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N,N′-Ethylenedisuccinimide

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Key indicators

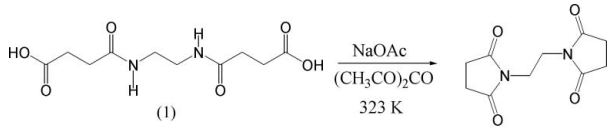
Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.002 Å
R factor = 0.048
wR factor = 0.137
Data-to-parameter ratio = 16.5

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The title compound, $C_{10}H_{12}N_2O_4$, crystallizes as discrete molecules disposed about crystallographic centres of symmetry, with two independent half-molecules constituting the asymmetric unit of the unit cell. The succinimide rings are essentially planar. No unusual features are observed in the molecular geometry.

Comment

As part of our ongoing research efforts into the synthesis of heterobifunctional linker molecules we have isolated the title molecule, *N,N′*-ethylenedisuccinimide, (2), as a product of intramolecular cyclization of *N,N′*-ethylenedisuccinimic acid, (1). The crystal structure of (2) consists of discrete centrosymmetric molecules (Fig. 1) with two independent half-molecules comprising the asymmetric unit of the unit cell. The molecules are separated by normal van der Waals distances with bond lengths in accord with conventional values (Allen *et al.*, 1987). The molecular fragments defined by Nn/C1*n*–C5*n*/O2*n*/O5*n* (n = 1, 2) are essentially coplanar with mean deviations from the planes of 0.020 and 0.010 Å for molecules 1 and 2, respectively.



(1) (2)

Experimental

A solution of *N,N′*-ethylenedisuccinimic acid, (1) (1.532 g, 5.9 mmol), with sodium acetate (0.100 g) in acetic anhydride (10 ml) was heated to 323 K for 2 h. The solvent was removed *in vacuo* and the product was extracted from the resulting residue with ethyl acetate. Removal of the solvent *in vacuo* afforded the title compound, (2), as a white crystalline solid (0.768 g, 3.4 mmol, 58%). Crystals suitable for X-ray analysis were obtained by slow evaporation of an ethyl acetate solution [m.p. 525–526 K; literature 522–523 K (Kato & Kogyo, 1968). (ESMS+) 225 (M^+, 80%), 231 (MLi$^+$, 100%). 247 (MNa$^+$, 100%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 3.73 (*s*, 4H, H1), 2.66 (*s*, 8H, H3, H4). ^{13}C NMR (100 MHz, $CDCl_3$): δ 177.89 (C2, C5), 37.30 (C1), 28.34 (C3, C4).

Crystal data

$C_{10}H_{12}N_2O_4$
M_r = 224.22
Monoclinic, $P2_1/c$
a = 12.5653 (13) Å
b = 8.3613 (10) Å
c = 9.9285 (15) Å
β = 90.694 (10)°
V = 1043.0 (2) Å^3
Z = 4
D_x = 1.428 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 8.3–10.6°
μ = 0.11 mm^{-1}
T = 295 K
Prism, colourless
0.50 × 0.40 × 0.30 mm

Data collection

Rigaku AFC-7*R* diffractometer
ω–2θ scans
Absorption correction: none
2655 measured reflections
2396 independent reflections
1825 reflections with $I > 2\sigma(I)$
$R_{int} = 0.031$
$\theta_{max} = 27.5^\circ$
$h = -7 \rightarrow 16$
$k = 0 \rightarrow 10$
$l = -12 \rightarrow 12$
3 standard reflections
every 150 reflections
intensity decay: 1.2%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.048$
$wR(F^2) = 0.137$
$S = 1.03$
2396 reflections
145 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0858P)^2 + 0.1556P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.20$ e Å^{-3}
$\Delta\rho_{min} = -0.34$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

O21—C21	1.2050 (18)	C11—C11^{i}	1.516 (2)
O51—C51	1.209 (2)	C21—C31	1.505 (2)
O22—C22	1.2042 (18)	C31—C41	1.518 (2)
O52—C52	1.2102 (19)	C41—C51	1.503 (2)
N1—C21	1.3889 (18)	C12—C12^{ii}	1.515 (2)
N1—C51	1.3841 (19)	C22—C32	1.507 (2)
N1—C11	1.4514 (18)	C32—C42	1.514 (2)
N2—C12	1.4539 (18)	C42—C52	1.504 (2)
N2—C52	1.3833 (18)	C12—H12*A*	0.9500
N2—C22	1.3866 (17)		
C11—N1—C21	123.21 (11)	O51—C51—N1	123.87 (14)
C11—N1—C51	123.64 (12)	O51—C51—C41	127.87 (14)
C21—N1—C51	113.07 (11)	N1—C51—C41	108.26 (12)
C12—N2—C52	123.29 (11)	N2—C12—C12^{ii}	110.79 (12)
C22—N2—C52	113.26 (11)	O22—C22—N2	124.18 (13)
C12—N2—C22	123.33 (11)	O22—C22—C32	128.18 (12)
N1—C11—C11^{i}	111.16 (11)	N2—C22—C32	107.64 (11)
O21—C21—N1	123.79 (13)	O52—C52—N2	123.45 (13)
O21—C21—C31	128.33 (13)	O52—C52—C42	128.24 (14)
N1—C21—C31	107.87 (12)	N2—C52—C42	108.31 (12)

Symmetry codes: (i) $1-x, -y, 1-z$; (ii) $-x, 1-y, -z$.

H atoms were placed in calculated positions, with C—H set at 0.95 Å, and included in the refinement in riding-model approximation, with U_{iso}(H) values set at $1.2U_{eq}$ of the parent atom.

Data collection: *MSC/AFC-7 Diffractometer Control Software* (Molecular Structure Corporation, 1999); cell refinement: *MSC/AFC-7 Diffractometer Control Software*; data reduction: *TEXSAN for Windows* (Molecular Structure Corporation, 2001); program(s) used to solve structure: *TEXSAN for Windows*; program(s) used to refine structure: *TEXSAN for Windows* and *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *TEXSAN for Windows* and *PLATON* (Spek, 2003).

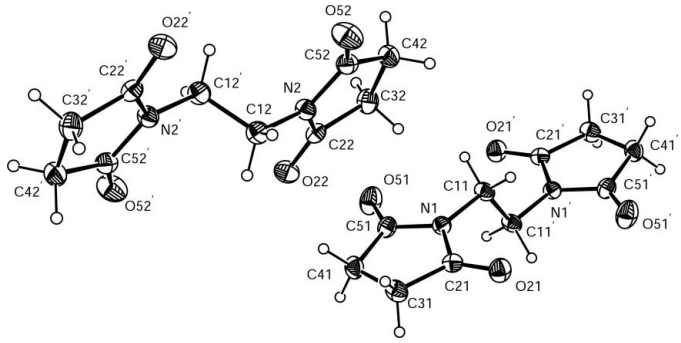


Figure 1
View of the title compound with the atom-numbering scheme. Displacement ellipsoids for non-H atoms are drawn at the 30% probability level. Primed atoms have symmetry codes $(1-x, -y, 1-z)$ for molecule 1 and $(-x, 1-y, -z)$ for molecule 2.

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