

Structure of 2,4,5,7-Tetranitro-9-fluorenone

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Abstract. $C_{13}H_4N_4O_9$, $M_r = 360.20$, monoclinic, $P2_1/a$, $a = 22.900$ (4), $b = 10.873$ (2), $c = 11.647$ (2) Å, $\beta = 103.20$ (1)°, $V = 2823.4$ (9) Å³, $Z = 8$, $D_x = 1.69$ Mg m⁻³, $\lambda(\text{Mo } K\alpha) = 0.71069$ Å, $\mu = 0.16$ mm⁻¹, $F(000) = 1456$, room temperature, $R = 0.053$ for 2213 reflections. The two independent molecules have similar conformations. Overcrowding between the 4- and 5-nitro groups is relieved by rotations (mean value 37°) and bends (mean value 10°) of these groups about the C–N bonds as well as by propeller-like deformations in the remaining molecular framework.

Introduction. Polynitro derivatives of 9-fluorenone are electron acceptors with photoelectronic properties (Pravednikov, Kotov & Tverskoi, 1978). The crystal structures are known for 2-nitro-9-fluorenone (Furmanova, Andrianov, Andrievsky & Poplavsky, 1985), 2,7-dinitro-9-fluorenone (Baughman, 1982) and 2,4,7-trinitro-9-fluorenone (Dorset, Hybl & Ammon, 1972) [and in a complex with hexamethylbenzene (Brown, Cheung, Trefonas & Majeste, 1974)]. However, the structure of 2,4,5,7-tetranitro-9-fluorenone (TNFL) is unknown so far, though this compound is widely used as a strong photosensitive substance. We began our investigations of the crystal and molecular structure of the other nitro derivatives of 9-fluorenone with TNFL. The attempt to determine the structure of TNFL in a complex with metalloporphyrin (Grigg, Trocha-Grimshaw & King, 1978) was unsuccessful because of the anomalous behaviour of the 4,5-dinitro groups. The same inexplicable deformation of the geometry of these nitro groups was observed also in the structure of 2,4,5-trinitro-7-piperidino-9-fluorenone (Chetkina, Povetieva, Belsky & Bepalov, 1985). Our results of the structure determination of 4-nitro-9-fluorenone, 2,5- and 4,5-dinitro-9-fluorenes, 2,4,5-trinitro-9-fluorenone and 4-cyano-2,5,7-trinitro-9-fluorenone are in the press.

Experimental. Yellow transparent crystals grown from *N,N*-dimethylformamide, m.p. 526.5–527 K, crystal size 0.18 × 0.30 × 0.35 mm. Syntex $P\bar{1}$ diffractometer, graphite-monochromated Mo $K\alpha$ radiation. Unit-cell dimensions determined by least-squares treatment of 12 reflections with $22 < 2\theta < 24^\circ$. Intensities collected at room temperature up to $2\theta = 46^\circ$ by $\theta/2\theta$ scan

technique; 2695 measured independent reflections, 2213 unique reflections with $I \geq 3\sigma(I)$, range of hkl : $h 0 \rightarrow 24$, $k 0 \rightarrow 11$, $l -11 \rightarrow 10$. Corrections for Lorentz–polarization effects, but not for extinction or absorption. Structure solved by direct methods (*SHELXTL*; Sheldrick, 1981) only after renormalization of structure factors (*XTL*, Syntex, 1980). An *E* map gave all C, N, O atomic positions, H-atom positions calculated. Refinement [$\ln F$, $w^{-1} = \sigma^2(F) + 0.0005F^2$] by full-matrix least squares with anisotropic thermal parameters for non-H atoms and isotropic for H atoms, $R = 0.053$, $wR = 0.056$, $S = 1.78$, $(\Delta/\sigma)_{\max} = 0.264$, in the final ΔF map $(\Delta\rho)_{\max} = 0.67$ e Å⁻³ near the positions of 4- and 5-nitro groups, $(\Delta\rho)_{\min} = -0.35$ e Å⁻³. Calculations carried out with *SHELXTL* (Sheldrick, 1981) on the Nova-3 computer incorporated in the Nicolet R3 system. Atomic scattering factors from *International Tables for X-ray Crystallography* (1974).

Discussion. Atomic coordinates, bond lengths and angles are given in Tables 1 and 2 respectively.* The atom-labelling system is shown in Fig. 1. There is generally good agreement between the geometry of the two independent molecules *A* and *B* except for bond distances O(5)–N(2) and O(6)–N(3). The molecular conformation of the polynitro aromatic compounds depends on steric factors (Sadova & Vilkov, 1982). Repulsion between the 4- and 5-nitro groups of TNFL causes rotation of these groups, inclination of C–N bonds and deformation of the fluorenone moiety. There are significant deviations from planarity of the fluorenone moiety of TNFL [dihedral angles between the outer rings are 12.5 (*A*) and 6.2° (*B*)] in contrast to the planar molecule of 9-fluorenone (Luss & Smith, 1972). This fragment has propeller-like deformations; maximum deviations from the plane through atoms C(1)–C(13) are 0.203 (*A*) and –0.105 Å (*B*). Rotation angles of the NO₂ groups around C–N bonds from the planes of the benzene rings are shown in Fig. 1. These

* Lists of structure factors, anisotropic thermal parameters and deviations of atoms from the least-squares planes have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 42945 (17 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

groups in positions 2 and 7 are planar within 0.010 (*A*) and 0.001 Å (*B*). The planarity of the CNO₂ groups in positions 4 and 5 is disturbed: deviations from the plane of the three neighbouring atoms are -0.034 (*A*), -0.037 Å (*B*) for the N(2) atom and -0.009 (*A*), 0.022 Å (*B*) for the N(3) atom. The bending angles of the C-N bond to the planes of benzene rings are 12.8 (*A*), 6.6° (*B*) for position 4 and -9.4 (*A*), -10.7° (*B*) for position 5. The CNO₂ groups in positions 4 and 5 are almost parallel with dihedral angles of 19.4 (*A*) and 6.5° (*B*) between the planes of

these groups. On the whole the molecular conformation of TNFL is similar to that of 9-(dicyanomethylene)-2,4,5,7-tetranitro-9-fluorene (Silverman, Yannoni & Krukoni, 1974) and 2,4,5-trinitro-7-piperidino-9-fluorenone (Chetkina *et al.*, 1985).

It should be noted that the O-N bond lengths in the 4- and 5-nitro groups are unequal (Table 2). The O(5)-N(2) and O(6)-N(3) bond distances exceed the

Table 1. Final fractional coordinates and isotropic thermal parameters (Å²)

For O, N, C atoms $U_{eq} = \frac{1}{3} \sum_i \sum_j U_{ij} a_i^* a_j^* a_i \cdot a_j$.

	<i>x</i>	<i>y</i>	<i>z</i>	U_{eq}/U_{iso}
O(1) <i>A</i>	0.2004 (2)	0.0140 (3)	0.3136 (3)	0.057 (1)
O(2) <i>A</i>	0.4247 (2)	0.1217 (4)	0.5271 (4)	0.080 (2)
O(3) <i>A</i>	0.4367 (2)	0.2484 (4)	0.6723 (3)	0.082 (2)
O(4) <i>A</i>	0.2725 (2)	0.3115 (4)	0.8630 (3)	0.063 (1)
O(5) <i>A</i>	0.1939 (2)	0.1988 (4)	0.7988 (3)	0.055 (1)
O(6) <i>A</i>	0.1529 (2)	0.4031 (3)	0.6631 (3)	0.068 (1)
O(7) <i>A</i>	0.0763 (2)	0.3295 (5)	0.7239 (4)	0.118 (2)
O(8) <i>A</i>	-0.0658 (1)	0.1218 (4)	0.4126 (4)	0.082 (2)
O(9) <i>A</i>	-0.0365 (2)	0.0565 (7)	0.2628 (5)	0.163 (3)
N(1) <i>A</i>	0.4060 (2)	0.1830 (4)	0.5978 (4)	0.057 (2)
N(2) <i>A</i>	0.2406 (2)	0.2502 (4)	0.7867 (4)	0.048 (2)
N(3) <i>A</i>	0.1114 (2)	0.3297 (4)	0.6594 (4)	0.066 (2)
N(4) <i>A</i>	-0.0274 (2)	0.0993 (5)	0.3607 (5)	0.074 (2)
C(1) <i>A</i>	0.3041 (2)	0.1273 (5)	0.4946 (4)	0.045 (2)
C(2) <i>A</i>	0.3409 (2)	0.1822 (4)	0.5914 (4)	0.042 (2)
C(3) <i>A</i>	0.3199 (2)	0.2279 (4)	0.6836 (4)	0.041 (2)
C(4) <i>A</i>	0.2592 (2)	0.2250 (4)	0.6773 (4)	0.032 (2)
C(5) <i>A</i>	0.1041 (2)	0.2309 (4)	0.5703 (4)	0.042 (2)
C(6) <i>A</i>	0.0457 (2)	0.2038 (5)	0.5136 (4)	0.053 (2)
C(7) <i>A</i>	0.0355 (2)	0.1265 (5)	0.4189 (4)	0.050 (2)
C(8) <i>A</i>	0.0810 (2)	0.0773 (5)	0.3750 (4)	0.047 (2)
C(9) <i>A</i>	0.1954 (2)	0.0726 (4)	0.3986 (4)	0.042 (2)
C(10) <i>A</i>	0.2434 (2)	0.1318 (4)	0.4881 (4)	0.038 (2)
C(11) <i>A</i>	0.2187 (2)	0.1849 (4)	0.5763 (4)	0.032 (2)
C(12) <i>A</i>	0.1523 (2)	0.1775 (4)	0.5366 (4)	0.036 (2)
C(13) <i>A</i>	0.1384 (2)	0.1032 (4)	0.4343 (4)	0.039 (2)
H(1) <i>A</i>	0.317 (2)	0.092 (4)	0.432 (4)	0.06 (1)
H(3) <i>A</i>	0.342 (2)	0.262 (4)	0.751 (4)	0.05 (1)
H(6) <i>A</i>	0.016 (2)	0.234 (4)	0.547 (4)	0.06 (2)
H(8) <i>A</i>	0.076 (2)	0.029 (4)	0.307 (4)	0.05 (1)
O(1) <i>B</i>	0.1674 (2)	-0.0343 (3)	-0.0699 (3)	0.056 (1)
O(2) <i>B</i>	0.4028 (2)	0.0112 (4)	0.0906 (4)	0.070 (2)
O(3) <i>B</i>	0.4333 (2)	0.1481 (4)	0.2244 (4)	0.081 (2)
O(4) <i>B</i>	0.2884 (2)	0.4200 (4)	0.3425 (3)	0.070 (2)
O(5) <i>B</i>	0.2195 (2)	0.4692 (3)	0.1855 (3)	0.068 (2)
O(6) <i>B</i>	0.1601 (2)	0.3420 (4)	0.3223 (4)	0.072 (2)
O(7) <i>B</i>	0.0941 (2)	0.4794 (4)	0.2326 (4)	0.080 (2)
O(8) <i>B</i>	-0.0716 (2)	0.2826 (5)	-0.0462 (4)	0.100 (2)
O(9) <i>B</i>	-0.0572 (2)	0.1040 (4)	-0.1132 (4)	0.074 (2)
N(1) <i>B</i>	0.3940 (2)	0.0938 (4)	0.1539 (4)	0.053 (2)
N(2) <i>B</i>	0.2564 (2)	0.3943 (4)	0.2480 (4)	0.061 (2)
N(3) <i>B</i>	0.1209 (2)	0.3833 (4)	0.2339 (4)	0.067 (2)
N(4) <i>B</i>	-0.0395 (2)	0.1977 (6)	-0.0592 (4)	0.060 (2)
C(1) <i>B</i>	0.2861 (2)	0.0675 (4)	0.0763 (4)	0.043 (2)
C(2) <i>B</i>	0.3315 (2)	0.1333 (5)	0.1464 (4)	0.041 (2)
C(3) <i>B</i>	0.3210 (2)	0.2361 (4)	0.2061 (4)	0.042 (2)
C(4) <i>B</i>	0.2625 (2)	0.2759 (4)	0.1938 (4)	0.040 (2)
C(5) <i>B</i>	0.1059 (2)	0.3031 (5)	0.1299 (4)	0.043 (2)
C(6) <i>B</i>	0.0454 (2)	0.2973 (5)	0.0778 (4)	0.047 (2)
C(7) <i>B</i>	0.0254 (2)	0.2089 (5)	-0.0064 (4)	0.045 (2)
C(8) <i>B</i>	0.0640 (2)	0.1268 (5)	-0.0393 (4)	0.048 (2)
C(9) <i>B</i>	0.1730 (2)	0.0549 (5)	-0.0072 (4)	0.043 (2)
C(10) <i>B</i>	0.2281 (2)	0.1072 (4)	0.0675 (4)	0.037 (2)
C(11) <i>B</i>	0.2141 (2)	0.2115 (4)	0.1261 (4)	0.033 (2)
C(12) <i>B</i>	0.1473 (2)	0.2272 (4)	0.0959 (4)	0.035 (2)
C(13) <i>B</i>	0.1240 (2)	0.1370 (5)	0.0118 (4)	0.041 (2)
H(1) <i>B</i>	0.296 (2)	0.001 (4)	0.035 (4)	0.06 (1)
H(3) <i>B</i>	0.354 (2)	0.281 (4)	0.248 (4)	0.05 (1)
H(6) <i>B</i>	0.022 (2)	0.350 (4)	0.097 (4)	0.06 (2)
H(8) <i>B</i>	0.051 (2)	0.072 (4)	-0.089 (3)	0.05 (1)

Table 2. Bond lengths (Å) and angles (°) for molecules *A* and *B*

	<i>A</i>	<i>B</i>	<i>A</i>	<i>B</i>
O(1)-C(9)	1.205 (6)	1.203 (6)	C(2)-C(3)	1.366 (7)
O(2)-N(1)	1.211 (7)	1.208 (6)	C(3)-C(4)	1.375 (6)
O(3)-N(1)	1.214 (6)	1.223 (6)	C(3)-H(3)	0.91 (5)
O(4)-N(2)	1.213 (6)	1.208 (6)	C(4)-C(11)	1.391 (7)
O(5)-N(2)	1.243 (6)	1.275 (6)	C(5)-C(6)	1.381 (6)
O(6)-N(3)	1.234 (6)	1.283 (6)	C(5)-C(12)	1.381 (6)
O(7)-N(3)	1.219 (7)	1.210 (6)	C(6)-C(7)	1.364 (7)
O(8)-N(4)	1.201 (6)	1.211 (8)	C(6)-H(6)	0.91 (5)
O(9)-N(4)	1.205 (8)	1.217 (7)	C(7)-C(8)	1.370 (7)
N(1)-C(2)	1.476 (6)	1.478 (6)	C(8)-C(13)	1.367 (6)
N(2)-C(4)	1.459 (7)	1.455 (6)	C(8)-H(8)	0.93 (5)
N(3)-C(5)	1.476 (6)	1.468 (7)	C(9)-C(10)	1.478 (6)
N(4)-C(7)	1.475 (6)	1.478 (6)	C(9)-C(13)	1.495 (6)
C(1)-C(2)	1.380 (7)	1.368 (7)	C(10)-C(11)	1.405 (7)
C(1)-C(10)	1.376 (6)	1.378 (6)	C(11)-C(12)	1.487 (6)
C(1)-H(1)	0.93 (5)	0.92 (5)	C(12)-C(13)	1.414 (7)
O(2)-N(1)-O(3)	124.8 (5)	124.7 (5)	C(6)-C(5)-C(12)	121.6 (4)
O(2)-N(1)-C(2)	118.2 (4)	118.3 (4)	C(5)-C(6)-C(7)	119.1 (5)
O(3)-N(1)-C(2)	116.9 (4)	117.0 (4)	C(5)-C(6)-H(6)	117 (3)
O(4)-N(2)-O(5)	123.6 (5)	123.9 (5)	C(7)-C(6)-H(6)	124 (3)
O(4)-N(2)-C(4)	119.7 (4)	120.1 (4)	N(4)-C(7)-C(6)	117.7 (5)
O(5)-N(2)-C(4)	116.4 (4)	115.7 (4)	N(4)-C(7)-C(8)	119.8 (5)
O(6)-N(3)-O(7)	126.2 (5)	124.9 (5)	C(6)-C(7)-C(8)	122.6 (5)
O(6)-N(3)-C(5)	117.2 (4)	116.3 (4)	C(7)-C(8)-C(13)	117.2 (5)
O(7)-N(3)-C(5)	116.6 (4)	118.7 (4)	C(7)-C(8)-H(8)	125 (3)
O(8)-N(4)-O(9)	124.5 (6)	124.2 (6)	C(13)-C(8)-H(8)	117 (3)
O(8)-N(4)-C(7)	118.6 (5)	117.8 (5)	O(1)-C(9)-C(10)	127.9 (4)
O(9)-N(4)-C(7)	116.9 (5)	117.9 (5)	O(1)-C(9)-C(13)	126.8 (4)
C(2)-C(1)-C(10)	116.8 (4)	118.0 (4)	C(10)-C(9)-C(13)	105.2 (4)
C(2)-C(1)-H(1)	125 (3)	118 (3)	C(11)-C(10)-C(9)	127.1 (4)
C(10)-C(1)-H(1)	118 (3)	124 (3)	C(11)-C(10)-C(11)	123.0 (4)
N(1)-C(2)-C(1)	117.7 (4)	118.5 (4)	C(9)-C(10)-C(11)	109.6 (4)
N(1)-C(2)-C(3)	119.4 (4)	119.2 (4)	C(4)-C(11)-C(10)	116.4 (4)
C(1)-C(2)-C(3)	122.7 (4)	122.2 (5)	C(4)-C(11)-C(12)	135.8 (4)
C(2)-C(3)-C(4)	118.9 (4)	118.8 (4)	C(10)-C(11)-C(12)	107.7 (4)
C(2)-C(3)-H(3)	127 (3)	118 (3)	C(5)-C(12)-C(11)	135.7 (4)
C(4)-C(3)-H(3)	114 (3)	122 (3)	C(5)-C(12)-C(13)	116.0 (4)
N(2)-C(4)-C(3)	116.2 (4)	114.7 (4)	C(11)-C(12)-C(13)	108.1 (4)
N(2)-C(4)-C(11)	121.7 (4)	123.2 (4)	C(8)-C(13)-C(9)	127.8 (4)
C(3)-C(4)-C(11)	121.5 (4)	121.8 (4)	C(8)-C(13)-C(12)	123.3 (4)
C(3)-C(5)-C(6)	115.7 (4)	114.3 (4)	C(9)-C(13)-C(12)	108.6 (4)
N(3)-C(5)-C(12)	122.4 (4)	123.0 (4)		

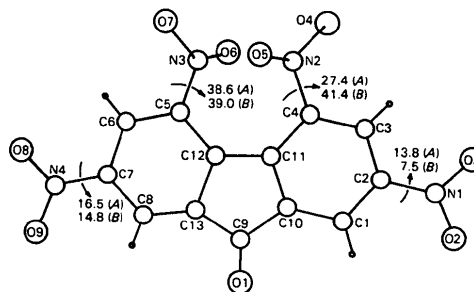


Fig. 1. Molecular structure of 2,4,5,7-tetranitro-9-fluorenone with atomic numbering and some dihedral angles for molecules *A* and *B*.

standard value of 1.22 Å (Sadova & Vilkov, 1982) especially in molecule *B*. For these groups intramolecular O...O distances are O(4)...O(5) 2.165 (6) Å (*A*) and 2.191 (6) Å (*B*), O(6)...O(7) 2.188 (6) Å (*A*) and 2.211 (6) Å (*B*), O(5)...O(6) 2.763 (5) Å (*A*) and 2.700 (6) Å (*B*).

The molecules are packed in layers perpendicular to the *b* axis. The 9-fluorenone plane is approximately perpendicular to the *bc* plane with dihedral angles 88.7° (*A*) and 85.2° (*B*). The intermolecular contacts correspond to normal van der Waals interactions with the shortest distances O(5)*A* (*x*, *y*, *z*)...C(9)*B* ($-x$, $-y$, $1-z$) 2.877 (6) Å, O(9)*A* (*x*, *y*, *z*)...H(8)*B* (*x*, *y*, *z*) 2.42 (4) Å and O(1)*B* (*x*, *y*, *z*)...C(3)*B* ($-\frac{1}{2}-x$, $\frac{1}{2}+y$, $-z$) 3.002 (6) Å.

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The Structure of 2,4,5,7-Tetranitro-9-fluorenone

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Abstract. C₁₃H₄N₄O₉, *M_r* = 360.19, monoclinic, *P*2₁/*a*, *a* = 22.955 (9), *b* = 10.873 (2), *c* = 11.659 (2) Å, β = 103.34 (4)°, *V* = 2832 (1) Å³, *Z* = 8, *D_x* = 1.690 g cm⁻³, monochromated Mo *K*α, λ = 0.71069 Å, μ = 1.59 cm⁻¹, *F*(000) = 1456, *T* = 300 K, *R* = 0.073 for 2747 observed reflections. The asymmetric unit consists of two molecules which differ slightly in their planarities and torsional angles about the C–N bonds. The two benzene rings in the fluorenone skeleton are not coplanar. Each of the C–NO₂ groups are planar. Within the molecules, the N2 and N3 nitro groups are not parallel.

Introduction. 2,4,7-Trinitro-9-fluorenone has been reported to form a charge-transfer complex with hexamethylbenzene (Brown, Cheung, Trefonas & Majeste, 1974). As a prelude to the study in this laboratory of a series of charge-transfer complexes (Baughman, 1982), reasonably accurate distance and angle information for the 2,4,5,7-tetranitro-9-fluorenone (TNF) molecule will be needed.

Experimental. A pale straw crystal 0.30 × 0.30 × 0.35 mm was selected from those recrystallized from an

acetone solution. *hkl* and *hk \bar{l}* octants ($2\theta \leq 45^\circ$, $0 \leq h \leq 24$, $0 \leq k \leq 11$, $-12 \leq l \leq 12$) collected with a Syntex *P*2₁ diffractometer. 4843 reflections yielded 2747 averaged *L_p*-corrected independent reflections with *F_o* > 3σ(*F_o*); 1052 unique reflections were considered unobserved. σ_{*i*}² = *C_T* + *k_iC_B* + (0.03*C_T*)² + (0.03*C_B*)², where *C_T*, *k_i* and *C_B* represent the total count, a counting time factor and the background count, respectively, and the factor 0.03 represents an estimate of nonstatistical errors. The e.s.d.'s in the structure factors were calculated by the finite difference method (Lawton & Jacobson, 1968). No absorption corrections were made (*T* max. = 0.953, *T* min. = 0.946); decomposition was not noted (*I*_{std} ≈ constant). All 52 non-H atoms (2 molecules/asymmetric unit) were located by *MULTAN76* (Main, Woolfson & Germain, 1976), using a partial set of coordinates from 2,4,7-trinitro-9-fluorenone (Brown, Cheung, Trefonas & Majeste, 1974) and a *K* curve to compute the *E* values. The H-atom positions were set at 1.00 Å from the respective C atoms while bisecting the C–C–C angle. Refinement by a full-matrix least-squares procedure (Lapp & Jacobson, 1979) minimizing Σ*w*(|*F_o*| – |*F_c*|)², where *w* = 1/σ_{*i*}², converged