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1,1′-(Naphthalene-1,4-diyldicarbonyl)-bis(1*H*-imidazole)

Lin-Hai Jing,* Shao-Jin Gu and Huan-Xia Zhang

Department of Chemistry, China West Normal University, Nanchong 637002, People's Republic of China

Correspondence e-mail: jlhhxg@yahoo.com.cn

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Key indicators

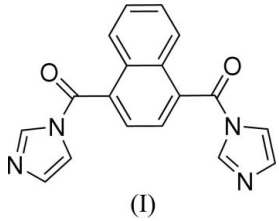
Single-crystal X-ray study
T = 153 K
Mean σ(C–C) = 0.002 Å
R factor = 0.036
wR factor = 0.123
Data-to-parameter ratio = 14.9

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

The title compound, $C_{18}H_{12}N_4O_2$, adopts a *cis* C═O conformation. The two amide groups are twisted away from the attached ring by 50.46 (1) and 55.79 (1)°. The molecules are linked into chains of rings by C—H···N and C—H···O hydrogen bonds.

Comment

1,4-Naphthalenedicarboxylic acid derivatives are a class of intermediates important for applications as monomers in the preparation of polymers (Fukuzumi *et al.*, 1994; Tsukada *et al.*, 1994). Previously, we have reported the crystal structures of *N*,*N*′-bis(4-nitrophenyl)naphthalene-1,4-dicarboxamide dimethylsulfoxide disolvate (Jing, Qin, Gu, Zhang & Mao 2006), *N*,*N*′-bis(2-methoxyphenyl)naphthalene-1,4-dicarboxamide (Jing, Qin, Gu, Zhang & Lei, 2006) and *N*,*N*′-bis(2-pyridyl)naphthalene-1,4-dicarboxamide (Jing, Gu & Zhang, 2006). We now report the crystal structure of the title compound, (I).



(I)

The bond lengths and angles in (I) are all normal. The two C═O groups are mutually *cis*. Probably as a result of steric effects, the substituent groups at atoms C1 and C4 are twisted away from the plane of the naphthalene ring system (Fig. 1). The O1/N1/C1/C11 and O2/N3/C4/C15 planes form dihedral angles of 50.46 (1) and 55.79 (1)°, respectively, with the plane formed by atoms C1–C4/C9/C10. The O1/N1/C1/C11 and N1/N2/C12–C14 planes are inclined at an angle of 15.24 (1)°, while the O2/N3/C4/C15 and N3/N4/C16–C18 planes make a dihedral angle of 7.19 (1)°. The molecules are linked into chains of rings along [011] by a combination of C—H···N and C—H···O hydrogen bonds (Table 1).

Experimental

Naphthalene-1,4-dicarboxylic acid (2 mmol) and an excess of thionyl chloride in dioxane (20 ml) were boiled under reflux for 6 h; the solution was distilled under reduced pressure and a yellow solid was formed. Imidazole (4 mmol) in tetrahydrofuran (20 ml) was added to the yellow solid and boiled under reflux for 1 d; the solution was cooled to ambient emperature and filtered to remove the tetrahydrofuran. The precipitate was dissolved in dimethyl sulfoxide and

allowed to stand for one month at ambient temperature; colourless single crystals suitable for X-ray diffraction were obtained.

Crystal data

$C_{18}H_{12}N_4O_2$	V = 723.81 (5) Å^3
M_r = 316.32	Z = 2
Triclinic, $P\overline{1}$	D_x = 1.451 Mg m^{-3}
a = 7.8010 (3) Å	Mo $K\alpha$ radiation
b = 8.1890 (3) Å	μ = 0.10 mm^{-1}
c = 11.9799 (6) Å	T = 153 (2) K
α = 75.900 (1)°	Block, colourless
β = 77.415 (2)°	0.57 × 0.22 × 0.13 mm
γ = 84.738 (1)°	

Data collection

Rigaku R-AXIS RAPID diffractometer	3259 independent reflections
ω scans	2823 reflections with $I > 2\sigma(I)$
Absorption correction: none	R_{int} = 0.012
7128 measured reflections	θ_{max} = 27.5°

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.089P)^2 + 0.138P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.036	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2)$ = 0.123	$\Delta\rho_{max}$ = 0.34 e Å^{-3}
S = 0.99	$\Delta\rho_{min}$ = −0.25 e Å^{-3}
3259 reflections	Extinction correction: *SHELXL97*
218 parameters	Extinction coefficient: 0.019 (5)
H-atom parameters constrained	

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

D—H···A	D—H	H···A	D···A	D—H···A
C12—H12···O1^{i}	0.95	2.40	3.349 (3)	174
C2—H2···N4^{ii}	0.95	2.56	3.351 (2)	141

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

H atoms were positioned geometricaly and treated as riding atoms, with C—H = 0.95 Å and U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *RAPID-AUTO* (Rigaku, 2004); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

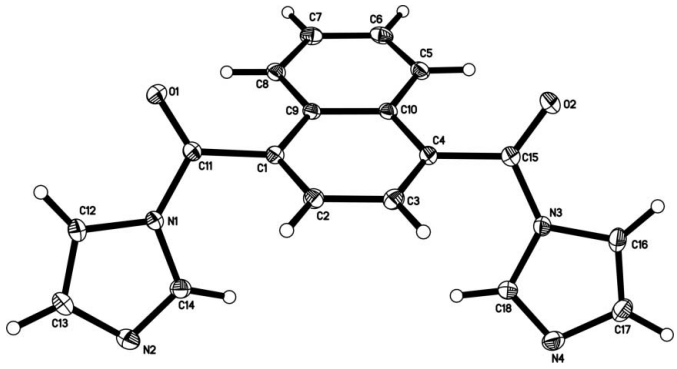


Figure 1
The molecular structure of (I), showing 30% probability displacement ellipsoids and the atomic numbering.

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