organic papers

N-[4-(2,2-Dimethylpropionylamino)phenyl]-2,2-dimethylpropionamide

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Key indicators

Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.004 Å
R factor = 0.068
wR factor = 0.174
Data-to-parameter ratio = 15.9

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

In the title compound, $C_{16}H_{24}N_2O_8$, the molecule is centrosymmetric. The crystal packing is stabilized by intermolecular N—H···O hydrogen bonds.

Comment

The luminescence features of some amide compounds have been studied by Frederick & Liu (1999). In this paper, we report the crystal structure of the title compound, (I), which is a new amide compound.

(I)
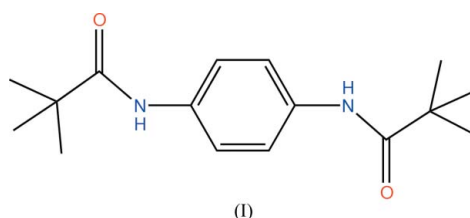
In the centrosymmetric molecule of (I) (Fig. 1), the bond lengths and angles present no unusual features. The crystal packing (Fig. 2) is stabilized by intermolecular hydrogen bonds (Table 1). The N···O distance of 2.14 (2) Å is shorter than those in benzanilide [2.34 (3) Å; Bowes *et al.*, 2003] and *N*-[4-(phenylethynyl)phenyl]benzamide [3.42 (2) Å; Yin *et al.*, 2005].

Experimental

To a mixture of benzene-1,4-diamine (0.54 g, 5 mmol) and Et$_3$N (5 ml) in tetrahydrofuran (30 ml), 2,2-dimethylpropionyl chloride (1.2 g, 10 mmol) was added dropwise and the mixture stirred at room temperature for 3 h. The solvent was then evaporated on a rotary evaporator and the mixture was extracted with EtOAc (50 ml) to obtain the title compound. Single crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of a solution in CH_2Cl_2–MeOH (1:1 *v/v*).
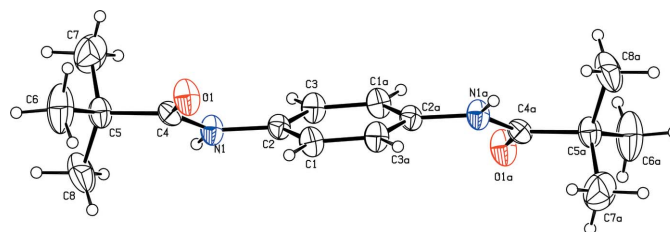
Figure 1
A view of the molecule of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are represented by circles of arbitrary size. [Symmetry code: (a) $2 - x$, $1 - y$, $2 - z$]

Crystal data

$C_{16}H_{24}N_2O_2$
$M_r = 276.37$
Monoclinic, $P2_1/c$
$a = 12.166\ (4)$ Å
$b = 7.677\ (3)$ Å
$c = 9.243\ (3)$ Å
$\beta = 96.613\ (6)°$
$V = 857.6\ (5)$ Å^3
$Z = 2$

$D_x = 1.070$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1225
 reflections
$\theta = 3.1–23.6°$
$\mu = 0.07$ mm^{-1}
$T = 292\ (2)$ K
Block, colourless
$0.30 \times 0.20 \times 0.10$ mm

Data collection

Bruker SMART 1K CCD area-
 detector diffractometer
φ and ω scans
Absorption correction: none
3943 measured reflections
1493 independent reflections

1136 reflections with $I > 2\sigma(I)$
$R_{int} = 0.026$
$\theta_{max} = 25.0°$
$h = -14 \rightarrow 12$
$k = -9 \rightarrow 9$
$l = -10 \rightarrow 9$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.068$
$wR(F^2) = 0.174$
$S = 1.09$
1493 reflections
94 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0699P)^2$
 $+ 0.4858P]$
 where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.25$ e Å^{-3}
$\Delta\rho_{min} = -0.15$ e Å^{-3}

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

$D—H\cdots A$	$D—H$	$H\cdots A$	$D\cdots A$	$D—H\cdots A$
N1—H1$A\cdots$O1^{i}	0.86	2.14	2.929 (3)	153

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

After their location in a difference Fourier map, H atoms were placed in calculated positions and allowed to ride on their parent atoms, with with C—H = 0.93 Å for aromatic C and 0.96 Å for methyl C, and N—H = 0.86 Å, and with U_{iso}(H) = 1.2 U_{eq}(C) for aromatic C and N, or 1.5$_{eq}$(C) for methyl C.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 2001); software used to prepare material for publication: *SHELXTL*.

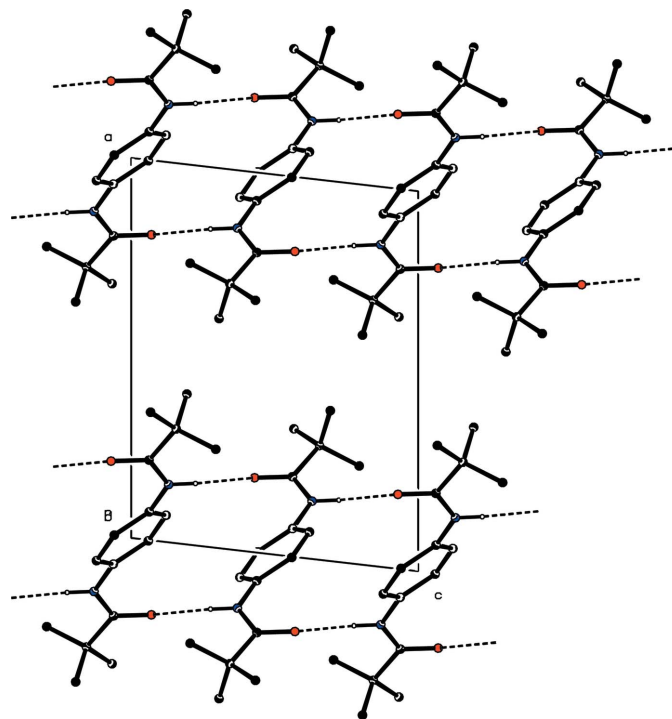**Figure 2**
N—H$\cdots$O intermolecular interactions (dashed lines) in the crystal structure of (I). H atoms have been omitted.

References

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