Molecular and crystal structure, optical properties and DFT studies of 1,4-dimethoxy-2,5-bis[2-(4-nitrophenyl)ethenyl]benzene

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The title compound DBNB, $C_{24}H_{20}N_2O_6$, has been crystallized and studied by X-ray diffraction, spectroscopic and computational methods. In the title molecule, which is based on a 1,4-distyryl-2,5-dimethoxybenzene core with p-nitro-substituted terminal benzene rings, the dihedral angle between mean planes of the central fragment and the terminal phenyl ring is 16.46 (6)°. The crystal packing is stabilized by π–π interactions. DFT calculations at the B3LYP/6–311 G(d,p) level of theory were used to compare the optimized structures with the experimental data. Energy parameters, including HOMO and LUMO energies, their difference, and vertical excitation and emission energies were obtained.

1. Chemical context

One method for the design of the organic two-photon absorbing (TPA) molecules is Donor–π-Bridge–Acceptor–π-Bridge–Donor or Acceptor–π-bridge–Donor–π-bridge–Acceptor (He *et al.*, 2008). Specific spectroscopic properties of such molecules make them useful for applications in different areas. For instance, about half a century ago it was found that the title compound and other substituted distyrylbenzenes would be highly efficient wavelength shifters in organic liquid scintillators (Nakaya *et al.*, 1966). It is important to mention that some molecules with such general structure possess not only plasminogen activator (tPA) activity but also demonstrate light emission, which make them useful for organic light-emitting diodes (OLEDs) (Cárdenas *et al.*, 2019) and/or chemical sensors (Xu *et al.*, 2013). For instance, for a molecule similar to the title molecule, 1,4-dimethoxy-2,5-bis(4′-dichlorostyryl)benzene, blue fluorescence emission was found, which makes it a prospective candidate for cell imaging. Another phenyleneethenylene derivative, 2,5-dimethoxy-1,4-bis[2-(4-carboxylatestyryl)]benzene, for which two polymorphs and one DMF solvate have been studied, demonstrated three different types of emission, depending on the molecular packing in the crystal (Cárdenas *et al.*, 2019). On this basis, we considered that an investigation of the molecular structure and crystal packing of the title compound would be useful for correlating its structural characteristics to its spectroscopic properties.

Figure 3
The packing in the crystal of the title compound.
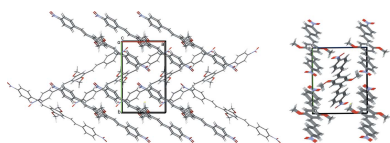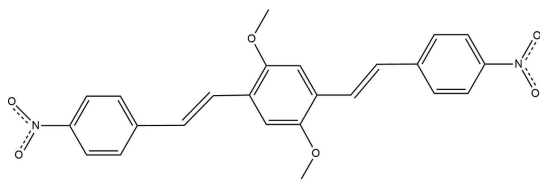
2. Structural commentary

The molecular structure of DBDB is presented in Fig. 1. The molecule lies on an inversion center and shows a slight deviation from planarity. The dihedral angle formed by mean planes of the central fragment and the terminal benzene ring is 16.46 (6)°. The methoxy group is rotated by 3.77 (11)° and the nitro group by 15.99 (8)° with respect to the central ring and the terminal benzene ring, respectively. In a similar compound with *para*-chlorine substitution, the angles between the central and terminal aromatic rings are 43.82 and 67.38° (Xu *et al.*, 2013), whereas in closely related structures these angles vary from 11.97 to 35.75° (Cárdenas *et al.*, 2019), demonstrating the flexibility of this type of molecule, even in the solid state.

3. Supramolecular features

In the crystal, the DBDB molecules are packed into ladder-like stacks (Fig. 2) along the *a*-axis direction, which in turn build a parquet-like structure (Fig. 3). An intermolecular distance of 3.451 (1) Å is found between the mean planes of the central rings in the molecular stacks, with a separation between the centroids of the central ring and the terminal benzene ring of 3.899 (1) Å, which suggests the presence of π–π interactions between the molecules.

4. Database survey

A search of the Cambridge Crystallographic Database (CSD version 5.40, update of September 2019; Groom *et al.*, 2016) for the title molecule returned no results. Two entries for compounds with the same core and unsubstituted terminal rings were found. Over 30 entries were found for variously substituted molecules with the same core, of which 10 entries correspond to *para*-substituted terminal aromatic groups. Among them halogen-substituted molecules [refcodes: VIQCAB (Xu *et al.*, 2013), ODOHOG (Sun *et al.*, 2013), ODOJAU (Sun *et al.*, 2013)], as well as molecules with cyano (OBUHAV; Xu *et al.*, 2013), carboxyl (TOJDEE, TOJDII; Cárdenas *et al.*, 2019) and alkylcarboxylate (TOJCUT; Cárdenas *et al.*, 2019) groups in the *para*-position have been reported. Most of the molecules demonstrate dihedral angles between the central fragment and the terminal rings ranging from 5.0 (1) to 36.1 (1)°. One notable exception is the chlorine-substituted compound (VIQCAB; Xu *et al.*, 2013), for which the angles between central and the terminal aromatic rings are 43.82 (16) and 67.38 (17)°.

5. Optical studies in solution

A solution of the title compound in dioxane (at 10 m*M* concentration) in a quartz sample cuvette (10 mm optical path length) was used for optical absorption and emission studies. All measurements were carried out at ambient temperature. The corresponding spectra are shown in Fig. 4. Peak positions,
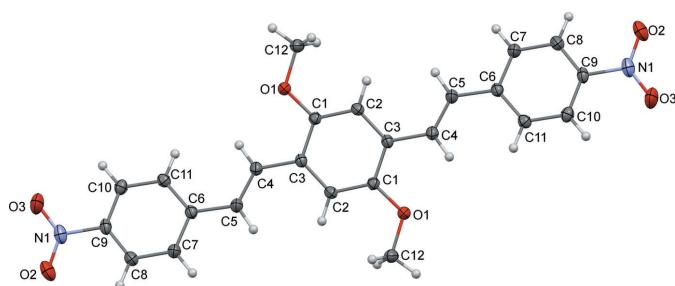

Figure 1
A view of the molecular structure of the title compound with the atom-labeling scheme. Displacement ellipsoids are drawn at the 50% probability level.
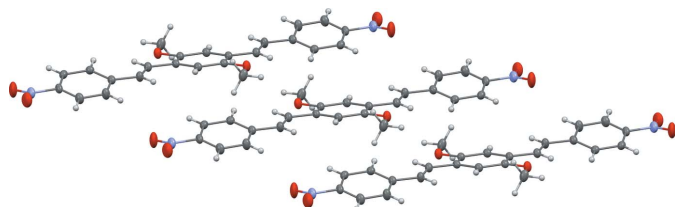

Figure 2
Ladder-like stack of DBDB molecules; the distance between the mean planes of the central phenyl rings within the stack is 3.451 (1) Å.
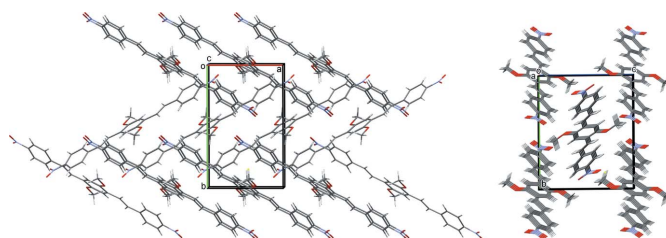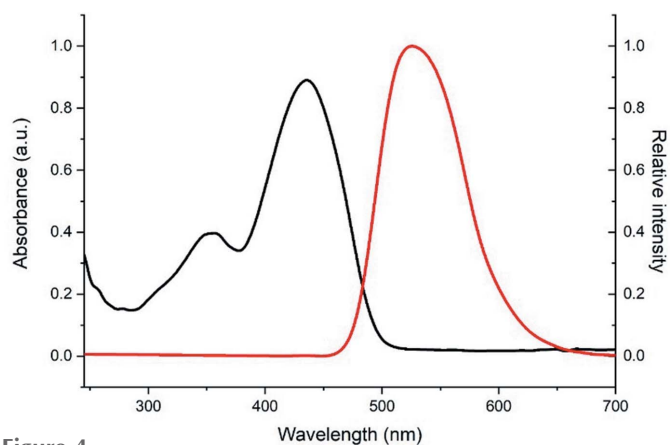

Figure 4
Normalized absorption (black) and emission (red) spectra of the title compound measured in dioxane solution.

Table 1
Selected energy parameters (gas phase).

Total Energy (eV)	−40479.535
E_{HOMO} (eV)	−5.813
E_{LUMO} (eV)	−3.096
HOMO–LUMO gap (eV)	2.717
S_0–S_1 vertical excitation (nm)	497.44
S_1–S_0 vertical emission (nm)	546.03

Table 2
Selected X-ray and DFT ground-state geometry parameter (Å, °) comparison.

Bonds/angles	Experimental	Calculated
O1—C1	1.3663 (14)	1.3652
O1—C12	1.4248 (15)	1.4207
O2—N1	1.2321 (16)	1.2253
N1—C9	1.4665 (16)	1.4723
C5—C4—C3	127.07 (11)	126.76
C4—C5—C6	125.13 (11)	126.38
C1—O1—C12	117.68 (9)	119.05
C8—C9—N1	118.92 (11)	119.26

Table 3
Experimental details.

Crystal data	
Chemical formula	$C_{24}H_{20}N_2O_6$
M_r	432.42
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	100
a, b, c (Å)	7.9074 (10), 12.4794 (16), 10.6248 (14)
β (°)	102.394 (3)
V (Å³)	1024.0 (2)
Z	2
Radiation type	Mo $K\alpha$
μ (mm⁻¹)	0.10
Crystal size (mm)	$0.22 \times 0.15 \times 0.11$
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2016)
T_{min}, T_{max}	0.653, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	32090, 3460, 2542
R_{int}	0.055
$(\sin\theta/\lambda)_{max}$ (Å⁻¹)	0.738
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.048, 0.145, 1.04
No. of reflections	3460
No. of parameters	146
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å⁻³)	0.49, −0.21

Computer programs: *APEX3* (Bruker, 2016), *SAINT* (Bruker, 2016), *SHELXT2017/1* (Sheldrick, 2015a), *SHELXL2017/1* (Sheldrick, 2015b), *OLEX2* (Dolomanov *et al.*, 2009), *Mercury* (Macrae *et al.*, 2020).

as well as band shapes are in good agreement with those previously reported (Nakaya *et al.*, 1966). Fluorescence was measured at the excitation wavelength of 434 nm, chosen from the absorption spectrum, and had a maximum at 525 nm. The E_{0-0} transition energy was estimated to be at 483 nm (2.57 eV).

6. DFT calculations

In an effort to further elucidate the nature of the electronic radiative transitions in the title compound, DFT and time-dependent (TD) DFT calculations were carried out with *GAUSSIAN 16* software (Frisch *et al.*, 2016). The standard B3LYP functional with the 6-311G(d,p) basis set was used to optimize both the ground and first excited states of the title molecule and to obtain vertical excitation and emission energies, HOMO (E_{HOMO}) and LUMO (E_{LUMO}) energies and their difference (Fig. 5). All of the calculated parameters are for the gas phase of the title compound. Both optimized geometries were confirmed to be the true minima *via* vibrational frequency analysis. The summary of calculated energy parameters is presented in Table 1. The calculated geometry parameters (bond lengths and angles) are in good agreement with the experimental data (Table 2).
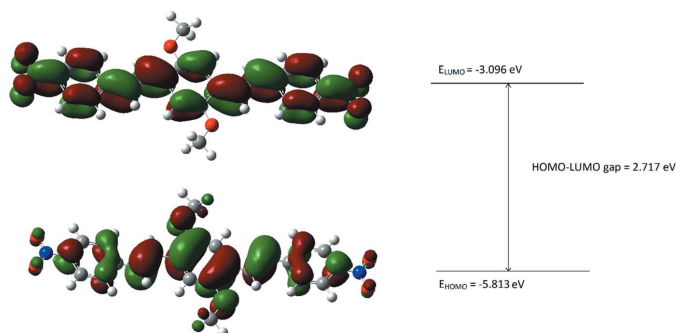
7. Synthesis and crystallization

The synthesis of title compound was carried out as described in the literature (Nakaya *et al.*, 1966; Caruso *et al.*, 2005). The obtained material was recrystallized by slow evaporation of ethanol solution giving dark-red block-shaped crystals.

8. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. H atoms were placed in calculated positions (0.95–0.98 Å) and refined as riding with $U_{iso}(H) = 1.2U_{eq}(C)$ or $1.5U_{eq}(C\text{-methyl})$.

Figure 5
HOMO and LUMO orbitals with corresponding energy values and gap.

E_LUMO = -3.096 eV

HOMO-LUMO gap = 2.717 eV

E_HOMO = -5.813 eV

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supporting information

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Computing details

Data collection: *APEX3* (Bruker, 2016); cell refinement: *SAINT* (Bruker, 2016); data reduction: *SAINT* (Bruker, 2016); program(s) used to solve structure: *SHELXT2017/1* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2017/1* (Sheldrick, 2015b), *OLEX2* (Dolomanov *et al.*, 2009); molecular graphics: *Mercury* (Macrae *et al.*, 2020); software used to prepare material for publication: *Mercury* (Macrae *et al.*, 2020).

1,4-Dimethoxy-2,5-bis[2-(4-nitrophenyl)ethenyl]benzene

Crystal data

$C_{24}H_{20}N_2O_6$	$F(000) = 452$
$M_r = 432.42$	$D_x = 1.403$ Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 7.9074$ (10) Å	Cell parameters from 6481 reflections
$b = 12.4794$ (16) Å	$\theta = 2.6–31.3°$
$c = 10.6248$ (14) Å	$\mu = 0.10$ mm^{-1}
$\beta = 102.394$ (3)°	$T = 100$ K
$V = 1024.0$ (2) Å^3	Block, red
$Z = 2$	$0.22 \times 0.15 \times 0.11$ mm

Data collection

Bruker APEXII CCD diffractometer	3460 independent reflections
φ and ω scans	2542 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Bruker, 2016)	$R_{int} = 0.055$
	$\theta_{max} = 31.7°$, $\theta_{min} = 2.6°$
$T_{min} = 0.653$, $T_{max} = 0.746$	$h = -11 \rightarrow 11$
32090 measured reflections	$k = -18 \rightarrow 18$
	$l = -15 \rightarrow 15$

Refinement

Refinement on F^2	Primary atom site location: dual
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.048$	
$wR(F^2) = 0.145$	Hydrogen site location: inferred from neighbouring sites
$S = 1.03$	
3460 reflections	H-atom parameters constrained
146 parameters	$w = 1/[\sigma^2(F_o^2) + (0.0723P)^2 + 0.3749P]$
0 restraints	where $P = (F_o^2 + 2F_c^2)/3$

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

$\Delta\rho_{max} = 0.49$ e Å^{-3}

$\Delta\rho_{min} = -0.21$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	1.12432 (11)	0.50902 (7)	0.27624 (8)	0.0223 (2)
O2	−0.13219 (13)	0.91355 (10)	0.42105 (12)	0.0423 (3)
O3	−0.08612 (15)	0.85312 (11)	0.61675 (12)	0.0453 (3)
N1	−0.04597 (14)	0.86252 (10)	0.51181 (12)	0.0301 (3)
C1	1.05803 (14)	0.50680 (9)	0.38485 (11)	0.0176 (2)
C2	0.90285 (14)	0.55533 (9)	0.39523 (11)	0.0185 (2)
H2	0.836944	0.592801	0.323366	0.022*
C3	0.84235 (14)	0.54988 (9)	0.50948 (11)	0.0178 (2)
C10	0.18811 (15)	0.73214 (10)	0.58176 (12)	0.0215 (2)
H10	0.137655	0.713154	0.652137	0.026*
C4	0.67887 (14)	0.59782 (10)	0.52387 (11)	0.0202 (2)
H4	0.640701	0.580352	0.600263	0.024*
C6	0.41503 (15)	0.71106 (10)	0.46101 (11)	0.0196 (2)
C11	0.33818 (15)	0.68241 (9)	0.56370 (11)	0.0198 (2)
H11	0.389852	0.627975	0.621909	0.024*
C9	0.11358 (14)	0.81049 (10)	0.49411 (12)	0.0217 (2)
C5	0.57748 (16)	0.66340 (10)	0.44141 (12)	0.0225 (2)
H5	0.613011	0.680685	0.363923	0.027*
C8	0.18426 (16)	0.84114 (11)	0.39171 (12)	0.0249 (3)
H8	0.131401	0.895451	0.333775	0.030*
C7	0.33514 (17)	0.79047 (11)	0.37539 (12)	0.0252 (3)
H7	0.384749	0.810152	0.304835	0.030*
C12	1.03435 (16)	0.57061 (12)	0.16982 (12)	0.0269 (3)
H12A	1.097995	0.568337	0.100234	0.040*
H12B	1.025026	0.645017	0.197031	0.040*
H12C	0.918153	0.540834	0.138992	0.040*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0212 (4)	0.0287 (5)	0.0177 (4)	0.0069 (3)	0.0058 (3)	0.0033 (3)
O2	0.0253 (5)	0.0519 (7)	0.0485 (7)	0.0170 (5)	0.0054 (5)	0.0069 (5)
O3	0.0363 (6)	0.0580 (8)	0.0491 (7)	0.0163 (5)	0.0260 (5)	0.0067 (6)
N1	0.0192 (5)	0.0331 (6)	0.0387 (6)	0.0057 (4)	0.0082 (4)	−0.0013 (5)
C1	0.0175 (5)	0.0183 (5)	0.0172 (5)	0.0007 (4)	0.0040 (4)	−0.0014 (4)
C2	0.0168 (5)	0.0200 (5)	0.0180 (5)	0.0027 (4)	0.0018 (4)	0.0010 (4)
C3	0.0152 (5)	0.0181 (5)	0.0198 (5)	0.0018 (4)	0.0029 (4)	−0.0014 (4)

C10	0.0191 (5)	0.0228 (6)	0.0237 (5)	−0.0025 (4)	0.0071 (4)	−0.0014 (4)
C4	0.0180 (5)	0.0234 (5)	0.0195 (5)	0.0026 (4)	0.0049 (4)	−0.0007 (4)
C6	0.0167 (5)	0.0211 (5)	0.0206 (5)	0.0023 (4)	0.0033 (4)	−0.0012 (4)
C11	0.0180 (5)	0.0199 (5)	0.0212 (5)	0.0000 (4)	0.0034 (4)	0.0003 (4)
C9	0.0148 (5)	0.0246 (6)	0.0257 (6)	0.0028 (4)	0.0045 (4)	−0.0043 (4)
C5	0.0211 (5)	0.0250 (6)	0.0235 (6)	0.0059 (4)	0.0092 (4)	0.0036 (4)
C8	0.0227 (6)	0.0284 (6)	0.0235 (6)	0.0083 (5)	0.0044 (4)	0.0030 (5)
C7	0.0247 (6)	0.0301 (6)	0.0225 (6)	0.0085 (5)	0.0091 (5)	0.0052 (5)
C12	0.0212 (5)	0.0388 (7)	0.0211 (6)	0.0048 (5)	0.0055 (4)	0.0086 (5)

Geometric parameters (Å, º)

O1—C1	1.3663 (14)	C4—C5	1.3337 (16)
O1—C12	1.4248 (15)	C6—C11	1.4043 (16)
O2—N1	1.2321 (16)	C6—C5	1.4704 (16)
O3—N1	1.2287 (16)	C6—C7	1.4007 (17)
N1—C9	1.4665 (16)	C11—H11	0.9500
C1—C2	1.3938 (15)	C9—C8	1.3796 (18)
C1—C3^i	1.4148 (16)	C5—H5	0.9500
C2—H2	0.9500	C8—H8	0.9500
C2—C3	1.3986 (16)	C8—C7	1.3936 (17)
C3—C4	1.4619 (15)	C7—H7	0.9500
C10—H10	0.9500	C12—H12A	0.9800
C10—C11	1.3885 (16)	C12—H12B	0.9800
C10—C9	1.3910 (17)	C12—H12C	0.9800
C4—H4	0.9500		
C1—O1—C12	117.68 (9)	C10—C11—C6	121.25 (11)
O2—N1—C9	118.37 (12)	C10—C11—H11	119.4
O3—N1—O2	123.52 (12)	C6—C11—H11	119.4
O3—N1—C9	118.11 (11)	C10—C9—N1	118.55 (11)
O1—C1—C2	124.19 (10)	C8—C9—N1	118.92 (11)
O1—C1—C3^i	115.54 (10)	C8—C9—C10	122.53 (11)
C2—C1—C3^i	120.27 (10)	C4—C5—C6	125.13 (11)
C1—C2—H2	119.4	C4—C5—H5	117.4
C1—C2—C3	121.23 (10)	C6—C5—H5	117.4
C3—C2—H2	119.4	C9—C8—H8	120.8
C1^i—C3—C4	118.41 (10)	C9—C8—C7	118.35 (11)
C2—C3—C1^i	118.50 (10)	C7—C8—H8	120.8
C2—C3—C4	123.08 (10)	C6—C7—H7	119.4
C11—C10—H10	120.9	C8—C7—C6	121.27 (11)
C11—C10—C9	118.26 (11)	C8—C7—H7	119.4
C9—C10—H10	120.9	O1—C12—H12A	109.5
C3—C4—H4	116.5	O1—C12—H12B	109.5
C5—C4—C3	127.07 (11)	O1—C12—H12C	109.5
C5—C4—H4	116.5	H12A—C12—H12B	109.5
C11—C6—C5	122.95 (11)	H12A—C12—H12C	109.5
C7—C6—C11	118.34 (10)	H12B—C12—H12C	109.5

C7—C6—C5	118.69 (11)		
O1—C1—C2—C3	179.95 (11)	C11—C10—C9—N1	179.35 (11)
O2—N1—C9—C10	−164.27 (12)	C11—C10—C9—C8	−0.84 (19)
O2—N1—C9—C8	15.92 (19)	C11—C6—C5—C4	−7.6 (2)
O3—N1—C9—C10	15.98 (19)	C11—C6—C7—C8	0.74 (19)
O3—N1—C9—C8	−163.83 (13)	C9—C10—C11—C6	0.93 (18)
N1—C9—C8—C7	−179.49 (12)	C9—C8—C7—C6	−0.6 (2)
C1—C2—C3—C1ⁱ	−0.34 (18)	C5—C6—C11—C10	177.54 (11)
C1—C2—C3—C4	−178.81 (11)	C5—C6—C7—C8	−177.76 (12)
C1ⁱ—C3—C4—C5	172.08 (12)	C7—C6—C11—C10	−0.89 (18)
C2—C3—C4—C5	−9.4 (2)	C7—C6—C5—C4	170.84 (13)
C3ⁱ—C1—C2—C3	0.34 (19)	C12—O1—C1—C2	4.15 (17)
C3—C4—C5—C6	−179.01 (12)	C12—O1—C1—C3ⁱ	−176.23 (11)
C10—C9—C8—C7	0.7 (2)		

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