

*N*-Phthaloyl-DL-alanineKraig A. Wheeler,<sup>a\*</sup>  
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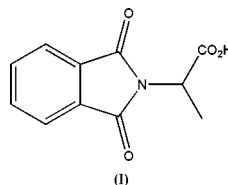
## Key indicators

Single-crystal X-ray study  
*T* = 93 K  
Mean  $\sigma$ (C–C) = 0.002 Å  
*R* factor = 0.036  
*wR* factor = 0.096  
Data-to-parameter ratio = 16.6For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

In the title compound [systematic name: DL-2-(1,3-dioxoisoindolin-2-yl)propanoic acid], C<sub>11</sub>H<sub>9</sub>NO<sub>4</sub>, the propanoic acid and planar phthaloyl moieties adopt a staggered conformation. Molecules crystallize as centrosymmetric dimers linked by carboxyl O–H···O hydrogen bonds [O···O = 2.6005 (12) Å and O–H···O = 174.8 (15)°].

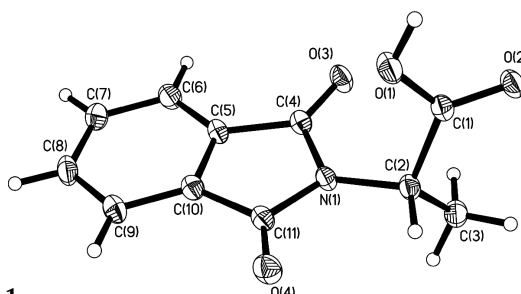
## Comment

By co-crystallizing two chemically unique compounds that are isosteric and opposite in handedness, we have recently been able to show the influence of molecular topology on the construction of molecular assemblies (Fomulu *et al.*, 2002*a,b*; Hendi *et al.*, 2001, 2004). These studies provided an opportunity to investigate systematically the isosteric relationship of several combinations of functional groups, such as Cl/NO<sub>2</sub>, O/NH, CH<sub>3</sub>/NO<sub>2</sub> and Cl/Br. In addition to functional group topologies, we have also considered the role of chemical frameworks and suggested several structural criteria to aid the formation of the observed bimolecular systems.



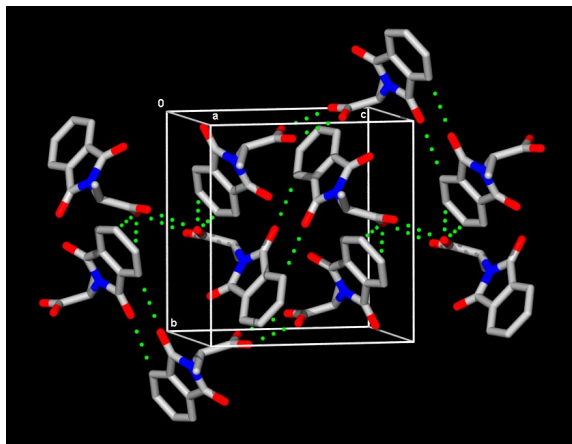
We report here the crystal structure of *N*-phthaloyl-DL-alanine, (I), as part of our effort to explore and develop new synthetically accessible molecular frameworks for future topological studies. The molecular conformation of (I), as observed in the crystal structure, is shown in Fig. 1. The planar phthaloyl moiety bisects the propanoic acid group to produce a staggered arrangement [C1–C2–N1–C4 = 58.1 (1)°]. Selected geometric parameters are given in Table 1.

Inspection of the crystal structure reveals molecules linked by carboxyl O1–H···O2<sup>i</sup> contacts to form the expected centrosymmetric hydrogen-bonded assemblies (Fig. 2 and Table 2). An interesting feature of this structure is the lack of



**Figure 1**  
The molecular structure of (I), showing the atom-labeling scheme and displacement ellipsoids at the 50% probability level.

Received 1 July 2004  
Accepted 6 July 2004  
Online 24 July 2004



**Figure 2**  
View of the molecular packing of (I) approximately down the *a* axis, showing the hydrogen-bond network. Hydrogen bonds are shown as dotted lines and H atoms have been omitted for clarity.

additional prominent non-bonded contacts. The absence of face-to-face  $\pi$ - $\pi$  stacking interactions and edge-to-face aromatic C-H $\cdots\pi$  interactions, and the possible occurrence of three very weak C-H $\cdots$ O interactions, suggests molecules of (I) assemble by favorable organization of van der Waals surfaces.

## Experimental

The title compound, (I), was prepared by reaction of phthalic anhydride with DL-alanine using a previously reported procedure (Taber & Malcolm, 2001). Suitable crystals were obtained by slow evaporation of a 70% ethanol-water solution at room temperature. Sample quality was assessed by polarized microscopy, and a single crystal was adhered with viscous oil to a glass fiber for subsequent crystallographic analysis.

### Crystal data

$C_{11}H_9NO_4$	$D_x = 1.411 \text{ Mg m}^{-3}$
$M_r = 219.19$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 5700 reflections
$a = 9.8777 (8) \text{ \AA}$	$\theta = 2.8\text{--}28.3^\circ$
$b = 10.4880 (8) \text{ \AA}$	$\mu = 0.11 \text{ mm}^{-1}$
$c = 9.9723 (8) \text{ \AA}$	$T = 93 (2) \text{ K}$
$\beta = 93.131 (2)^\circ$	Block, transparent light yellow
$V = 1031.56 (14) \text{ \AA}^3$	$0.58 \times 0.34 \times 0.31 \text{ mm}$
$Z = 4$	

### Data collection

Bruker SMART 1000 CCD diffractometer	2477 independent reflections
$\varphi$ and $\omega$ scans	2132 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Bruker, 2000)	$R_{\text{int}} = 0.026$
$T_{\text{min}} = 0.943$ , $T_{\text{max}} = 0.964$	$\theta_{\text{max}} = 28.3^\circ$
8006 measured reflections	$h = -12 \rightarrow 11$
	$k = -13 \rightarrow 13$
	$l = -12 \rightarrow 13$

### Refinement

Refinement on $F^2$	$w = 1/[\sigma^2(F_o^2) + (0.046P)^2 + 0.3545P]$
$R[F^2 > 2\sigma(F^2)] = 0.036$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.096$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.05$	$\Delta\rho_{\text{max}} = 0.40 \text{ e \AA}^{-3}$
2477 reflections	$\Delta\rho_{\text{min}} = -0.23 \text{ e \AA}^{-3}$
149 parameters	
H atoms treated by a mixture of independent and constrained refinement	

**Table 1**

Selected geometric parameters ( $\text{\AA}$ ,  $^\circ$ ).

O1—C1	1.3044 (14)	N1—C11	1.4026 (14)
O2—C1	1.2314 (14)	N1—C2	1.4569 (13)
O3—C4	1.2138 (14)	C1—C2	1.5239 (15)
O4—C11	1.2076 (14)	C2—C3	1.5222 (16)
N1—C4	1.3979 (14)		
C1—O1—H1	110.5 (10)	N1—C2—C1	109.53 (9)
C4—N1—C11	112.15 (9)	C3—C2—C1	113.00 (9)
C4—N1—C2	122.95 (9)	O3—C4—N1	123.93 (10)
C11—N1—C2	124.00 (9)	O3—C4—C5	130.33 (11)
O2—C1—O1	124.51 (10)	N1—C4—C5	105.70 (9)
O2—C1—C2	121.79 (10)	O4—C11—N1	125.05 (10)
O1—C1—C2	113.65 (9)	O4—C11—C10	129.57 (10)
N1—C2—C3	112.82 (9)	N1—C11—C10	105.35 (9)

**Table 2**

Hydrogen-bonding geometry ( $\text{\AA}$ ,  $^\circ$ ).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1—H1 $\cdots$ O2 <sup>i</sup>	0.910 (17)	1.692 (17)	2.6005 (12)	174.8 (15)
C7—H7 $\cdots$ O1 <sup>ii</sup>	0.95	2.69	3.3659 (15)	129
C8—H8 $\cdots$ O1 <sup>ii</sup>	0.95	2.85	3.4413 (15)	122
C9—H9 $\cdots$ O4 <sup>iii</sup>	0.95	2.56	3.3654 (14)	143

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

The carboxyl H atom (H1) was located in a difference density map and refined independently with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{O})$ . The remaining H atoms were treated as riding, with C—H distances of 0.95 (aromatic), 0.98 ( $\text{CH}_3$ ) and 1.0  $\text{\AA}$  (CH) and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ . Riding methyl H atoms were allowed to rotate freely during refinement.

Data collection: SMART (Bruker, 2001); cell refinement: SAINT (Bruker, 2002); data reduction: SAINT and XPREP (Bruker, 2001); program(s) used to solve structure: SHELXTL (Bruker, 2000); program(s) used to refine structure: SHELXTL; molecular graphics: XSEED (Barbour, 2001); software used to prepare material for publication: XSEED.

Acknowledgment is made to the Donors of the American Chemical Society Petroleum Research Fund, the Office of Naval Research (ONR) and the Naval Research Laboratory (NRL) for support of this crystallographic investigation.

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