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Diisopropyl *N*,*N*′-(4-methyl-*m*-phenylene)-dicarbamate

Yong-Yan Lu, Qiu-Xiang Yin,* Jing-Kang Wang and Lina Zhou

School of Chemical Engineering and Technology, Tianjin University, Tianjin 300072, People's Republic of China

Correspondence e-mail: srcict_chem@yahoo.com

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.040
wR factor = 0.104
Data-to-parameter ratio = 16.6

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

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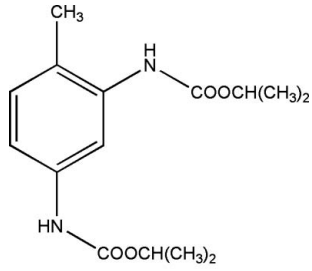
The crystal structure of the title compound, $C_{15}H_{22}N_2O_4$, is stabilized by two intermolecular N—H···O hydrogen bonds.

Comment

The title compound, (I), is a derivative of toluene-2,4-bis-(isocyanate), prepared by the reaction of 4-methylbenzene-1,3-diamine and isopropyl carbonochloridate according to the method of Baskakow & Mel'nikow (1954). In the present paper, the crystal structure of (I) (Fig. 1) is reported. The crystal packing projected on to the *bc* face is shown in Fig. 2. Selected geometric parameters are given in Table 1. In the crystal structure, there are two intermolecular N—H···O hydrogen bonds (Table 2).



(I)

Experimental

Toluene-2,4-bis(isocyanate) (TDI) was provided by Hebei Cangzhou Dahua Co. Ltd. The raw material was purified twice by a melt crystallization process. Compound (I) was prepared by the reaction of purified TDI (98%) with isopropyl alcohol (m.p. 408.7 K; differential scanning calorimetry). Colourless block-shaped single crystals suitable for X-ray diffraction were obtained by slow evaporation of a methanol solution at room temperature over a period of 5 d.

Crystal data

$C_{15}H_{22}N_2O_4$
M_r = 294.35
Monoclinic, *Cc*
a = 9.0708 (18) Å
b = 15.997 (6) Å
c = 12.113 (2) Å
β = 111.28 (3)°
V = 1637.8 (7) Å^3
Z = 4
D_x = 1.194 Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 8078 reflections
θ = 3.1–27.5°
μ = 0.09 mm^{-1}
T = 293 (2) K
Block, colourless
0.31 × 0.24 × 0.14 mm

Data collection

Rigaku R-AXIS RAPID IP area-detector diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.973, T_{max} = 0.988
7930 measured reflections
3520 independent reflections
2978 reflections with $I > 2\sigma(I)$
R_{int} = 0.038
θ_{max} = 27.5°
h = −11 → 11
k = −20 → 18
l = −15 → 15

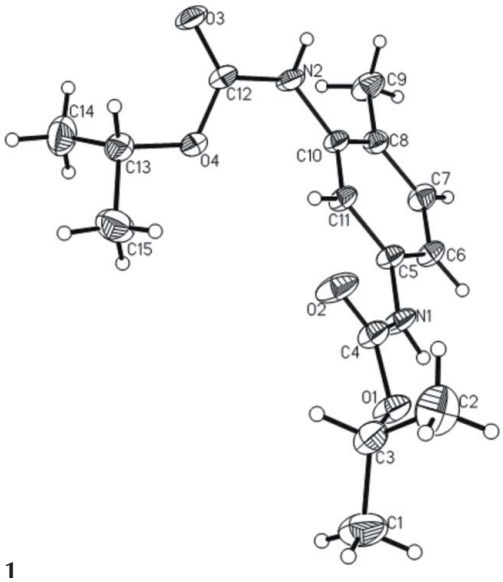


Figure 1
An *ORTEPII* (Johnson, 1976) view of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

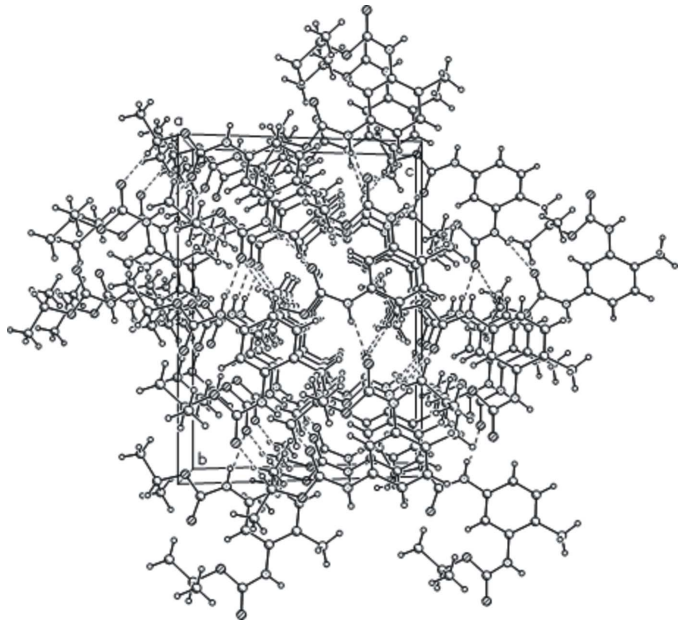


Figure 2
The molecular packing of compound (I), viewed along the *a* axis. Dashed lines indicate hydrogen bonds.

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0584P)^2 + 0.1074P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.040$	$(\Delta/\sigma)_{max} = 0.008$
$wR(F^2) = 0.104$	$\Delta\rho_{max} = 0.13$ e Å^{-3}
$S = 1.03$	$\Delta\rho_{min} = -0.16$ e Å^{-3}
3520 reflections	
212 parameters	
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

N1—C4	1.343 (3)	N2—C12	1.348 (2)
N1—C5	1.406 (2)	N2—C10	1.425 (2)
C4—N1—C5	127.87 (15)	C12—N2—C10	128.96 (16)
C3—O1—C4—O2	−3.6 (3)	C13—O4—C12—O3	−4.5 (3)
C3—O1—C4—N1	177.11 (17)	C13—O4—C12—N2	176.84 (16)
C8—C10—N2—C12	145.9 (2)	C6—C5—N1—C4	168.6 (2)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O3^{i}	0.86	2.03	2.873 (2)	166
N2—H2A···O2^{ii}	0.86	2.13	2.975 (2)	168

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

H atoms were placed in calculated positions and constrained to ride on their parent atoms, with C—H = 0.93–0.96 Å and N—H = 0.86 Å, and U_{iso}(H) = 1.2U_{eq}(C,N) and 1.5U_{eq}(methyl 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: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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