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(*E*)-Ethyl 4-[4-(diethylamino)styryl]-benzoate

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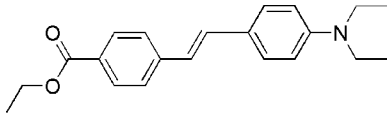
Key indicators: single-crystal X-ray study; T = 292 K; mean σ(C–C) = 0.005 Å; disorder in main residue; R factor = 0.044; wR factor = 0.112; data-to-parameter ratio = 7.8.

In the title molecule, $C_{21}H_{25}NO_2$, the dihedral angle between the two benzene rings is 4.8 (2)°. Both the ethyl group of the ester group and one of the ethyl groups attached to the N atom are disordered over two sites, the approximate occupancies being 66:34 and 81:19, respectively. In the cystal structure, there are no direction-specific interactions.

Related literature

For related literature, see: Boggess *et al.* (1986); Iwase *et al.* (2003); Marynaoff & Reitz (1989); Reinhardt *et al.* (1998). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{21}H_{25}NO_2$
M_r = 323.42
Orthorhombic, $Pna2_1$
a = 7.8689 (11) Å
b = 8.8441 (11) Å
c = 26.404 (3) Å
V = 1837.6 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.07 mm^{-1}
T = 292 (2) K
0.25 × 0.20 × 0.18 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: none
10027 measured reflections
2043 independent reflections
1118 reflections with $I > 2\sigma(I)$
R_{int} = 0.121

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.112
S = 0.88
2043 reflections
261 parameters
6 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 e Å^{-3}

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2575).

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(*E*)-Ethyl 4-[4-(diethylamino)styryl]benzoate

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S1. Comment

Two-photon absorption (TPA) of organic materials has attracted much attention because of its various applications in photonics (Iwase *et al.*, 2003). For these applications, it is important to prepare materials having a TPA cross-section at the wavelength of available laser sources (Reinhardt *et al.*,1998). We report here the structure of a new compound containing a TPA cross-section. The measurement of the TPA cross-section was performed by the nonlinear transmission method (Boggess *et al.*, 1986).

In the molecular structure, the two benzene rings are almost coplanar with a dihedral angle of only 4.8 (2)° between them (Fig.1). The bond lengths and angles in the molecule are as expected (Allen *et al.*, 1987).

In the crystal structure, no H-bonding, C—H···π, or π-π interactions are observed. The crystal is stablized only by van der Waals interactions.

S2. Experimental

All reagents and solvents were used as obtained without further purification. The title compound was prepared according to literature procedure (Marynaoff *et al.*, 1989). The solid product was dissolved in ether and the solution kept in air for one week. Crystals of of the title compound suitable for single-crystal X-ray diffraction analysis were grown by slow evaporation of the solution at the bottom of the vessel.

S3. Refinement

All H atoms were included in calculated positions with C—H = 0.93Å (aromatic and –CH=CH– moiety), 0.97Å (methylene), 0.96Å (methyl); U_{iso}(H)=1.2U_{eq}C (aromatic, –CH=CH–, methylene) and U_{iso}(H)=1.5U_{eq}C (methyl). Two ethyl groups (C16/C17/O2 & C20/C21/N1) are disordered over two sites and the corresponding N—C, C—C and O—C bond distances were refined by using the *SHELXL97* (Sheldrick, 1997) commands; *DFIX*, EADP and EXYZ with the ratios of the refined occupancies being 0.66 (1):0.34 (1) and 0.81 (1):0.19 (1) for the major and minor components, respectively. In the absence of significant anomalous dispersion effects Fridel pairs were merged.

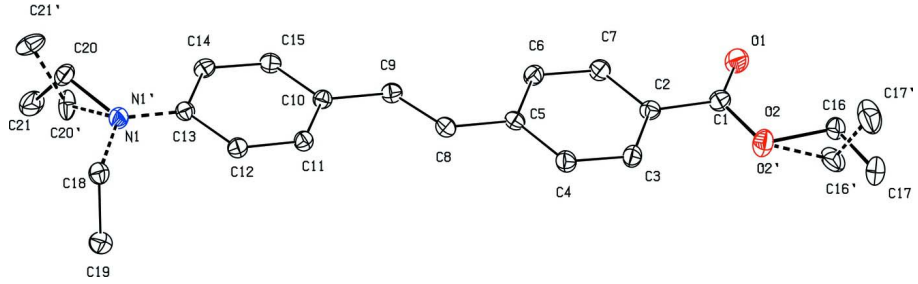

Figure 1

The molecular structure showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. The disorder is not shown.

(*E*)-Ethyl 4-[4-(diethylamino)styryl]benzoate

Crystal data

$C_{21}H_{25}NO_2$
$M_r = 323.42$
Orthorhombic, $Pna2_1$
Hall symbol: P 2c -2n
$a = 7.8689$ (11) Å
$b = 8.8441$ (11) Å
$c = 26.404$ (3) Å
$V = 1837.6$ (4) Å^3
$Z = 4$
$F(000) = 696$
$D_x = 1.169$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1356 reflections
$\theta = 2.6$–$26.4°$
$\mu = 0.07$ mm^{-1}
$T = 292$ K
Prism, orange
0.25 × 0.20 × 0.18 mm

Data collection

Bruker SMART CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
10027 measured reflections
2043 independent reflections
1118 reflections with $I > 2\sigma(I)$
$R_{int} = 0.121$
$\theta_{max} = 27.0°$, $\theta_{min} = 2.4°$
$h = -10 \rightarrow 8$
$k = -11 \rightarrow 9$
$l = -33 \rightarrow 33$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.044$
$wR(F^2) = 0.112$
$S = 0.88$
2043 reflections
261 parameters
6 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0476P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.15$ e Å^{-3}
$\Delta\rho_{min} = -0.14$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 1997), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0030 (12)

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 $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
C1	0.3128 (5)	−0.0493 (5)	0.53178 (16)	0.0725 (10)	
C2	0.4421 (5)	−0.0245 (4)	0.49197 (13)	0.0623 (9)	
C3	0.4259 (5)	0.0791 (4)	0.45313 (14)	0.0757 (10)	
H3	0.3282	0.1378	0.4508	0.091*	
C4	0.5536 (5)	0.0961 (4)	0.41782 (14)	0.0755 (11)	
H4	0.5395	0.1659	0.3918	0.091*	
C5	0.7031 (4)	0.0120 (4)	0.41986 (13)	0.0600 (8)	
C6	0.7157 (5)	−0.0933 (4)	0.45886 (14)	0.0700 (10)	
H6	0.8119	−0.1540	0.4611	0.084*	
C7	0.5887 (5)	−0.1088 (4)	0.49398 (14)	0.0716 (10)	
H7	0.6022	−0.1786	0.5200	0.086*	
C8	0.8356 (5)	0.0350 (4)	0.38217 (13)	0.0636 (9)	
H8	0.8129	0.1074	0.3575	0.076*	
C9	0.9833 (5)	−0.0335 (4)	0.37851 (14)	0.0652 (9)	
H9	1.0058	−0.1062	0.4031	0.078*	
C10	1.1164 (4)	−0.0102 (4)	0.34089 (13)	0.0576 (8)	
C11	1.1104 (4)	0.0989 (3)	0.30381 (14)	0.0613 (9)	
H11	1.0181	0.1646	0.3031	0.074*	
C12	1.2348 (4)	0.1150 (4)	0.26768 (13)	0.0639 (9)	
H12	1.2244	0.1901	0.2432	0.077*	
C13	1.3780 (4)	0.0193 (4)	0.26715 (13)	0.0598 (9)	
C14	1.3851 (5)	−0.0887 (4)	0.30509 (15)	0.0700 (9)	
H14	1.4784	−0.1531	0.3067	0.084*	
C15	1.2587 (5)	−0.1030 (4)	0.34012 (14)	0.0678 (9)	
H15	1.2683	−0.1782	0.3646	0.081*	
O2	0.1775 (4)	0.0376 (3)	0.52482 (12)	0.1001 (9)	0.663 (19)
C16	0.0545 (15)	0.0316 (14)	0.5682 (5)	0.076 (3)	0.663 (19)
H16A	−0.0044	−0.0648	0.5691	0.091*	0.663 (19)
H16B	0.1127	0.0462	0.6002	0.091*	0.663 (19)
C17	−0.0668 (12)	0.1578 (11)	0.5583 (5)	0.091 (4)	0.663 (19)
H17A	−0.0072	0.2524	0.5597	0.137*	0.663 (19)
H17B	−0.1548	0.1569	0.5835	0.137*	0.663 (19)
H17C	−0.1164	0.1453	0.5254	0.137*	0.663 (19)
O2′	0.1775 (4)	0.0376 (3)	0.52482 (12)	0.1001 (9)	0.337 (19)
C16′	0.009 (5)	0.025 (4)	0.5492 (11)	0.107 (10)	0.337 (19)

H16C	−0.0081	−0.0725	0.5651	0.128*	0.337 (19)
H16D	−0.0833	0.0452	0.5257	0.128*	0.337 (19)
C17′	0.029 (5)	0.149 (4)	0.5871 (11)	0.153 (12)	0.337 (19)
H17D	0.1412	0.1442	0.6015	0.230*	0.337 (19)
H17E	−0.0537	0.1371	0.6135	0.230*	0.337 (19)
H17F	0.0135	0.2448	0.5708	0.230*	0.337 (19)
C18	1.4744 (5)	0.1303 (4)	0.18598 (12)	0.0739 (10)	
H18A	1.5819	0.1448	0.1687	0.089*	
H18B	1.4349	0.2289	0.1970	0.089*	
C19	1.3479 (5)	0.0668 (5)	0.14881 (15)	0.0886 (11)	
H19A	1.3934	−0.0232	0.1337	0.133*	
H19B	1.3255	0.1403	0.1229	0.133*	
H19C	1.2441	0.0429	0.1662	0.133*	
N1	1.5034 (4)	0.0366 (3)	0.23066 (12)	0.0738 (9)	0.811 (11)
C20	1.6626 (7)	−0.0480 (8)	0.2327 (3)	0.0763 (19)	0.811 (11)
H20A	1.6920	−0.0665	0.2679	0.092*	0.811 (11)
H20B	1.7525	0.0126	0.2179	0.092*	0.811 (11)
C21	1.6527 (8)	−0.1943 (8)	0.2057 (3)	0.110 (2)	0.811 (11)
H21A	1.5812	−0.2625	0.2243	0.166*	0.811 (11)
H21B	1.7645	−0.2368	0.2027	0.166*	0.811 (11)
H21C	1.6059	−0.1785	0.1725	0.166*	0.811 (11)
N1′	1.5034 (4)	0.0366 (3)	0.23066 (12)	0.0738 (9)	0.189 (11)
C20′	1.599 (3)	−0.1001 (14)	0.2184 (12)	0.083 (10)	0.189 (11)
H20C	1.5948	−0.1209	0.1823	0.100*	0.189 (11)
H20D	1.5548	−0.1867	0.2366	0.100*	0.189 (11)
C21′	1.775 (4)	−0.065 (3)	0.2346 (19)	0.113 (19)	0.189 (11)
H21D	1.7960	0.0410	0.2307	0.170*	0.189 (11)
H21E	1.8538	−0.1212	0.2141	0.170*	0.189 (11)
H21F	1.7893	−0.0932	0.2695	0.170*	0.189 (11)
O1	0.3244 (3)	−0.1352 (3)	0.56591 (12)	0.0978 (9)	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.064 (3)	0.076 (2)	0.078 (3)	−0.010 (2)	−0.002 (2)	−0.003 (2)
C2	0.061 (2)	0.063 (2)	0.063 (2)	−0.0091 (17)	−0.0039 (18)	0.0026 (18)
C3	0.065 (3)	0.087 (2)	0.075 (3)	0.014 (2)	0.010 (2)	0.005 (2)
C4	0.081 (3)	0.081 (2)	0.065 (2)	0.0169 (19)	0.006 (2)	0.0128 (19)
C5	0.069 (2)	0.0576 (18)	0.053 (2)	−0.0048 (16)	−0.0036 (19)	−0.0054 (16)
C6	0.060 (2)	0.078 (2)	0.072 (2)	0.0067 (17)	0.001 (2)	0.009 (2)
C7	0.071 (3)	0.073 (2)	0.071 (2)	0.0006 (19)	0.002 (2)	0.0177 (18)
C8	0.072 (3)	0.0589 (19)	0.059 (2)	−0.0024 (18)	0.0006 (18)	0.0005 (16)
C9	0.067 (2)	0.062 (2)	0.066 (2)	−0.0011 (18)	−0.0025 (19)	0.0040 (18)
C10	0.059 (2)	0.057 (2)	0.057 (2)	0.0024 (16)	−0.0021 (18)	−0.0014 (16)
C11	0.065 (2)	0.056 (2)	0.063 (2)	0.0083 (16)	0.0024 (19)	0.0015 (18)
C12	0.068 (2)	0.059 (2)	0.065 (2)	0.0102 (16)	0.0009 (19)	0.0066 (17)
C13	0.061 (2)	0.0586 (19)	0.059 (2)	0.0038 (17)	−0.0026 (19)	−0.0067 (17)
C14	0.065 (2)	0.073 (2)	0.071 (2)	0.0174 (18)	−0.009 (2)	0.007 (2)

C15	0.074 (2)	0.066 (2)	0.063 (2)	0.0069 (18)	−0.003 (2)	0.0139 (18)
O2	0.080 (2)	0.109 (2)	0.111 (2)	0.0086 (16)	0.0270 (18)	0.0163 (19)
C16	0.066 (6)	0.091 (7)	0.071 (8)	−0.006 (4)	0.011 (5)	−0.001 (6)
C17	0.083 (6)	0.080 (5)	0.110 (7)	0.008 (4)	0.036 (5)	0.004 (4)
O2′	0.080 (2)	0.109 (2)	0.111 (2)	0.0086 (16)	0.0270 (18)	0.0163 (19)
C16′	0.11 (2)	0.145 (19)	0.070 (16)	−0.042 (15)	0.007 (11)	−0.034 (13)
C17′	0.15 (3)	0.18 (2)	0.13 (2)	−0.044 (19)	0.050 (18)	−0.067 (18)
C18	0.071 (2)	0.080 (2)	0.071 (2)	−0.0031 (18)	0.007 (2)	0.005 (2)
C19	0.088 (3)	0.100 (3)	0.078 (2)	0.000 (2)	−0.004 (2)	0.005 (2)
N1	0.070 (2)	0.082 (2)	0.0688 (19)	0.0183 (16)	0.0061 (17)	0.0071 (17)
C20	0.050 (5)	0.090 (5)	0.090 (4)	0.003 (3)	0.002 (3)	0.002 (3)
C21	0.092 (4)	0.113 (5)	0.126 (5)	0.035 (4)	−0.013 (4)	−0.026 (4)
N1′	0.070 (2)	0.082 (2)	0.0688 (19)	0.0183 (16)	0.0061 (17)	0.0071 (17)
C20′	0.071 (17)	0.062 (19)	0.12 (2)	−0.031 (12)	0.046 (17)	−0.037 (13)
C21′	0.067 (19)	0.09 (2)	0.13 (6)	−0.012 (17)	−0.03 (3)	0.06 (2)
O1	0.079 (2)	0.120 (2)	0.095 (2)	−0.0136 (15)	0.0086 (16)	0.0296 (19)

Geometric parameters (Å, º)

C1—O1	1.182 (4)	C16—H16A	0.9700
C1—O2	1.326 (4)	C16—H16B	0.9700
C1—C2	1.479 (5)	C17—H17A	0.9600
C2—C7	1.374 (5)	C17—H17B	0.9600
C2—C3	1.381 (5)	C17—H17C	0.9600
C3—C4	1.379 (5)	C16′—C17′	1.492 (8)
C3—H3	0.9300	C16′—H16C	0.9700
C4—C5	1.393 (5)	C16′—H16D	0.9700
C4—H4	0.9300	C17′—H17D	0.9600
C5—C6	1.392 (5)	C17′—H17E	0.9600
C5—C8	1.456 (4)	C17′—H17F	0.9600
C6—C7	1.370 (5)	C18—N1	1.460 (3)
C6—H6	0.9300	C18—C19	1.506 (5)
C7—H7	0.9300	C18—H18A	0.9700
C8—C9	1.314 (4)	C18—H18B	0.9700
C8—H8	0.9300	C19—H19A	0.9600
C9—C10	1.458 (5)	C19—H19B	0.9600
C9—H9	0.9300	C19—H19C	0.9600
C10—C11	1.376 (4)	N1—C20	1.460 (4)
C10—C15	1.389 (5)	C20—C21	1.480 (7)
C11—C12	1.374 (4)	C20—H20A	0.9700
C11—H11	0.9300	C20—H20B	0.9700
C12—C13	1.409 (4)	C21—H21A	0.9600
C12—H12	0.9300	C21—H21B	0.9600
C13—C14	1.386 (5)	C21—H21C	0.9600
C13—N1	1.388 (4)	C20′—C21′	1.481 (7)
C14—C15	1.364 (5)	C20′—H20C	0.9700
C14—H14	0.9300	C20′—H20D	0.9700
C15—H15	0.9300	C21′—H21D	0.9600

O2—C16	1.502 (14)	C21′—H21E	0.9600
C16—C17	1.492 (8)	C21′—H21F	0.9600
O1—C1—O2	122.7 (4)	C17—C16—O2	104.6 (8)
O1—C1—C2	125.7 (4)	C17—C16—H16A	110.8
O2—C1—C2	111.6 (4)	O2—C16—H16A	110.8
C7—C2—C3	117.8 (3)	C17—C16—H16B	110.8
C7—C2—C1	118.0 (3)	O2—C16—H16B	110.8
C3—C2—C1	124.2 (4)	H16A—C16—H16B	108.9
C4—C3—C2	120.5 (3)	C17′—C16′—H16C	112.1
C4—C3—H3	119.8	C17′—C16′—H16D	112.2
C2—C3—H3	119.8	H16C—C16′—H16D	109.8
C3—C4—C5	122.1 (3)	C16′—C17′—H17D	109.5
C3—C4—H4	119.0	C16′—C17′—H17E	109.5
C5—C4—H4	119.0	H17D—C17′—H17E	109.5
C6—C5—C4	116.5 (3)	C16′—C17′—H17F	109.5
C6—C5—C8	123.3 (3)	H17D—C17′—H17F	109.5
C4—C5—C8	120.3 (3)	H17E—C17′—H17F	109.5
C7—C6—C5	121.1 (3)	N1—C18—C19	114.7 (3)
C7—C6—H6	119.5	N1—C18—H18A	108.6
C5—C6—H6	119.5	C19—C18—H18A	108.6
C6—C7—C2	122.1 (3)	N1—C18—H18B	108.6
C6—C7—H7	118.9	C19—C18—H18B	108.6
C2—C7—H7	118.9	H18A—C18—H18B	107.6
C9—C8—C5	128.2 (3)	C18—C19—H19A	109.5
C9—C8—H8	115.9	C18—C19—H19B	109.5
C5—C8—H8	115.9	H19A—C19—H19B	109.5
C8—C9—C10	128.3 (3)	C18—C19—H19C	109.5
C8—C9—H9	115.8	H19A—C19—H19C	109.5
C10—C9—H9	115.8	H19B—C19—H19C	109.5
C11—C10—C15	115.6 (3)	C13—N1—C18	120.8 (3)
C11—C10—C9	124.0 (3)	C13—N1—C20	121.9 (3)
C15—C10—C9	120.4 (3)	C18—N1—C20	117.1 (4)
C12—C11—C10	122.8 (3)	N1—C20—C21	112.6 (6)
C12—C11—H11	118.6	N1—C20—H20A	109.1
C10—C11—H11	118.6	C21—C20—H20A	109.1
C11—C12—C13	120.9 (3)	N1—C20—H20B	109.1
C11—C12—H12	119.5	C21—C20—H20B	109.1
C13—C12—H12	119.5	H20A—C20—H20B	107.8
C14—C13—N1	123.3 (3)	C21′—C20′—H20C	110.9
C14—C13—C12	116.1 (3)	C21′—C20′—H20D	110.9
N1—C13—C12	120.6 (3)	H20C—C20′—H20D	108.9
C15—C14—C13	121.6 (3)	C20′—C21′—H21D	109.5
C15—C14—H14	119.2	C20′—C21′—H21E	109.5
C13—C14—H14	119.2	H21D—C21′—H21E	109.5
C14—C15—C10	122.9 (3)	C20′—C21′—H21F	109.5
C14—C15—H15	118.5	H21D—C21′—H21F	109.5
C10—C15—H15	118.5	H21E—C21′—H21F	109.5

C1—O2—C16	113.1 (4)		
O1—C1—C2—C7	0.6 (5)	C9—C10—C11—C12	−177.6 (3)
O2—C1—C2—C7	−179.1 (3)	C10—C11—C12—C13	−0.5 (5)
O1—C1—C2—C3	−178.6 (4)	C11—C12—C13—C14	−0.6 (5)
O2—C1—C2—C3	1.6 (5)	C11—C12—C13—N1	−179.8 (3)
C7—C2—C3—C4	0.0 (5)	N1—C13—C14—C15	−179.6 (3)
C1—C2—C3—C4	179.3 (3)	C12—C13—C14—C15	1.3 (5)
C2—C3—C4—C5	−0.6 (6)	C13—C14—C15—C10	−1.0 (6)
C3—C4—C5—C6	1.5 (5)	C11—C10—C15—C14	−0.2 (5)
C3—C4—C5—C8	−179.2 (3)	C9—C10—C15—C14	178.4 (3)
C4—C5—C6—C7	−1.9 (5)	O1—C1—O2—C16	8.3 (8)
C8—C5—C6—C7	178.8 (3)	C2—C1—O2—C16	−172.0 (7)
C5—C6—C7—C2	1.4 (5)	C1—O2—C16—C17	168.7 (10)
C3—C2—C7—C6	−0.5 (5)	C14—C13—N1—C18	167.6 (3)
C1—C2—C7—C6	−179.8 (3)	C12—C13—N1—C18	−13.4 (5)
C6—C5—C8—C9	−0.9 (5)	C14—C13—N1—C20	−6.7 (6)
C4—C5—C8—C9	179.8 (3)	C12—C13—N1—C20	172.3 (5)
C5—C8—C9—C10	−179.8 (3)	C19—C18—N1—C13	−69.5 (4)
C8—C9—C10—C11	4.4 (5)	C19—C18—N1—C20	105.0 (5)
C8—C9—C10—C15	−174.1 (3)	C13—N1—C20—C21	89.9 (6)
C15—C10—C11—C12	0.9 (5)	C18—N1—C20—C21	−84.6 (6)