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1-Naphthaleneacetic acid–piperidine (2/1)

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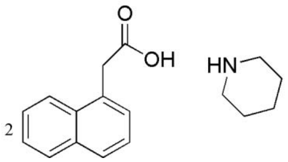
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.006 Å; R factor = 0.064; wR factor = 0.137; data-to-parameter ratio = 14.7.

The asymmetric unit of the title compound, $2C_{12}H_{10}O_2 \cdot C_5H_{11}N$, contains two naphthaleneacetic acid molecules and one piperidine molecule, which are held together by intermolecular O—H⋯O and O—H⋯N hydrogen bonds. The piperidine ring has a chair conformation. In the crystal structure, intermolecular N—H⋯O hydrogen bonds link the molecules into dimers.

Related literature

For general background, see: Prasad & Williams (1991); Pal *et al.* (2003); Anwar *et al.* (2000); Muthuraman *et al.* (2001); Kotler *et al.* (1992); Wang *et al.* (2006); Brasselet *et al.* (1999); Rodrigues *et al.* (2001); Goswami *et al.* (1999); Cremer & Pople (1975). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$2C_{12}H_{10}O_2 \cdot C_5H_{11}N$
M_r = 457.55
Monoclinic, $P2_1/n$
a = 9.7415 (16) Å
b = 19.174 (3) Å
c = 13.6232 (19) Å
β = 105.757 (11)°
V = 2449.0 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 295 (2) K
0.4 × 0.3 × 0.2 mm

Data collection

Bruker P4 diffractometer
Absorption correction: none
5745 measured reflections
4550 independent reflections
2552 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.034
3 standard reflections
every 97 reflections
intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.064
$wR(F^2)$ = 0.137
S = 1.05
4550 reflections
309 parameters
H-atom parameters constrained
$\Delta\rho_{\rm max}$ = 0.56 e Å^{-3}
$\Delta\rho_{\rm min}$ = −0.27 e Å^{-3}

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

D—H⋯*A*	*D*—H	H⋯*A*	*D*⋯*A*	*D*—H⋯*A*
N1—H1*A*⋯O1$^{\rm i}$	0.90	1.85	2.736 (3)	168
O2—H2*B*⋯N1	0.82	1.94	2.759 (3)	175
O4—H4*B*⋯O2	0.82	1.77	2.578 (3)	166

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

Data collection: *XSCANS* (Bruker, 1997*a*); cell refinement: *XSCANS*; data reduction: *XSCANS*; program(s) used to solve structure: *SHELXTL* (Bruker, 1997*b*); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2300).

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supplementary materials

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1-Naphthaleneacetic acid-piperidine (2/1)

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Comment

Numerous highly efficient nonlinear optical (NLO) crystals for visible and ultraviolet (UV) regions have been synthesized and studied. They attract considerable attention due to their extreme importance for both laser spectroscopy and laser processing (Prasad & Williams, 1991; Pal *et al.*, 2003). In recent years, many new non-linear optical second harmonic generation (SHG) materials of organic adduct were reported, which have main merits. The main advantage of organic adduct materials compared with inorganic materials for such second-harmonic generation devices are the large macroscopic second-order nonlinear optical susceptibilities, ultrafast optical response time and high optical damage thresholds (Anwar *et al.*, 2000; Muthuraman *et al.*, 2001; Kotler *et al.*, 1992; Wang *et al.*, 2006). At present, adduct assembly is a hot point in designing solid state structures with outstanding conductance, electronic, nonlinear optical or magnetic properties (Brasselet *et al.*, 1999; Rodrigues *et al.*, 2001; Goswami *et al.*, 1999). We report herein the synthesis and structure of a new organic adduct of 1-naphthalene-acetic acid and piperidine.

The asymmetric unit of the title compound, (I), contains two naphthalene-acetic acid and one piperidine moieties (Fig. 1), in which they are held together by intramolecular O—H···O and O—H···N hydrogen bonds (Table 1). The bond lengths and angles are generally within normal ranges (Allen *et al.*, 1987). The two oxygen atoms of each carboxyl groups are conjugated [O1—C12 =1.237 (3) Å, O2—C12 = 1.268 (4) Å and O3—C24 = 1.196 (3) Å, O4—C24 1.322 (4) Å].

Rings A (C1—C10) and B (C13—C22) are, of course, planar and the dihedral angle between them is A/B = 14.20 (2)°. Ring C (N1/C25—C29) is not planar, having total puckering amplitude, Q_T, of 0.568 (3) Å, and chair conformation [φ = 1.36 (3)° and θ = 1.39 (3)°] (Cremer & Pople, 1975).

In the crystal structure, intermolecular N—H···O hydrogen bonds (Table 1) link the molecules into dimers (Fig. 2), in which they seem to be effective in the stabilization of the structure.

Experimental

The title compound was synthesized by the reaction of 1-naphthalene-acetic acid (1.86 g, 10 mmol) with excessive piperidine (7.1 g, 100 mmol), they were put in a flask, equipped with a magnetic stirrer bar, and the reaction mixture was subjected to microwave irradiation for 10 min under 400 W, then piperidine was refluxed. The reaction flask was allowed to cool to room temperature and the colorless crystals were obtained. They were recrystallized from methanol (yield; 80%, m.p. 417–419 K).

Refinement

H atoms were positioned geometrically with O—H = 0.82 Å (for OH), N—H = 0.90 Å (for NH), C—H = 0.93 and 0.97 Å for aromatic and methylene atoms, respectively, and constrained to ride on their parent atoms, with $U_{iso}(H) = 1.2U_{eq}(C,N,O)$.

Figures

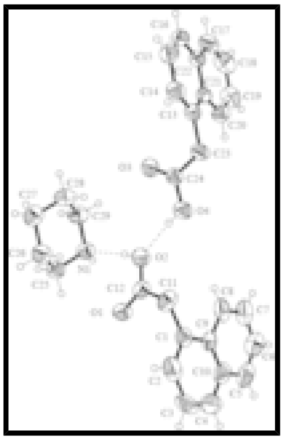

Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 35% probability level. Hydrogen bonds are shown as dashed lines.

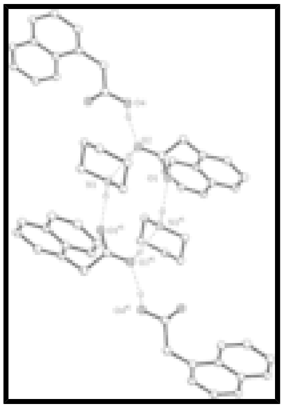

Fig. 2. A partial packing diagram of (I). Hydrogen bonds are shown as dashed lines [symmetry code (#1): $2 - x$, $1 - y$, $1 - z$].

1-Naphthaleneacetic acid–piperidine (2/1)

Crystal data

$2C_{12}H_{10}O_2\cdot C_5H_{11}N$	$F_{000} = 976$
$M_r = 457.55$	$D_x = 1.241$ Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -P 2yn	Cell parameters from 43 reflections
$a = 9.7415$ (16) Å	$\theta = 3.1$–13.2°
$b = 19.174$ (3) Å	$\mu = 0.08$ mm^{-1}
$c = 13.6232$ (19) Å	$T = 295$ (2) K
$\beta = 105.757$ (11)°	Plate, colorless
$V = 2449.0$ (7) Å^3	0.4 × 0.3 × 0.2 mm
$Z = 4$	

Data collection

Bruker P4 diffractometer	$R_{\text{int}} = 0.034$

Radiation source: fine-focus sealed tube	$\theta_{\max} = 25.5°$
Monochromator: graphite	$\theta_{\min} = 1.9°$
$T = 295(2)$ K	$h = -1 \rightarrow 11$
ω scans	$k = -1 \rightarrow 23$
Absorption correction: none	$l = -16 \rightarrow 16$
5745 measured reflections	3 standard reflections
4550 independent reflections	every 97 reflections
2552 reflections with $I > 2\sigma(I)$	intensity decay: none

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.064$	H-atom parameters constrained
$wR(F^2) = 0.137$	$w = 1/[\sigma^2(F_o^2) + (0.001P)^2 + 2P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.05$	$(\Delta/\sigma)_{\max} < 0.001$
4550 reflections	$\Delta\rho_{\max} = 0.56$ e Å^{-3}
309 parameters	$\Delta\rho_{\min} = -0.27$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

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

	x	y	z	U_{iso}*/U_{eq}
O1	0.8603 (2)	0.55184 (12)	0.57310 (17)	0.0701 (6)
O2	0.6931 (2)	0.52314 (13)	0.43362 (19)	0.0784 (7)
H2B	0.7446	0.4890	0.4362	0.094*
O3	0.4475 (2)	0.44149 (12)	0.23853 (17)	0.0738 (6)
O4	0.4474 (2)	0.54627 (13)	0.30738 (19)	0.0825 (7)
H4B	0.5274	0.5344	0.3405	0.099*
N1	0.8800 (3)	0.41263 (14)	0.4533 (2)	0.0651 (7)
H1A	0.9587	0.4285	0.4381	0.078*
C1	0.7313 (3)	0.68434 (17)	0.5729 (3)	0.0648 (8)
C2	0.7634 (5)	0.7012 (2)	0.6751 (3)	0.1009 (15)

H2A	0.7263	0.6742	0.7185	0.121*
C3	0.8531 (6)	0.7598 (3)	0.7158 (3)	0.123 (2)
H3A	0.8731	0.7714	0.7845	0.148*
C4	0.9082 (6)	0.7981 (3)	0.6505 (5)	0.123 (2)
H4A	0.9682	0.8354	0.6763	0.148*
C5	0.9406 (5)	0.8249 (2)	0.4817 (5)	0.1051 (15)
H5A	1.0026	0.8618	0.5057	0.126*
C6	0.9017 (5)	0.8058 (3)	0.3821 (5)	0.1069 (15)
H6A	0.9412	0.8306	0.3378	0.128*
C7	0.8084 (5)	0.7527 (2)	0.3411 (4)	0.1053 (15)
H7A	0.7826	0.7441	0.2712	0.126*
C8	0.7559 (4)	0.7137 (2)	0.4036 (3)	0.0854 (12)
H8A	0.6958	0.6767	0.3768	0.102*
C9	0.7899 (3)	0.72764 (17)	0.5117 (3)	0.0631 (8)
C10	0.8784 (4)	0.7834 (2)	0.5487 (4)	0.0867 (12)
C11	0.6487 (3)	0.62008 (17)	0.5313 (3)	0.0742 (10)
H11A	0.5782	0.6317	0.4682	0.089*
H11B	0.5982	0.6040	0.5794	0.089*
C12	0.7427 (3)	0.56126 (17)	0.5112 (3)	0.0601 (8)
C13	0.1607 (3)	0.46038 (16)	0.1131 (2)	0.0583 (8)
C14	0.0605 (3)	0.41947 (19)	0.1382 (3)	0.0704 (9)
H14A	0.0440	0.4250	0.2019	0.084*
C15	−0.0180 (4)	0.36970 (19)	0.0714 (3)	0.0799 (11)
H15A	−0.0850	0.3427	0.0913	0.096*
C16	0.0026 (4)	0.36042 (18)	−0.0217 (3)	0.0747 (10)
H16A	−0.0499	0.3269	−0.0655	0.090*
C17	0.1252 (4)	0.3946 (2)	−0.1509 (3)	0.0835 (11)
H17A	0.0730	0.3615	−0.1957	0.100*
C18	0.2196 (5)	0.4348 (3)	−0.1812 (3)	0.0993 (14)
H18A	0.2317	0.4295	−0.2462	0.119*
C19	0.2995 (4)	0.4847 (2)	−0.1145 (3)	0.0895 (12)
H19A	0.3644	0.5125	−0.1356	0.107*
C20	0.2828 (4)	0.49275 (19)	−0.0192 (3)	0.0715 (9)
H20A	0.3372	0.5258	0.0245	0.086*
C21	0.1844 (3)	0.45178 (16)	0.0143 (2)	0.0556 (7)
C22	0.1035 (3)	0.40139 (17)	−0.0530 (3)	0.0636 (8)
C23	0.2388 (3)	0.51424 (18)	0.1867 (2)	0.0663 (9)
H23A	0.1846	0.5238	0.2353	0.080*
H23B	0.2422	0.5570	0.1494	0.080*
C24	0.3882 (3)	0.49526 (17)	0.2449 (2)	0.0568 (7)
C25	0.9207 (4)	0.38701 (19)	0.5601 (3)	0.0777 (10)
H25A	0.9607	0.4251	0.6059	0.093*
H25B	0.9930	0.3511	0.5679	0.093*
C26	0.7930 (4)	0.3579 (2)	0.5876 (3)	0.0845 (11)
H26A	0.7247	0.3949	0.5860	0.101*
H26B	0.8222	0.3393	0.6564	0.101*
C27	0.7229 (4)	0.3007 (2)	0.5146 (3)	0.0856 (11)
H27A	0.7870	0.2612	0.5220	0.103*
H27B	0.6367	0.2854	0.5308	0.103*

C28	0.6867 (4)	0.3268 (2)	0.4067 (3)	0.0817 (11)
H28A	0.6139	0.3626	0.3976	0.098*
H28B	0.6478	0.2887	0.3606	0.098*
C29	0.8154 (4)	0.35637 (19)	0.3797 (3)	0.0786 (10)
H29A	0.8849	0.3197	0.3821	0.094*
H29B	0.7872	0.3751	0.3110	0.094*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0458 (12)	0.0723 (15)	0.0858 (16)	0.0051 (11)	0.0072 (11)	−0.0115 (12)
O2	0.0636 (15)	0.0706 (16)	0.0902 (17)	0.0176 (12)	0.0026 (13)	−0.0111 (14)
O3	0.0680 (14)	0.0683 (15)	0.0795 (16)	0.0157 (12)	0.0107 (12)	−0.0041 (12)
O4	0.0659 (15)	0.0759 (16)	0.0880 (17)	0.0128 (13)	−0.0095 (13)	−0.0141 (14)
N1	0.0507 (15)	0.0678 (17)	0.0759 (18)	−0.0024 (13)	0.0154 (13)	−0.0070 (15)
C1	0.063 (2)	0.061 (2)	0.070 (2)	0.0162 (16)	0.0173 (17)	0.0018 (17)
C2	0.138 (4)	0.101 (3)	0.067 (3)	0.054 (3)	0.033 (3)	0.011 (2)
C3	0.161 (5)	0.129 (5)	0.054 (3)	0.063 (4)	−0.014 (3)	−0.032 (3)
C4	0.122 (4)	0.094 (4)	0.122 (4)	0.048 (3)	−0.022 (4)	−0.032 (3)
C5	0.088 (3)	0.062 (3)	0.164 (5)	0.018 (2)	0.032 (3)	0.019 (3)
C6	0.101 (4)	0.085 (3)	0.141 (5)	0.008 (3)	0.044 (3)	0.015 (3)
C7	0.129 (4)	0.093 (3)	0.103 (3)	0.034 (3)	0.048 (3)	0.031 (3)
C8	0.105 (3)	0.083 (3)	0.076 (3)	0.039 (2)	0.039 (2)	0.022 (2)
C9	0.0586 (19)	0.055 (2)	0.076 (2)	0.0179 (16)	0.0189 (17)	0.0119 (17)
C10	0.068 (2)	0.060 (2)	0.122 (4)	0.0175 (19)	0.009 (2)	0.003 (2)
C11	0.0539 (19)	0.068 (2)	0.106 (3)	0.0099 (17)	0.0300 (19)	0.003 (2)
C12	0.0462 (18)	0.0548 (19)	0.081 (2)	0.0000 (15)	0.0196 (17)	−0.0013 (17)
C13	0.0489 (17)	0.0574 (18)	0.0630 (19)	0.0078 (15)	0.0055 (15)	0.0010 (15)
C14	0.061 (2)	0.079 (2)	0.071 (2)	0.0017 (19)	0.0173 (17)	0.0084 (19)
C15	0.061 (2)	0.072 (2)	0.102 (3)	−0.0088 (19)	0.015 (2)	0.015 (2)
C16	0.059 (2)	0.060 (2)	0.091 (3)	−0.0033 (17)	−0.0026 (19)	−0.005 (2)
C17	0.078 (3)	0.091 (3)	0.073 (3)	0.011 (2)	0.005 (2)	−0.018 (2)
C18	0.095 (3)	0.138 (4)	0.068 (3)	0.023 (3)	0.028 (2)	−0.003 (3)
C19	0.077 (3)	0.109 (3)	0.089 (3)	0.007 (2)	0.033 (2)	0.016 (3)
C20	0.063 (2)	0.076 (2)	0.073 (2)	−0.0056 (18)	0.0153 (18)	0.0029 (19)
C21	0.0485 (17)	0.0523 (17)	0.0614 (19)	0.0034 (14)	0.0073 (14)	0.0002 (15)
C22	0.0572 (19)	0.060 (2)	0.066 (2)	0.0059 (16)	0.0038 (16)	−0.0040 (16)
C23	0.0571 (19)	0.072 (2)	0.0639 (19)	0.0090 (17)	0.0069 (16)	−0.0058 (17)
C24	0.0563 (18)	0.0602 (19)	0.0531 (18)	0.0007 (16)	0.0134 (15)	0.0040 (15)
C25	0.065 (2)	0.074 (2)	0.083 (3)	0.0026 (19)	0.0019 (19)	−0.005 (2)
C26	0.088 (3)	0.087 (3)	0.078 (2)	−0.004 (2)	0.020 (2)	−0.003 (2)
C27	0.079 (3)	0.076 (3)	0.105 (3)	−0.006 (2)	0.030 (2)	−0.002 (2)
C28	0.066 (2)	0.094 (3)	0.085 (3)	−0.013 (2)	0.0201 (19)	−0.024 (2)
C29	0.062 (2)	0.088 (3)	0.088 (3)	−0.0053 (19)	0.0233 (19)	−0.021 (2)

Geometric parameters (Å, °)

O1—C12	1.237 (3)	C14—C15	1.394 (5)
O2—C12	1.268 (4)	C14—H14A	0.9300

O2—H2B	0.8200	C15—C16	1.349 (5)
O3—C24	1.196 (3)	C15—H15A	0.9300
O4—C24	1.322 (4)	C16—C22	1.411 (5)
O4—H4B	0.8200	C16—H16A	0.9300
N1—C25	1.484 (4)	C17—C18	1.348 (5)
N1—C29	1.491 (4)	C17—C22	1.413 (5)
N1—H1A	0.9001	C17—H17A	0.9300
C1—C2	1.381 (5)	C18—C19	1.401 (6)
C1—C9	1.403 (4)	C18—H18A	0.9300
C1—C11	1.496 (5)	C19—C20	1.361 (5)
C2—C3	1.438 (7)	C19—H19A	0.9300
C2—H2A	0.9300	C20—C21	1.408 (4)
C3—C4	1.371 (7)	C20—H20A	0.9300
C3—H3A	0.9300	C21—C22	1.415 (4)
C4—C10	1.366 (6)	C23—C24	1.500 (4)
C4—H4A	0.9300	C23—H23A	0.9700
C5—C6	1.357 (6)	C23—H23B	0.9700
C5—C10	1.460 (6)	C25—C26	1.501 (5)
C5—H5A	0.9300	C25—H25A	0.9700
C6—C7	1.378 (6)	C25—H25B	0.9700
C6—H6A	0.9300	C26—C27	1.511 (5)
C7—C8	1.335 (5)	C26—H26A	0.9700
C7—H7A	0.9300	C26—H26B	0.9700
C8—C9	1.444 (5)	C27—C28	1.502 (5)
C8—H8A	0.9300	C27—H27A	0.9700
C9—C10	1.381 (5)	C27—H27B	0.9700
C11—C12	1.524 (4)	C28—C29	1.510 (4)
C11—H11A	0.9700	C28—H28A	0.9700
C11—H11B	0.9700	C28—H28B	0.9700
C13—C14	1.367 (4)	C29—H29A	0.9700
C13—C21	1.436 (4)	C29—H29B	0.9700
C13—C23	1.496 (4)		
C12—O2—H2B	109.5	C18—C17—H17A	119.2
C24—O4—H4B	109.5	C22—C17—H17A	119.2
C25—N1—C29	111.8 (3)	C17—C18—C19	119.9 (4)
C25—N1—H1A	108.6	C17—C18—H18A	120.1
C29—N1—H1A	108.7	C19—C18—H18A	120.1
C2—C1—C9	116.3 (4)	C20—C19—C18	120.4 (4)
C2—C1—C11	121.7 (4)	C20—C19—H19A	119.8
C9—C1—C11	121.8 (3)	C18—C19—H19A	119.8
C1—C2—C3	121.3 (4)	C19—C20—C21	121.0 (4)
C1—C2—H2A	119.4	C19—C20—H20A	119.5
C3—C2—H2A	119.4	C21—C20—H20A	119.5
C4—C3—C2	118.1 (4)	C20—C21—C22	118.7 (3)
C4—C3—H3A	120.9	C20—C21—C13	122.5 (3)
C2—C3—H3A	120.9	C22—C21—C13	118.8 (3)
C10—C4—C3	122.4 (5)	C16—C22—C17	121.9 (3)
C10—C4—H4A	118.8	C16—C22—C21	119.7 (3)
C3—C4—H4A	118.8	C17—C22—C21	118.4 (3)

C6—C5—C10	115.3 (5)
C6—C5—H5A	122.3
C10—C5—H5A	122.3
C5—C6—C7	125.4 (5)
C5—C6—H6A	117.3
C7—C6—H6A	117.3
C8—C7—C6	118.6 (5)
C8—C7—H7A	120.7
C6—C7—H7A	120.7
C7—C8—C9	121.7 (4)
C7—C8—H8A	119.1
C9—C8—H8A	119.1
C10—C9—C1	123.8 (4)
C10—C9—C8	117.6 (4)
C1—C9—C8	118.6 (3)
C4—C10—C9	118.0 (5)
C4—C10—C5	120.8 (5)
C9—C10—C5	121.2 (4)
C1—C11—C12	112.9 (3)
C1—C11—H11A	109.0
C12—C11—H11A	109.0
C1—C11—H11B	109.0
C12—C11—H11B	109.0
H11A—C11—H11B	107.8
O1—C12—O2	123.8 (3)
O1—C12—C11	118.4 (3)
O2—C12—C11	117.7 (3)
C14—C13—C21	118.5 (3)
C14—C13—C23	119.7 (3)
C21—C13—C23	121.7 (3)
C13—C14—C15	122.1 (3)
C13—C14—H14A	118.9
C15—C14—H14A	118.9
C16—C15—C14	120.6 (3)
C16—C15—H15A	119.7
C14—C15—H15A	119.7
C15—C16—C22	120.2 (3)
C15—C16—H16A	119.9
C22—C16—H16A	119.9
C18—C17—C22	121.7 (4)
C13—C23—C24	115.5 (3)
C13—C23—H23A	108.4
C24—C23—H23A	108.4
C13—C23—H23B	108.4
C24—C23—H23B	108.4
H23A—C23—H23B	107.5
O3—C24—O4	123.3 (3)
O3—C24—C23	126.1 (3)
O4—C24—C23	110.6 (3)
N1—C25—C26	110.4 (3)
N1—C25—H25A	109.6
C26—C25—H25A	109.6
N1—C25—H25B	109.6
C26—C25—H25B	109.6
H25A—C25—H25B	108.1
C25—C26—C27	111.3 (3)
C25—C26—H26A	109.4
C27—C26—H26A	109.4
C25—C26—H26B	109.4
C27—C26—H26B	109.4
H26A—C26—H26B	108.0
C28—C27—C26	110.3 (3)
C28—C27—H27A	109.6
C26—C27—H27A	109.6
C28—C27—H27B	109.6
C26—C27—H27B	109.6
H27A—C27—H27B	108.1
C27—C28—C29	111.9 (3)
C27—C28—H28A	109.2
C29—C28—H28A	109.2
C27—C28—H28B	109.2
C29—C28—H28B	109.2
H28A—C28—H28B	107.9
N1—C29—C28	109.6 (3)
N1—C29—H29A	109.8
C28—C29—H29A	109.8
N1—C29—H29B	109.8
C28—C29—H29B	109.8
H29A—C29—H29B	108.2

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1A···O1^{i}	0.90	1.85	2.736 (3)	168
O2—H2B···N1	0.82	1.94	2.759 (3)	175
O4—H4B···O2	0.82	1.77	2.578 (3)	166

Symmetry codes: (i) $-x+2$, $-y+1$, $-z+1$.

Fig. 1

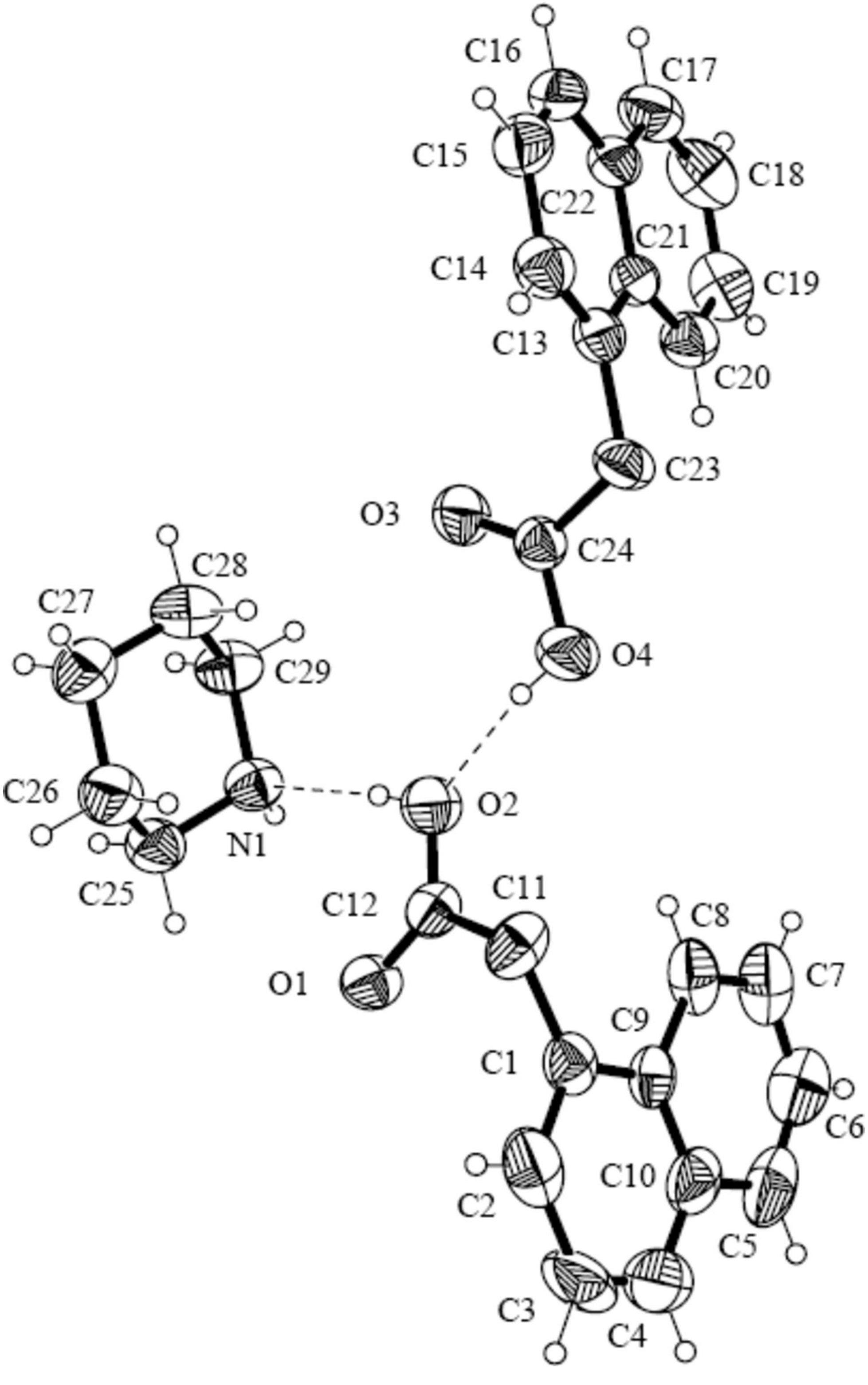
C16
C17
C15
C18
C22
C21
C14
C19
C13
C20
C23
O3
C24
C28
C27
C29
O4
C26
O2
N1
C25
C12
C11
C8
C7
O1
C9
C1
C6
C10
C2
C5
C3
C4

Fig. 2