804 (3)
H23B	0.238720	0.951551	0.531667	0.055*	0.804 (3)
H23C	0.293469	0.870156	0.478167	0.055*	0.804 (3)
O4A	−0.0743 (8)	0.7207 (12)	0.4693 (4)	0.0496 (19)	0.196 (3)
N2A	0.1243 (8)	0.8380 (9)	0.4771 (4)	0.0332 (12)	0.196 (3)
C20A	0.0371 (9)	0.7362 (11)	0.4923 (4)	0.0369 (12)	0.196 (3)
C21A	0.064 (3)	0.694 (3)	0.5513 (6)	0.039 (2)	0.196 (3)
H21D	0.129391	0.761244	0.567808	0.059*	0.196 (3)
H21E	0.099197	0.594970	0.552752	0.059*	0.196 (3)
H21F	−0.019839	0.699037	0.571807	0.059*	0.196 (3)
C22A	0.083 (3)	0.933 (3)	0.4313 (10)	0.035 (2)	0.196 (3)
H22D	0.102444	1.034030	0.440877	0.053*	0.196 (3)
H22E	−0.013882	0.921667	0.424344	0.053*	0.196 (3)
H22F	0.131343	0.905840	0.398021	0.053*	0.196 (3)
C23A	0.2596 (15)	0.836 (3)	0.5004 (8)	0.040 (3)	0.196 (3)
H23D	0.320334	0.885391	0.475125	0.060*	0.196 (3)
H23E	0.288775	0.735411	0.505731	0.060*	0.196 (3)
H23F	0.260857	0.886607	0.536101	0.060*	0.196 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0203 (2)	0.01784 (18)	0.01676 (18)	−0.00194 (14)	0.00182 (13)	0.00343 (13)
O1	0.0255 (6)	0.0321 (6)	0.0213 (6)	0.0003 (5)	0.0022 (5)	0.0035 (5)
O2	0.0273 (6)	0.0448 (7)	0.0209 (6)	0.0008 (5)	−0.0034 (5)	0.0087 (5)
C1	0.0164 (7)	0.0172 (7)	0.0166 (7)	0.0000 (5)	−0.0002 (5)	0.0038 (5)
C2	0.0179 (7)	0.0180 (7)	0.0161 (7)	0.0015 (5)	0.0010 (5)	0.0016 (5)
C3	0.0270 (8)	0.0231 (7)	0.0171 (7)	0.0010 (6)	0.0038 (6)	0.0013 (6)
C4	0.0355 (9)	0.0251 (8)	0.0196 (8)	0.0025 (7)	0.0030 (7)	−0.0056 (6)
C5	0.0334 (9)	0.0191 (7)	0.0293 (8)	−0.0021 (7)	0.0003 (7)	−0.0062 (6)
C6	0.0270 (8)	0.0180 (7)	0.0235 (8)	−0.0031 (6)	0.0029 (6)	0.0014 (6)
C7	0.0176 (7)	0.0161 (7)	0.0177 (7)	0.0009 (5)	−0.0002 (5)	0.0006 (5)
C8	0.0203 (8)	0.0197 (7)	0.0176 (7)	−0.0021 (6)	0.0019 (6)	0.0035 (6)
C9	0.0246 (8)	0.0144 (6)	0.0144 (7)	−0.0005 (6)	0.0046 (6)	0.0001 (5)
C10	0.0251 (8)	0.0206 (7)	0.0193 (7)	0.0002 (6)	0.0024 (6)	0.0030 (6)
C11	0.0246 (8)	0.0245 (8)	0.0264 (8)	−0.0031 (6)	0.0068 (7)	0.0019 (6)
C12	0.0337 (9)	0.0196 (7)	0.0211 (8)	−0.0006 (6)	0.0098 (7)	0.0030 (6)
C13	0.0333 (9)	0.0184 (7)	0.0153 (7)	0.0030 (6)	0.0047 (6)	0.0007 (5)
C14	0.0268 (8)	0.0169 (7)	0.0151 (7)	0.0013 (6)	0.0037 (6)	−0.0023 (5)
C15	0.0280 (8)	0.0181 (7)	0.0171 (7)	0.0030 (6)	0.0006 (6)	−0.0015 (6)
O3	0.0269 (12)	0.0420 (17)	0.0365 (11)	−0.0029 (11)	−0.0087 (9)	0.0098 (13)
N1	0.0231 (9)	0.0343 (10)	0.0281 (9)	0.0025 (8)	−0.0027 (7)	−0.0040 (8)
C16	0.0213 (10)	0.0370 (11)	0.0240 (10)	0.0014 (8)	0.0025 (8)	−0.0010 (8)
C17	0.033 (3)	0.0390 (15)	0.034 (3)	−0.0047 (13)	0.0030 (16)	0.0056 (16)
C18	0.0321 (19)	0.0303 (16)	0.048 (2)	0.0022 (14)	−0.0077 (14)	−0.0056 (14)
C19	0.0286 (19)	0.048 (2)	0.0311 (15)	0.0058 (17)	−0.0070 (13)	0.0038 (15)
O3A	0.027 (4)	0.042 (5)	0.037 (4)	0.000 (4)	−0.005 (3)	0.007 (4)
N1A	0.022 (2)	0.038 (2)	0.029 (2)	0.001 (2)	−0.001 (2)	0.001 (2)
C16A	0.023 (2)	0.037 (2)	0.029 (2)	0.002 (2)	0.002 (2)	−0.002 (2)
C17A	0.030 (5)	0.034 (4)	0.040 (5)	−0.002 (4)	−0.002 (4)	−0.005 (4)
C18A	0.022 (4)	0.043 (5)	0.036 (5)	−0.003 (4)	−0.008 (4)	0.001 (4)
C19A	0.024 (5)	0.042 (4)	0.033 (6)	−0.005 (4)	0.001 (4)	0.003 (4)
O4	0.0313 (10)	0.0784 (17)	0.0403 (11)	−0.0231 (11)	−0.0036 (8)	−0.0016 (11)
N2	0.0279 (10)	0.0325 (10)	0.0374 (11)	−0.0028 (8)	0.0053 (8)	0.0029 (8)
C20	0.0284 (11)	0.0387 (11)	0.0282 (10)	−0.0058 (9)	0.0042 (8)	−0.0080 (9)
C21	0.0410 (15)	0.040 (2)	0.0293 (17)	−0.0050 (15)	0.0059 (13)	0.0024 (12)
C22	0.056 (2)	0.070 (3)	0.040 (2)	−0.0181 (19)	0.0098 (19)	0.0103 (19)
C23	0.0215 (12)	0.0405 (18)	0.047 (2)	0.0020 (11)	−0.0001 (13)	−0.0004 (14)
O4A	0.033 (3)	0.063 (4)	0.052 (4)	−0.013 (3)	−0.004 (3)	−0.001 (4)
N2A	0.029 (2)	0.040 (2)	0.031 (2)	−0.001 (2)	0.004 (2)	0.001 (2)
C20A	0.032 (2)	0.045 (2)	0.034 (2)	−0.005 (2)	0.004 (2)	−0.002 (2)
C21A	0.043 (5)	0.037 (5)	0.038 (4)	−0.003 (4)	0.008 (4)	0.008 (4)
C22A	0.035 (5)	0.040 (5)	0.030 (5)	0.004 (4)	0.002 (4)	−0.005 (3)
C23A	0.028 (4)	0.051 (5)	0.042 (5)	0.002 (4)	0.005 (4)	0.003 (5)

Geometric parameters (Å, º)

S1—C9	1.7721 (14)	C19—H19C	0.9800
S1—C8	1.8245 (15)	O3A—C16A	1.241 (12)
O1—C15	1.2169 (18)	N1A—C16A	1.318 (10)
O2—C15	1.3222 (18)	N1A—C19A	1.473 (14)
O2—H2	0.8400	N1A—C18A	1.477 (14)
C1—C7	1.406 (2)	C16A—C17A	1.497 (14)
C1—C2	1.408 (2)	C17A—H17D	0.9800
C1—C8	1.5086 (19)	C17A—H17E	0.9800
C2—C3	1.430 (2)	C17A—H17F	0.9800
C2—C7^{i}	1.4405 (19)	C18A—H18D	0.9800
C3—C4	1.360 (2)	C18A—H18E	0.9800
C3—H3	0.9500	C18A—H18F	0.9800
C4—C5	1.412 (2)	C19A—H19D	0.9800
C4—H4	0.9500	C19A—H19E	0.9800
C5—C6	1.360 (2)	C19A—H19F	0.9800
C5—H5	0.9500	O4—C20	1.229 (3)
C6—C7^{i}	1.431 (2)	N2—C20	1.339 (3)
C6—H6	0.9500	N2—C23	1.472 (4)
C8—H8A	0.9900	N2—C22	1.478 (6)
C8—H8B	0.9900	C20—C21	1.511 (4)
C9—C10	1.398 (2)	C21—H21A	0.9800
C9—C14	1.411 (2)	C21—H21B	0.9800
C10—C11	1.386 (2)	C21—H21C	0.9800
C10—H10	0.9500	C22—H22A	0.9800
C11—C12	1.382 (2)	C22—H22B	0.9800
C11—H11	0.9500	C22—H22C	0.9800
C12—C13	1.379 (2)	C23—H23A	0.9800
C12—H12	0.9500	C23—H23B	0.9800
C13—C14	1.402 (2)	C23—H23C	0.9800
C13—H13	0.9500	O4A—C20A	1.243 (10)
C14—C15	1.485 (2)	N2A—C20A	1.335 (10)
O3—C16	1.249 (4)	N2A—C23A	1.454 (13)
N1—C16	1.336 (3)	N2A—C22A	1.466 (13)
N1—C19	1.464 (5)	C20A—C21A	1.497 (13)
N1—C18	1.467 (5)	C21A—H21D	0.9800
C16—C17	1.502 (5)	C21A—H21E	0.9800
C17—H17A	0.9800	C21A—H21F	0.9800
C17—H17B	0.9800	C22A—H22D	0.9800
C17—H17C	0.9800	C22A—H22E	0.9800
C18—H18A	0.9800	C22A—H22F	0.9800
C18—H18B	0.9800	C23A—H23D	0.9800
C18—H18C	0.9800	C23A—H23E	0.9800
C19—H19A	0.9800	C23A—H23F	0.9800
C19—H19B	0.9800		
C9—S1—C8	103.13 (7)	H19B—C19—H19C	109.5

C15—O2—H2	109.5	C16A—N1A—C19A	121.7 (14)
C7—C1—C2	120.14 (12)	C16A—N1A—C18A	124.4 (12)
C7—C1—C8	120.23 (13)	C19A—N1A—C18A	114.0 (16)
C2—C1—C8	119.57 (13)	O3A—C16A—N1A	122.5 (10)
C1—C2—C3	121.59 (13)	O3A—C16A—C17A	118.2 (12)
C1—C2—C7^{i}	120.19 (13)	N1A—C16A—C17A	119.4 (11)
C3—C2—C7^{i}	118.22 (13)	C16A—C17A—H17D	109.5
C4—C3—C2	121.46 (14)	C16A—C17A—H17E	109.5
C4—C3—H3	119.3	H17D—C17A—H17E	109.5
C2—C3—H3	119.3	C16A—C17A—H17F	109.5
C3—C4—C5	120.48 (14)	H17D—C17A—H17F	109.5
C3—C4—H4	119.8	H17E—C17A—H17F	109.5
C5—C4—H4	119.8	N1A—C18A—H18D	109.5
C6—C5—C4	120.22 (14)	N1A—C18A—H18E	109.5
C6—C5—H5	119.9	H18D—C18A—H18E	109.5
C4—C5—H5	119.9	N1A—C18A—H18F	109.5
C5—C6—C7^{i}	121.72 (14)	H18D—C18A—H18F	109.5
C5—C6—H6	119.1	H18E—C18A—H18F	109.5
C7^{i}—C6—H6	119.1	N1A—C19A—H19D	109.5
C1—C7—C6^{i}	122.42 (13)	N1A—C19A—H19E	109.5
C1—C7—C2^{i}	119.68 (13)	H19D—C19A—H19E	109.5
C6^{i}—C7—C2^{i}	117.90 (13)	N1A—C19A—H19F	109.5
C1—C8—S1	104.70 (10)	H19D—C19A—H19F	109.5
C1—C8—H8A	110.8	H19E—C19A—H19F	109.5
S1—C8—H8A	110.8	C20—N2—C23	122.1 (3)
C1—C8—H8B	110.8	C20—N2—C22	120.4 (3)
S1—C8—H8B	110.8	C23—N2—C22	117.5 (4)
H8A—C8—H8B	108.9	O4—C20—N2	121.6 (2)
C10—C9—C14	118.61 (13)	O4—C20—C21	121.4 (3)
C10—C9—S1	121.23 (11)	N2—C20—C21	116.9 (3)
C14—C9—S1	120.16 (11)	C20—C21—H21A	109.5
C11—C10—C9	120.66 (14)	C20—C21—H21B	109.5
C11—C10—H10	119.7	H21A—C21—H21B	109.5
C9—C10—H10	119.7	C20—C21—H21C	109.5
C12—C11—C10	120.88 (15)	H21A—C21—H21C	109.5
C12—C11—H11	119.6	H21B—C21—H21C	109.5
C10—C11—H11	119.6	N2—C22—H22A	109.5
C13—C12—C11	119.28 (14)	N2—C22—H22B	109.5
C13—C12—H12	120.4	H22A—C22—H22B	109.5
C11—C12—H12	120.4	N2—C22—H22C	109.5
C12—C13—C14	121.20 (14)	H22A—C22—H22C	109.5
C12—C13—H13	119.4	H22B—C22—H22C	109.5
C14—C13—H13	119.4	N2—C23—H23A	109.5
C13—C14—C9	119.34 (14)	N2—C23—H23B	109.5
C13—C14—C15	119.55 (13)	H23A—C23—H23B	109.5
C9—C14—C15	121.04 (13)	N2—C23—H23C	109.5
O1—C15—O2	122.88 (15)	H23A—C23—H23C	109.5
O1—C15—C14	122.95 (14)	H23B—C23—H23C	109.5

O2—C15—C14	114.17 (13)	C20A—N2A—C23A	119.4 (12)
C16—N1—C19	124.1 (3)	C20A—N2A—C22A	116.6 (11)
C16—N1—C18	119.9 (3)	C23A—N2A—C22A	123.3 (14)
C19—N1—C18	115.9 (3)	O4A—C20A—N2A	122.7 (9)
O3—C16—N1	120.5 (2)	O4A—C20A—C21A	122.7 (13)
O3—C16—C17	120.8 (3)	N2A—C20A—C21A	109.7 (12)
N1—C16—C17	118.7 (3)	C20A—C21A—H21D	109.5
C16—C17—H17A	109.5	C20A—C21A—H21E	109.5
C16—C17—H17B	109.5	H21D—C21A—H21E	109.5
H17A—C17—H17B	109.5	C20A—C21A—H21F	109.5
C16—C17—H17C	109.5	H21D—C21A—H21F	109.5
H17A—C17—H17C	109.5	H21E—C21A—H21F	109.5
H17B—C17—H17C	109.5	N2A—C22A—H22D	109.5
N1—C18—H18A	109.5	N2A—C22A—H22E	109.5
N1—C18—H18B	109.5	H22D—C22A—H22E	109.5
H18A—C18—H18B	109.5	N2A—C22A—H22F	109.5
N1—C18—H18C	109.5	H22D—C22A—H22F	109.5
H18A—C18—H18C	109.5	H22E—C22A—H22F	109.5
H18B—C18—H18C	109.5	N2A—C23A—H23D	109.5
N1—C19—H19A	109.5	N2A—C23A—H23E	109.5
N1—C19—H19B	109.5	H23D—C23A—H23E	109.5
H19A—C19—H19B	109.5	N2A—C23A—H23F	109.5
N1—C19—H19C	109.5	H23D—C23A—H23F	109.5
H19A—C19—H19C	109.5	H23E—C23A—H23F	109.5

C7—C1—C2—C3	−179.61 (14)	C10—C9—C14—C13	−0.2 (2)
C8—C1—C2—C3	3.3 (2)	S1—C9—C14—C13	179.70 (11)
C7—C1—C2—C7^{i}	−0.1 (2)	C10—C9—C14—C15	−177.18 (13)
C8—C1—C2—C7^{i}	−177.13 (13)	S1—C9—C14—C15	2.68 (19)
C1—C2—C3—C4	179.07 (15)	C13—C14—C15—O1	−164.05 (14)
C7^{i}—C2—C3—C4	−0.5 (2)	C9—C14—C15—O1	13.0 (2)
C2—C3—C4—C5	0.4 (2)	C13—C14—C15—O2	15.89 (19)
C3—C4—C5—C6	−0.3 (3)	C9—C14—C15—O2	−167.10 (13)
C4—C5—C6—C7^{i}	0.2 (3)	C19—N1—C16—O3	178.2 (5)
C2—C1—C7—C6^{i}	−179.13 (14)	C18—N1—C16—O3	3.2 (6)
C8—C1—C7—C6^{i}	−2.1 (2)	C19—N1—C16—C17	−0.5 (7)
C2—C1—C7—C2^{i}	0.1 (2)	C18—N1—C16—C17	−175.6 (6)
C8—C1—C7—C2^{i}	177.11 (13)	C19A—N1A—C16A—O3A	−1 (3)
C7—C1—C8—S1	−95.52 (14)	C18A—N1A—C16A—O3A	180 (2)
C2—C1—C8—S1	81.56 (14)	C19A—N1A—C16A—C17A	−180 (3)
C9—S1—C8—C1	178.13 (9)	C18A—N1A—C16A—C17A	0 (3)
C8—S1—C9—C10	−11.00 (14)	C23—N2—C20—O4	−174.3 (3)
C8—S1—C9—C14	169.14 (11)	C22—N2—C20—O4	4.3 (4)
C14—C9—C10—C11	1.3 (2)	C23—N2—C20—C21	5.4 (5)
S1—C9—C10—C11	−178.57 (12)	C22—N2—C20—C21	−175.9 (4)
C9—C10—C11—C12	−1.0 (2)	C23A—N2A—C20A—O4A	−171.1 (13)
C10—C11—C12—C13	−0.5 (2)	C22A—N2A—C20A—O4A	0 (2)
C11—C12—C13—C14	1.6 (2)	C23A—N2A—C20A—C21A	33.2 (17)

C12—C13—C14—C9	−1.3 (2)	C22A—N2A—C20A—C21A	−155.7 (19)
C12—C13—C14—C15	175.77 (13)		

Symmetry code: (i) −*x*+1, −*y*+1, −*z*+1.

Hydrogen-bond geometry (Å, º)

*Cg*1 is the centroid of the C9–C14 ring of (**1**).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···O3*A*^{ii}	0.84	1.94	2.770 (14)	169
C8—H8*B*···O4*A*^{iii}	0.99	2.48	3.126 (8)	122
C17—H17*A*···O4^{iv}	0.98	2.62	3.518 (8)	152
C18*A*—H18*D*···S1^{iv}	0.98	3.02	3.83 (3)	142
C19*A*—H19*E*···O4*A*^{iv}	0.98	2.43	3.40 (4)	168
C21—H21*C*···O1	0.98	2.49	3.422 (7)	158
C22*A*—H22*F*···O1	0.98	2.54	3.51 (3)	168
C4—H4···*Cg*1	0.95	2.76	3.49	135

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

4,4′-{[Anthracene-9,10-diylbis(methylene)]bis(oxy)}dibenzoic acid dimethylformamide disolvate (2)

Crystal data

$C_{30}H_{22}O_6·2C_3H_7NO$
M_r = 624.67
Monoclinic, $P2_1/n$
a = 10.8761 (10) Å
b = 9.6711 (9) Å
c = 14.8968 (14) Å
β = 100.519 (3)°
V = 1540.6 (2) Å^3
Z = 2
F(000) = 660
D_x = 1.347 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 1406 reflections
θ = 2.6–18.7°
μ = 0.10 mm^{-1}
T = 104 K
Plate, clear yellowish yellow
0.26 × 0.19 × 0.16 mm

Data collection

Bruker APEXII CCD diffractometer
φ and *ω* scans
Absorption correction: multi-scan (Olex2; Dolomanov *et al.*, 2009)
T_{min} = 0.666, T_{max} = 0.745
49734 measured reflections
3169 independent reflections
1669 reflections with $I > 2\sigma(I)$
R_{int} = 0.179
θ_{max} = 26.5°, θ_{min} = 2.1°
h = −13→13
k = −12→12
l = −18→18

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.069
$wR(F^2)$ = 0.182
S = 1.02
3169 reflections
211 parameters
0 restraints
Primary atom site location: dual
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0696P)^2 + 0.9349P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.4625 (2)	0.3352 (2)	0.09997 (14)	0.0337 (6)
O2	0.3683 (2)	0.8009 (2)	0.38061 (15)	0.0411 (6)
O3	0.4259 (2)	0.9259 (2)	0.26840 (16)	0.0466 (7)
H3	0.420178	0.991287	0.304515	0.070*
O4	0.4165 (2)	1.1349 (2)	0.37398 (17)	0.0503 (7)
N1	0.3426 (3)	1.1942 (3)	0.50255 (19)	0.0422 (7)
C7	0.3906 (3)	0.0820 (3)	−0.0203 (2)	0.0250 (7)
C1	0.4710 (3)	0.0961 (3)	0.0652 (2)	0.0255 (7)
C9	0.4409 (3)	0.4460 (3)	0.1518 (2)	0.0303 (8)
C2	0.5807 (3)	0.0166 (3)	0.0859 (2)	0.0259 (7)
C13	0.3834 (3)	0.5569 (3)	0.2809 (2)	0.0316 (8)
H13	0.353304	0.551391	0.336760	0.038*
C14	0.3968 (3)	0.4365 (3)	0.2335 (2)	0.0313 (8)
H14	0.376246	0.349338	0.256255	0.038*
C6	0.7205 (3)	−0.1639 (3)	0.0447 (2)	0.0312 (8)
H6	0.740356	−0.229858	0.002326	0.037*
C8	0.4362 (3)	0.1987 (3)	0.1318 (2)	0.0299 (7)
H8A	0.346404	0.190190	0.134842	0.036*
H8B	0.485761	0.181983	0.193453	0.036*
C3	0.6662 (3)	0.0280 (3)	0.1708 (2)	0.0336 (8)
H3A	0.649564	0.092861	0.215009	0.040*
C15	0.4000 (3)	0.8076 (3)	0.3059 (2)	0.0368 (8)
C12	0.4126 (3)	0.6845 (3)	0.2495 (2)	0.0309 (8)
C10	0.4707 (3)	0.5746 (3)	0.1194 (2)	0.0335 (8)
H10	0.501582	0.580681	0.063815	0.040*
C11	0.4557 (3)	0.6929 (3)	0.1676 (2)	0.0354 (8)
H11	0.474846	0.780492	0.144782	0.042*
C5	0.7977 (3)	−0.1500 (4)	0.1261 (2)	0.0378 (8)
H5	0.870193	−0.206227	0.140562	0.045*
C4	0.7702 (3)	−0.0514 (4)	0.1897 (2)	0.0410 (9)
H4	0.825451	−0.040790	0.246538	0.049*
C16	0.3683 (3)	1.1049 (4)	0.4424 (3)	0.0443 (9)
H16	0.349206	1.010445	0.450942	0.053*
C17	0.3683 (4)	1.3394 (4)	0.4945 (3)	0.0541 (11)
H17A	0.433156	1.351418	0.457255	0.081*
H17B	0.397436	1.378518	0.555323	0.081*
H17C	0.291892	1.387089	0.465295	0.081*
C18	0.2832 (4)	1.1503 (4)	0.5779 (3)	0.0540 (11)
H18A	0.198205	1.188036	0.569478	0.081*

H18B	0.331843	1.184320	0.635586	0.081*
H18C	0.279500	1.049111	0.579376	0.081*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0475 (14)	0.0227 (12)	0.0350 (12)	−0.0027 (10)	0.0182 (10)	−0.0034 (10)
O2	0.0483 (15)	0.0389 (14)	0.0400 (14)	−0.0043 (11)	0.0181 (12)	−0.0065 (11)
O3	0.0656 (17)	0.0302 (14)	0.0507 (15)	−0.0051 (12)	0.0288 (14)	−0.0078 (12)
O4	0.0652 (17)	0.0386 (15)	0.0510 (16)	−0.0080 (13)	0.0210 (14)	−0.0086 (12)
N1	0.0441 (18)	0.0409 (19)	0.0423 (17)	0.0027 (14)	0.0098 (14)	−0.0051 (15)
C7	0.0250 (16)	0.0212 (16)	0.0303 (17)	−0.0032 (13)	0.0094 (14)	0.0010 (13)
C1	0.0303 (17)	0.0182 (16)	0.0307 (18)	−0.0031 (13)	0.0127 (14)	0.0004 (13)
C9	0.0343 (18)	0.0233 (18)	0.0336 (18)	−0.0003 (14)	0.0067 (15)	−0.0047 (14)
C2	0.0303 (17)	0.0198 (17)	0.0288 (17)	−0.0061 (13)	0.0087 (14)	0.0007 (13)
C13	0.0363 (19)	0.0305 (19)	0.0299 (18)	−0.0025 (15)	0.0111 (15)	−0.0001 (15)
C14	0.0357 (18)	0.0251 (18)	0.0342 (19)	−0.0054 (14)	0.0092 (15)	0.0015 (14)
C6	0.0329 (18)	0.0256 (18)	0.0373 (19)	0.0005 (14)	0.0123 (15)	0.0019 (14)
C8	0.0346 (18)	0.0242 (18)	0.0318 (17)	−0.0009 (14)	0.0087 (14)	0.0019 (14)
C3	0.0365 (19)	0.034 (2)	0.0316 (19)	−0.0036 (16)	0.0103 (15)	−0.0064 (15)
C15	0.039 (2)	0.033 (2)	0.041 (2)	−0.0043 (16)	0.0153 (17)	−0.0025 (17)
C12	0.0315 (18)	0.0288 (19)	0.0338 (18)	−0.0002 (14)	0.0096 (14)	−0.0025 (15)
C10	0.041 (2)	0.033 (2)	0.0285 (18)	−0.0005 (15)	0.0106 (15)	−0.0011 (15)
C11	0.042 (2)	0.0290 (19)	0.0372 (19)	−0.0008 (15)	0.0112 (16)	0.0018 (16)
C5	0.0330 (19)	0.042 (2)	0.039 (2)	0.0063 (16)	0.0078 (16)	0.0054 (17)
C4	0.035 (2)	0.052 (2)	0.034 (2)	0.0015 (18)	0.0020 (16)	−0.0005 (17)
C16	0.042 (2)	0.040 (2)	0.052 (2)	−0.0043 (17)	0.0091 (19)	−0.0013 (19)
C17	0.075 (3)	0.039 (2)	0.052 (2)	0.004 (2)	0.019 (2)	−0.0032 (18)
C18	0.062 (3)	0.057 (3)	0.050 (2)	−0.001 (2)	0.026 (2)	0.001 (2)

Geometric parameters (Å, º)

O1—C9	1.366 (3)	C6—C5	1.348 (4)
O1—C8	1.448 (3)	C6—H6	0.9500
O2—C15	1.225 (4)	C8—H8A	0.9900
O3—C15	1.326 (4)	C8—H8B	0.9900
O3—H3	0.8400	C3—C4	1.353 (4)
O4—C16	1.262 (4)	C3—H3A	0.9500
N1—C16	1.311 (4)	C15—C12	1.477 (4)
N1—C17	1.442 (5)	C12—C11	1.387 (4)
N1—C18	1.457 (4)	C10—C11	1.377 (4)
C7—C1	1.414 (4)	C10—H10	0.9500
C7—C6^{i}	1.435 (4)	C11—H11	0.9500
C7—C2^{i}	1.439 (4)	C5—C4	1.415 (5)
C1—C2	1.405 (4)	C5—H5	0.9500
C1—C8	1.499 (4)	C4—H4	0.9500
C9—C14	1.391 (4)	C16—H16	0.9500
C9—C10	1.394 (4)	C17—H17A	0.9800

C2—C3	1.431 (4)	C17—H17B	0.9800
C13—C12	1.377 (4)	C17—H17C	0.9800
C13—C14	1.383 (4)	C18—H18A	0.9800
C13—H13	0.9500	C18—H18B	0.9800
C14—H14	0.9500	C18—H18C	0.9800

C9—O1—C8	117.8 (2)	C2—C3—H3A	119.2
C15—O3—H3	109.5	O2—C15—O3	123.0 (3)
C16—N1—C17	121.1 (3)	O2—C15—C12	123.0 (3)
C16—N1—C18	121.0 (3)	O3—C15—C12	114.0 (3)
C17—N1—C18	117.9 (3)	C13—C12—C11	119.1 (3)
C1—C7—C6^{i}	121.9 (3)	C13—C12—C15	118.6 (3)
C1—C7—C2^{i}	120.0 (3)	C11—C12—C15	122.3 (3)
C6^{i}—C7—C2^{i}	118.1 (3)	C11—C10—C9	120.2 (3)
C2—C1—C7	120.4 (3)	C11—C10—H10	119.9
C2—C1—C8	121.6 (3)	C9—C10—H10	119.9
C7—C1—C8	118.1 (3)	C10—C11—C12	120.1 (3)
O1—C9—C14	124.4 (3)	C10—C11—H11	119.9
O1—C9—C10	115.5 (3)	C12—C11—H11	119.9
C14—C9—C10	120.1 (3)	C6—C5—C4	119.8 (3)
C1—C2—C3	122.7 (3)	C6—C5—H5	120.1
C1—C2—C7^{i}	119.6 (3)	C4—C5—H5	120.1
C3—C2—C7^{i}	117.7 (3)	C3—C4—C5	120.9 (3)
C12—C13—C14	122.0 (3)	C3—C4—H4	119.5
C12—C13—H13	119.0	C5—C4—H4	119.5
C14—C13—H13	119.0	O4—C16—N1	124.9 (3)
C13—C14—C9	118.4 (3)	O4—C16—H16	117.6
C13—C14—H14	120.8	N1—C16—H16	117.6
C9—C14—H14	120.8	N1—C17—H17A	109.5
C5—C6—C7^{i}	122.0 (3)	N1—C17—H17B	109.5
C5—C6—H6	119.0	H17A—C17—H17B	109.5
C7^{i}—C6—H6	119.0	N1—C17—H17C	109.5
O1—C8—C1	107.4 (2)	H17A—C17—H17C	109.5
O1—C8—H8A	110.2	H17B—C17—H17C	109.5
C1—C8—H8A	110.2	N1—C18—H18A	109.5
O1—C8—H8B	110.2	N1—C18—H18B	109.5
C1—C8—H8B	110.2	H18A—C18—H18B	109.5
H8A—C8—H8B	108.5	N1—C18—H18C	109.5
C4—C3—C2	121.6 (3)	H18A—C18—H18C	109.5
C4—C3—H3A	119.2	H18B—C18—H18C	109.5

C6^{i}—C7—C1—C2	−178.4 (3)	C7^{i}—C2—C3—C4	−0.5 (4)
C2^{i}—C7—C1—C2	1.5 (4)	C14—C13—C12—C11	0.5 (5)
C6^{i}—C7—C1—C8	1.0 (4)	C14—C13—C12—C15	−177.8 (3)
C2^{i}—C7—C1—C8	−179.1 (2)	O2—C15—C12—C13	2.2 (5)
C8—O1—C9—C14	0.8 (4)	O3—C15—C12—C13	−177.7 (3)
C8—O1—C9—C10	178.4 (3)	O2—C15—C12—C11	−176.1 (3)
C7—C1—C2—C3	179.2 (3)	O3—C15—C12—C11	4.0 (5)

C8—C1—C2—C3	−0.2 (4)	O1—C9—C10—C11	−178.3 (3)
C7—C1—C2—C7^{i}	−1.5 (4)	C14—C9—C10—C11	−0.6 (5)
C8—C1—C2—C7^{i}	179.2 (3)	C9—C10—C11—C12	1.0 (5)
C12—C13—C14—C9	0.0 (5)	C13—C12—C11—C10	−1.0 (5)
O1—C9—C14—C13	177.6 (3)	C15—C12—C11—C10	177.3 (3)
C10—C9—C14—C13	0.1 (5)	C7^{i}—C6—C5—C4	−0.6 (5)
C9—O1—C8—C1	−178.3 (2)	C2—C3—C4—C5	−0.6 (5)
C2—C1—C8—O1	104.5 (3)	C6—C5—C4—C3	1.1 (5)
C7—C1—C8—O1	−74.8 (3)	C17—N1—C16—O4	0.2 (5)
C1—C2—C3—C4	178.9 (3)	C18—N1—C16—O4	178.0 (3)

Symmetry code: (i) −*x*+1, −*y*, −*z*.

Hydrogen-bond geometry (Å, º)

*Cg*2 is the centroid of the C9–C14 ring of (**2**).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3···O4	0.84	1.74	2.575 (3)	175
C8—H8*A*···O2^{ii}	0.99	2.54	3.429 (4)	149
C16—H16···O2	0.95	2.31	3.080 (4)	138
C4—H4···*Cg*2	0.95	3.07	3.96	157

Symmetry code: (ii) −*x*+1/2, *y*−1/2, −*z*+1/2.