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Key indicators

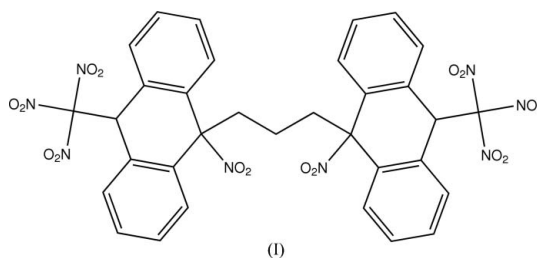
Single-crystal X-ray study
 $T = 295$ K
Mean $\sigma(C-C) = 0.006$ Å
 R factor = 0.061
 wR factor = 0.140
Data-to-parameter ratio = 11.8For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.**(*E,E*)-1,3-Bis[9,10-dihydro-9-nitro-10-(trinitromethyl)-9-anthryl]propane**

The title compound, $C_{33}H_{24}N_8O_{16}$, was obtained as a product of the photoreaction between 1,3-di-9-anthrylpropane and tetranitromethane. The molecule occupies a special position on a twofold axis. The trinitromethyl and nitro substituents on the 9,10-dihydroacridine system are *E* oriented.

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Comment

Aromatic amine compounds are of interest due to their potential uses as photoconductive materials in a wide range of electrophotographic devices (Hara & Omae, 1978; Thelakkat, 2002). One common method for the preparation of aromatic amines is the reduction of the corresponding nitro compounds which are commonly prepared through the reaction of aromatic compounds with concentrated nitric acid in the presence of concentrated sulfuric acid. Nitration through the irradiation of the charge-transfer complexes formed between aromatic compounds and tetranitromethane (TNM) offers an alternative route to the use of concentrated acids (Kochi, 1991; Butts *et al.*, 1996; Cox, 1998; Lehnig & Schürmann, 1998). We have already reported the crystal structure of (*E*)-9,10-dihydro-9-methyl-9-nitro-10-(trinitromethyl)anthracene as the product of the photoreaction between 9-methylantracene and TNM (Arslan *et al.*, 2005). In the present paper, we report the crystal structure of the title compound, (I), which is a product of the photoreaction between 1,3-di-9-anthrylpropane, a dimeric analogue to 9-methylantracene, with TNM.



The asymmetric unit contains one half-molecule; the other half is generated by a crystallographic twofold axis operation. Bond lengths and angles (Table 1) are similar to those of (*E*)-9,10-dihydro-9-methyl-9-nitro-10-(trinitromethyl)anthracene (Arslan *et al.*, 2005).

The propylene bridge connecting the two rings shows an *anti-anti* conformation. The central ring of the 9,10-dihydroanthracene unit adopts a boat conformation with a dihedral angle between the two benzene ring planes of 25.86 (13)°. The trinitromethyl group is attached pseudoaxially at the C10 position of the *meso* ring. The trinitromethyl and nitro groups on the *meso* ring are *E* oriented.

The crystal packing is mainly determined by van der Waals forces and, contrary to the structure of the monomeric analogue (Arslan *et al.*, 2005), no intermolecular π - π stacking interactions are observed.

Experimental

The title compound was synthesized by irradiation for 60 min of a solution of 1,3-di-9-anthrylpropane (20 mg, 0.051 mmol) and TNM (325 mg, 1.67 mmol) in a 40 ml pentane/5 ml CCl_4 mixture, according to the procedure reported earlier (Arslan *et al.*, 2005). Single crystals suitable for X-ray diffraction studies were grown from a concentrated solution of (I) in chloroform through slow evaporation of solvent at ambient conditions [22.36% yield (9.0 mg, 0.0114 mmol), m.p. 439–440 K].

Crystal data

$\text{C}_{33}\text{H}_{24}\text{N}_8\text{O}_{16}$
 $M_r = 788.6$
 Monoclinic, $C2/c$
 $a = 23.388$ (3) Å
 $b = 9.4054$ (10) Å
 $c = 16.3442$ (11) Å
 $\beta = 107.161$ (7)°
 $V = 3435.2$ (6) Å³

$Z = 4$
 $D_x = 1.525$ Mg m⁻³
 Mo $K\alpha$ radiation
 $\mu = 0.13$ mm⁻¹
 $T = 295$ (2) K
 Thick plate, colorless
 $0.2 \times 0.2 \times 0.1$ mm

Data collection

Enraf–Nonius CAD-4 diffractometer
 ω scans
 Absorption correction: none
 3049 measured reflections
 3049 independent reflections

1481 reflections with $I > 2\sigma(I)$
 $\theta_{\text{max}} = 25.1^\circ$
 3 standard reflections
 frequency: 120 min
 intensity decay: 2.6%

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.061$
 $wR(F^2) = 0.140$
 $S = 1.11$
 3049 reflections
 258 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0444P)^2 + 3.4205P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.21$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.23$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

N1–C13	1.529 (5)	N9–C9	1.561 (4)
N2–C13	1.534 (5)	C9–C11	1.542 (5)
N3–C13	1.538 (5)	C10–C13	1.570 (5)
C8A–C9–C9A	113.8 (3)	C9A–C9–C11	114.5 (3)
C8A–C9–C11	108.8 (3)	C4A–C10–C10A	113.3 (3)

All H atoms were placed geometrically and allowed to ride on their parent atoms with C–H distances of 0.93, 0.97 and 0.98 Å for

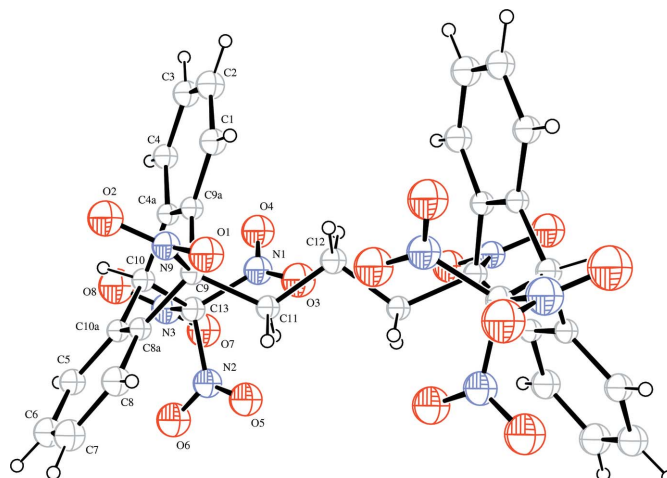


Figure 1

Molecular structure of (I) with the atom-numbering scheme. Displacement ellipsoids for non-H atoms are drawn at the 30% probability level. Unlabeled atoms are related to labeled atoms by the symmetry operator $(1 - x, y, \frac{1}{2} - z)$.

aromatic, methylene, and methine H atoms, respectively, and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Data collection: *CAD-4-PC Software* (Enraf–Nonius, 1993); cell refinement: *CAD-4-PC Software*; data reduction: *DATRD2* in *NRCVAX* (Gabe *et al.*, 1989); 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) and *PLATON* (Spek, 2003); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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