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Tri-*tert*-butyl 3,3′,3″-(aminomethanetriyl)-tripropanoate

Edwin Weber,* Joachim Langer and Wilhelm Seichter

Institut für Organische Chemie, TU Bergakademie Freiberg, Leipziger Strasse 29, D-09596 Freiberg/Sachsen, Germany

Correspondence e-mail:
edwin.weber@chemie.tu-freiberg.de

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Key indicators

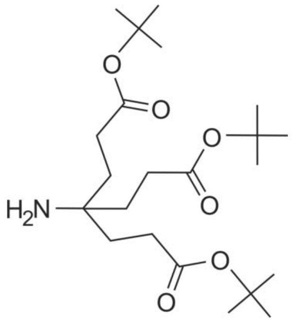
Single-crystal X-ray study
T = 93 K
Mean σ(C–C) = 0.002 Å
R factor = 0.034
wR factor = 0.111
Data-to-parameter ratio = 16.7

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

The crystal structure of the title compound, $C_{22}H_{41}NO_6$, is stabilized by intermolecular N—H···O hydrogen-bonding contacts.

Comment

Dendrimers are particular macromolecules characterized by the controlled branching structure radiating from the core to the periphery (Fréchet *et al.*, 2001). This architecture gives rise to a number of very interesting properties which can be used in many applications, including catalysis, materials design and drug delivery (Gittins *et al.*, 2003). A basic building block for the assembly of this remarkable type of molecular structure is the title compound, (I) (Newkome *et al.*, 2001), the crystal structure of which is reported here.



(I)

Although compound (I) has intrinsic molecular symmetry, it crystallizes in a general position without crystallographic symmetry (Fig. 1). The C1—N1 distance of 1.481 (1) Å is within the expected range and the N—C—C angles are 105.6 (1), 107.5 (1) and 112.3 (1)°. The torsion angles within the oxycarbonylethyl fragments all adopt an *anti* conformation and are in the range 152.3 (1)–179.6 (1)°. The torsion angles around the core atom C1 are *gauche* and *anti*, reflecting the *trans*–*syn*–*trans* orientation of the three carbonyl groups. Thus, the overall conformation of (I) resembles that found in the corresponding nitro compound (Newkome *et al.*, 1994).

There are intramolecular C—H···O hydrogen bonds with O1, O3 and O5 acting as bifurcated acceptors. The amino H atoms, the positions of which could be located in a difference Fourier map, form weak N—H···O contacts (Table 1) to carbonyl O atoms of two neighbouring molecules, resulting in supramolecular strands which extend in the c-axis direction (Fig. 2). The peripheral regions of the molecular chains are formed by *tert*-butyl groups. In this way, they participate in packing stabilization by forming weak hydrophobic interactions.

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Experimental

The title compound, (I), was synthesized by hydrogenation of the corresponding nitro compound following a modification of the original literature procedure (Newkome *et al.*, 1991, 1996) to give a product of higher purity and yield (Akpo *et al.*, 2006). Recrystallization from *n*-heptane produced colourless crystals.

Crystal data

$C_{22}H_{41}NO_6$
$M_r = 415.56$
Orthorhombic, $Pna2_1$
$a = 11.6788\ (4)$ Å
$b = 20.0635\ (7)$ Å
$c = 10.4288\ (4)$ Å
$V = 2443.65\ (15)$ Å^3
$Z = 4$
Mo $K\alpha$ radiation
$\mu = 0.08$ mm^{-1}
$T = 93\ (2)$ K
$0.53 \times 0.47 \times 0.38$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Blessing, 1995; Sheldrick, 2002)
$T_{\min} = 0.895$, $T_{\max} = 0.970$
43711 measured reflections
4672 independent reflections
4424 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.029$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.034$
$wR(F^2) = 0.111$
$S = 1.12$
4672 reflections
280 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{\max} = 0.38$ e Å^{-3}
$\Delta\rho_{\min} = -0.36$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C22—H22*A*···O5	0.98	2.57	3.093 (2)	114
C21—H21*B*···O5	0.98	2.39	2.925 (2)	114
C15—H15*A*···O3	0.98	2.45	3.0005 (19)	115
C13—H13*B*···O3	0.98	2.40	2.986 (2)	118
C6—H6*B*···O1	0.98	2.42	2.973 (2)	115
C8—H8*A*···O1	0.98	2.47	3.039 (2)	116
N1—H1*A*···O3$^{\rm i}$	0.869 (9)	2.390 (13)	3.2009 (15)	155.5 (19)
N1—H1*B*···O5$^{\rm ii}$	0.859 (10)	2.597 (10)	3.4466 (17)	170 (2)

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

In the absence of significant anomalous scattering effects, Friedel pairs were merged. The amino H atoms were located in difference-density maps. All other H atoms were constrained to ideal geometry, with C—H = 0.96 Å and $U_{\rm iso}({\rm H}) = 1.5U_{\rm eq}$(methyl C) or $1.2U_{\rm eq}$(methylene C).

Data collection: *SMART* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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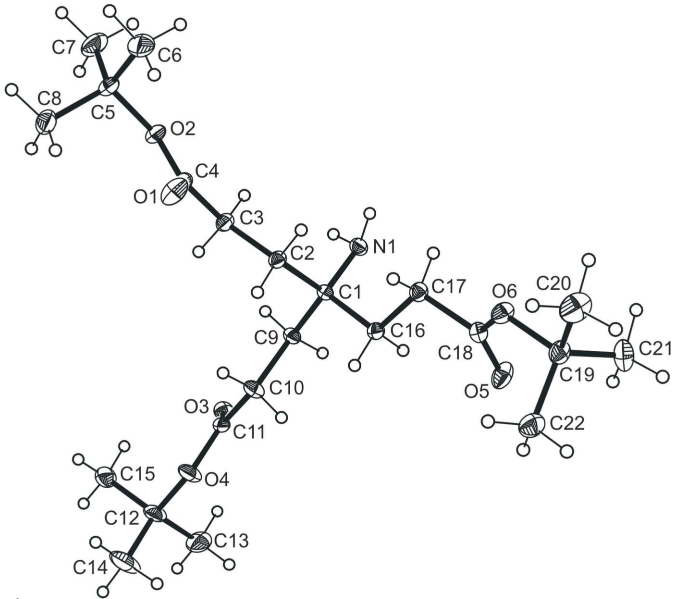

Figure 1
The molecular stucture of (I), showing 50% probability displacement ellipsoids.

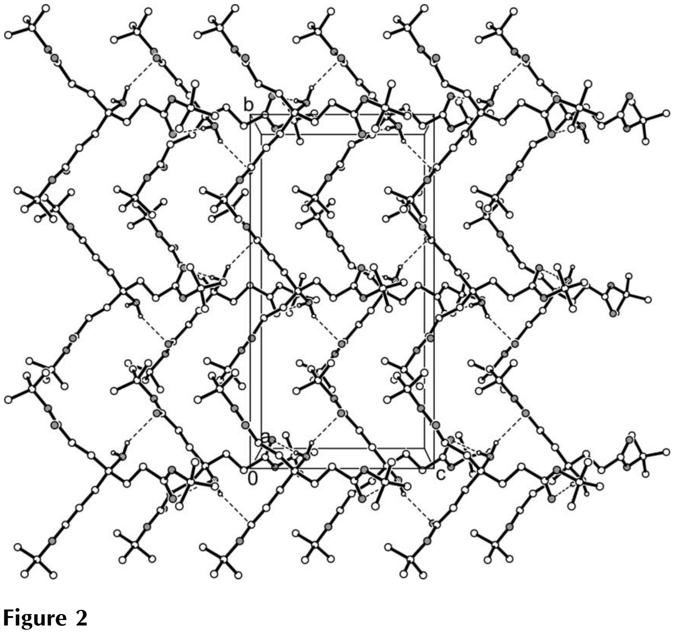

Figure 2
Packing diagram of (I). All but the amino H atoms have been omitted. Dashed lines represent hydrogen bonds.

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