main bond lengths, bond and torsion angles are given in Table 2. Fig. 1 represents a general view of molecule (II), with atomic numbering.

The geometry of the molecule in the monoclinic structure (II) does not differ significantly from that in the triclinic form (I): the maximal difference between the corresponding CSCC torsion angles, which fully define molecular conformations in these structures, is equal to 16°. The configuration of the molecule in structure (II) is closer to the ideal *mm*2 symmetry than in (I): the absolute values of the CSCC torsion angles related by the approximate mirror planes normal to the *A* macrocycle and passing through the midpoints of its S···S edges (Fig. 1) differ on average by 16°, while in the triclinic form the corresponding average difference is 26°. The S_4 tetragon in structure (II) has a much more planar conformation than in structure (I), the dihedral angles between the S(1) S(2) S(3) and the S(1) S(4) S(3) planes being 15·6 and 27·0° respectively. The observed higher symmetry of the molecule in the monoclinic form (II) may be a consequence of a rather interesting trend of simultaneous increase in molecular and packing symmetry, observed to a different extent in crystals of other phenylenesulfides (Sergeev, Ovchinnikov, Nedel'kin, Astankov, Andrianova, Shklover, Zamaev, Struchkov, 1988): the centre of the S_4 cycle is located in the vicinity of $\frac{1}{4},\frac{1}{4},0$ (its exact coordinates are 0·257, 0·248, 0·043) and the enantiomers of one type form layers in the *bc* plane (Fig. 2).

According to Kitaigorodsky (1971), an increase in the packing symmetry is accompanied as a rule by a decrease in the density. Nevertheless, crystal (II) has a higher density than crystal (I): 1·408 and 1·368 Mg m^{-3} respectively. This peculiarity of (II) may be caused by its stronger net intermolecular interaction owing to the contribution of the stacking interactions, in which two (*C* and *E*) of the four benzene rings of each molecule take part (Fig. 2). The higher energy of the intermolecular interaction is also reflected in the higher (by 32 K) melting point of the monoclinic form (II).

The average values of S—C bond lengths, 1·772 Å, and CSC bond angles, 103·6°, in structure (II) differ only slightly from those in structure (I) (1·777 Å and 104·2° respectively); the deviations of the S atoms from the planes of the benzene rings bonded to them do not exceed 0·12 Å, as compared to 0·14 Å in (I). Thus the steric-strain energies in both conformers (I) and (II) are quite close.

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The Structure of T-2 Toxin

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Abstract. T-2 toxin, 12,13-epoxytrichothec-9-ene-3,4,8,15-tetraol 4,15-diacetate 8-(3-methylbutanoate), $C_{24}H_{34}O_9$, M_r = 466·53, orthorhombic, $P2_12_12_1$, a = 7·808 (2), b = 15·800 (4), c = 40·891 (9) Å, V = 5044 (2) Å^3, Z = 8, D_x = 1·228 Mg m^{-3}, λ(Cu $K\alpha$) = 1·54178 Å, μ = 0·74 mm^{-1}, F(000) = 2000, T = 295 K, final R = 0·055, wR = 0·063 for 3434 independent observed reflections. The chemically established structural formula was corroborated. The two molecules in the asymmetric unit differ only in the torsion angles of the ester side chains.

Introduction. T-2 toxin, produced by a mold growing on stored corn, was the first trichothecene to be implicated in animal-feed toxicosis in 1971; since then more than a score have been found which are

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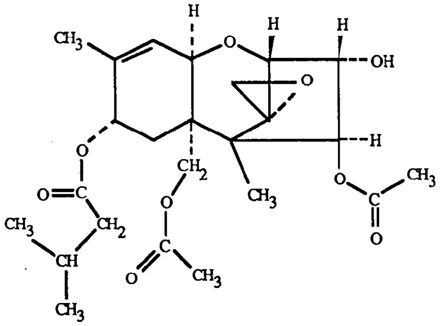
toxic. Trichothecene mycotoxins produce a variety of potent biological effects which damage all types of living cells. They are produced by grain molds and soil fungi (primarily *Fusaria, Myrothecia* and *Trichothecia* species) and may have a natural antimicrobial or phytotoxic role. However, they can damage the health of animals whether ingested, inhaled or topically applied and are thus a public health problem.



The structure of this molecule was determined to aid in the study of the structure–activity relationships in the trichothecene family. Detailed studies are complicated by the existence of a plethora of effects (interference with protein synthesis and DNA replication *in vitro*, local inflammation, internal hemorrhaging, and immunosuppressive disease *in vivo*). Many separate assays of toxicity have been published (Ueno, 1983) using different hosts and measures of damage; although the differences in toxicity of the various trichothecenes range from slight to major in these tests the rank is generally the same. Macrocyclic trichothecenes, so called because a large ring links carbon atoms C4 and C6, are the most toxic. Next most toxic are the non-macrocyclic members which have bulky ester side chains such as T-2 toxin. However, unsubstituted trichothecenes which contain 12,13-epoxy and 9-ene substitution still retain appreciable toxicity.

Table 1. *Atomic coordinates* ($\times 10^4$) *and equivalent isotropic displacement parameters* ($Å^2 \times 10^3$)

	x	*y*	*z*	U_{eq}
O1	951 (4)	6919 (2)	9056 (1)	56 (1)
O2	1522 (4)	7911 (2)	9858 (1)	65 (1)
O3	2440 (4)	9835 (2)	8755 (1)	78 (1)
O4	1487 (7)	10415 (3)	8297 (1)	131 (2)
O5	−1484 (4)	9101 (2)	9564 (1)	68 (1)
O6	−3131 (6)	9814 (2)	9217 (1)	122 (2)
O7	−2544 (4)	7376 (2)	9148 (1)	67 (1)
O8	4839 (4)	8677 (2)	8403 (1)	85 (1)
O9	7576 (5)	8327 (4)	8349 (1)	171 (3)
C2	409 (6)	7173 (3)	9372 (1)	55 (2)
C3	−1285 (6)	7657 (3)	9370 (1)	55 (2)
C4	−813 (6)	8578 (3)	9299 (1)	56 (2)
C5	1188 (5)	8611 (3)	9298 (1)	51 (1)
C6	1836 (5)	8402 (3)	8941 (1)	47 (1)
C7	3796 (6)	8238 (3)	8934 (1)	58 (2)
C8	4506 (6)	7931 (3)	8612 (1)	68 (2)
C9	3391 (7)	7349 (3)	8430 (1)	72 (2)
C10	1803 (6)	7200 (3)	8522 (1)	67 (2)
C11	956 (6)	7588 (3)	8813 (1)	51 (1)
C12	1586 (6)	7829 (3)	9504 (1)	50 (1)
C13	3120 (6)	7664 (3)	9698 (1)	66 (2)
C14	1916 (6)	9434 (3)	9438 (1)	65 (2)
C15	1356 (6)	9101 (3)	8693 (1)	61 (2)
C16	4212 (9)	6880 (4)	8141 (1)	109 (3)
C17	2399 (7)	10441 (3)	8529 (1)	86 (2)
C18	3563 (8)	11148 (3)	8618 (2)	115 (3)
C19	−2677 (6)	9680 (3)	9494 (1)	74 (2)
C20	−3334 (7)	10113 (4)	9787 (1)	100 (3)
C21	6431 (7)	8836 (5)	8307 (1)	113 (3)
C22	6622 (10)	9662 (4)	8113 (1)	128 (3)
C23	6365 (16)	9611 (6)	7791 (2)	258 (8)
C24	6722 (16)	10391 (8)	7603 (2)	344 (10)
C25	4764 (18)	9219 (9)	7670 (3)	487 (15)
O1*A*	5754 (4)	5802 (2)	8993 (1)	65 (1)
O2*A*	2229 (4)	4630 (2)	9376 (1)	87 (1)
O3*A*	7759 (4)	2864 (2)	8925 (1)	73 (1)
O4*A*	10547 (5)	2570 (2)	8921 (1)	98 (2)
O5*A*	5538 (4)	4088 (2)	9848 (1)	70 (1)
O6*A*	8012 (6)	3401 (3)	9888 (1)	163 (2)
O7*A*	6924 (5)	5994 (2)	9629 (1)	76 (1)
O8*A*	8101 (5)	3619 (2)	8257 (1)	87 (1)
O9*A*	6202 (7)	2795 (3)	8014 (1)	172 (3)
C2*A*	4621 (6)	5602 (3)	9254 (1)	63 (2)
C3*A*	5533 (6)	5430 (3)	9575 (1)	64 (2)
C4*A*	6110 (6)	4511 (3)	9556 (1)	55 (2)
C5*A*	5251 (6)	4140 (3)	9242 (1)	58 (2)
C6*A*	6536 (5)	4271 (3)	8945 (1)	51 (1)
C7*A*	5684 (6)	4078 (3)	8611 (1)	69 (2)
C8*A*	6794 (7)	4270 (3)	8318 (1)	77 (2)
C9*A*	7781 (7)	5076 (3)	8347 (1)	76 (2)
C10*A*	7918 (7)	5477 (3)	8629 (1)	70 (2)
C11*A*	7128 (6)	5205 (3)	8941 (1)	57 (2)
C12*A*	3795 (6)	4771 (3)	9192 (1)	64 (2)
C13*A*	2187 (6)	4641 (3)	9023 (1)	85 (2)
C14*A*	4619 (7)	3223 (3)	9283 (1)	73 (2)
C15*A*	8165 (6)	3741 (3)	8985 (1)	57 (2)
C16*A*	8576 (10)	5388 (4)	8032 (1)	118 (3)
C17*A*	9114 (7)	2349 (3)	8901 (1)	77 (2)
C18*A*	8537 (8)	1448 (3)	8847 (2)	115 (3)
C19*A*	6633 (8)	3537 (3)	9992 (1)	90 (2)
C20*A*	5862 (10)	3158 (4)	10288 (1)	119 (3)
C21*A*	7670 (10)	2920 (4)	8088 (1)	112 (3)
C22*A*	9185 (11)	2394 (4)	8010 (2)	121 (3)
C23*A*	10236 (10)	2699 (5)	7738 (2)	141 (4)
C24*A*	11760 (13)	2149 (6)	7669 (2)	185 (5)
C25*A*	9326 (15)	2730 (9)	7429 (2)	308 (9)

Equivalent isotropic *U* defined as one-third of the trace of the orthogonalized U_{ij} tensor.

Experimental. A clear colorless $0{\cdot}10 \times 0{\cdot}15 \times 0{\cdot}62$ mm data crystal was provided by S. Missler of the US Army Medical Research Institute for Infectious Diseases. An automated Nicolet *R*3*m* diffractometer with incident-beam monochromator used 25 centered reflections within $30 \leq 2\theta \leq 53°$ for determining lattice parameters. $[\sin(\theta)/\lambda]_{\max} = 0{\cdot}56$ Å^{-1}, range of *hkl*: $0 \leq h \leq 8$, $0 \leq k \leq 17$, $0 \leq l \leq 45$. Standards 200, 040, 006, monitored every 60 reflections with a random variation of 2·5% over data collection, $\theta/2\theta$ mode, scan width $[2\theta(K\alpha_1) - 1{\cdot}0]$ to $[2\theta(K\alpha_2) + 1{\cdot}0]°$, scan rate a function of count rate (4·0° min^{-1} minimum, 29° min^{-1} maximum), 4528 reflections measured, 4267 unique, $R_{\rm int} = 0{\cdot}0045$, 3434 observed with $F_o > 3\sigma(F_o)$. Data corrected for Lorentz and polarization, but not absorption effects. Structure solved by trial of 1000 random phase set assignments followed by tangent-formula expansion of phase sets and assessment by NQEST criterion (*SHELXTL*; Sheldrick, 1980). The least-squares refinement also used program *SHELXTL*. $\sum w(|F_o| - |F_c|)^2$ minimized where $w = 1/[\sigma^2(|F_o|) + gF_o^2]$, $g = 0{\cdot}0006$. Secondary-extinction parameter *p*

$= 0{\cdot}0008$ (1) in $F_c^* = F_c/[1{\cdot}0 + 0{\cdot}002pF_o^2/\sin(2\theta)]^{0{\cdot}25}$. 638 parameters were refined: atom coordinates, anisotropic thermal parameters for all non-H atoms, atom coordinates for hydroxyl H atoms, other H atoms included using riding model in *SHELXTL*, H riding on C, C—H = 0·96 Å, $U(\mathrm{H}) = 1{\cdot}1\ U_{\mathrm{eq}}(\mathrm{C})$ (methylenes, methines), $U(\mathrm{H}) = 1{\cdot}2\ U_{\mathrm{eq}}(\mathrm{C})$ (methyls, hydroxyls). $(\Delta/\sigma)_{\max} = 0{\cdot}7$ (methyl rotations), $R = 0{\cdot}055$, $wR = 0{\cdot}062$, $S = 1{\cdot}54$. Final difference Fourier excursions 0·21 and −0·23 e Å^{-3}. Atomic scattering factors from *International Tables for X-ray Crystallography* (1974).†

Discussion. Table 1 lists the coordinates and U_{eq} for the two T-2 toxin molecules in the asymmetric unit and atom numbering follows that given in Fig. 1; molecule *A*, not displayed, is numbered similarly. The chirality shown in the figure was chosen to conform to the absolute configuration of verrucarin A (McPhail & Sim, 1966). The primary difference between the molecules in the asymmetric unit is the respective orientation of the methylbutanoate group; torsions C7—C8—O8—C21 and C21—C22—C23—C25 are 118·0 and 52·4° (83·4 and −61·8° for molecule *A*). The methyls of this side chain have large thermal parameters for C23, C24, C25, and to a lesser extent C25*A*, which indicate the presence of a disorder; however, it was not resolvable as a discrete disorder. Bond lengths and angles are listed in Table 2.

In T-2 toxin the hydroxyl at C3 is *endo* with respect to the ring system and *trans* to both the acetate at C4 and the methyl at C5. The bond distances, bond angles, and torsion angles of the trichothecene moiety are very similar to those found

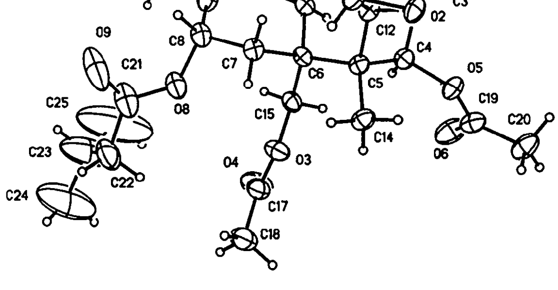


Fig. 1. Thermal-ellipsoid plot of T-2 toxin with ellipsoids drawn at the 20% probability level. The second molecule in the asymmetric unit is very similar and is not shown.

Table 2. *Bond lengths* (Å) *and bond angles* (°)

C2—O1	1·417 (5)	C2—C3	1·527 (6)
C2—C12	1·486 (6)	C3—O7	1·409 (5)
C3—C4	1·530 (6)	C4—O5	1·461 (5)
C4—C5	1·564 (6)	C5—C6	1·578 (5)
C5—C12	1·528 (6)	C5—C14	1·530 (6)
C6—C7	1·552 (6)	C6—C11	1·549 (6)
C6—C15	1·546 (6)	C7—C8	1·507 (6)
C8—O8	1·479 (6)	C8—C9	1·471 (7)
C9—C10	1·317 (7)	C9—C16	1·534 (7)
C10—C11	1·494 (6)	C11—O1	1·450 (5)
C12—O2	1·458 (4)	C12—C13	1·461 (6)
C13—O2	1·462 (6)	C15—O3	1·459 (5)
C17—O3	1·330 (6)	C17—O4	1·186 (7)
C17—C18	1·485 (8)	C19—O5	1·337 (5)
C19—O6	1·204 (6)	C19—C20	1·474 (7)
C21—O8	1·327 (7)	C21—O9	1·214 (8)
C21—C22	1·535 (9)	C22—C23	1·336 (9)
C23—C24	1·480 (9)	C23—C25	1·481 (9)
C2*A*—O1*A*	1·422 (5)	C2*A*—C3*A*	1·519 (6)
C2*A*—C12*A*	1·484 (7)	C3*A*—O7*A*	1·422 (6)
C3*A*—C4*A*	1·523 (6)	C4*A*—O5*A*	1·440 (5)
C4*A*—C5*A*	1·562 (6)	C5*A*—C12*A*	1·526 (6)
C5*A*—C14*A*	1·539 (6)	C6*A*—C7*A*	1·549 (6)
C6*A*—C11*A*	1·547 (6)	C6*A*—C15*A*	1·531 (6)
C7*A*—C8*A*	1·511 (6)	C8*A*—O8*A*	1·471 (6)
C8*A*—C9*A*	1·493 (7)	C9*A*—C10*A*	1·320 (7)
C9*A*—C16*A*	1·514 (8)	C10*A*—C11*A*	1·480 (6)
C11*A*—O1*A*	1·444 (5)	C11*A*—C10*A*	1·480 (6)
C12*A*—O2*A*	1·454 (6)	C12*A*—C13*A*	1·448 (7)
C13*A*—O2*A*	1·446 (6)	C15*A*—O3*A*	1·443 (5)
C17*A*—O3*A*	1·338 (6)	C17*A*—O4*A*	1·174 (7)
C17*A*—C18*A*	1·510 (7)	C19*A*—O5*A*	1·357 (6)
C19*A*—O6*A*	1·178 (7)	C19*A*—C20*A*	1·476 (8)
C21*A*—O8*A*	1·345 (7)	C21*A*—O9*A*	1·201 (9)
C21*A*—C22*A*	1·480 (9)	C22*A*—C23*A*	1·463 (9)
C23*A*—C24*A*	1·500 (2)	C23*A*—C25*A*	1·452 (2)

C2—O1—C11	114·7 (3)	C12—O2—C13	60·1 (3)
C15—O3—C17	116·0 (4)	C4—O5—C19	118·5 (3)
C8—O8—C21	119·1 (4)	O1—C2—C3	113·3 (3)
O1—C2—C12	110·1 (3)	C3—C2—C12	100·9 (3)
O7—C3—C2	116·7 (3)	O7—C3—C4	110·1 (3)
C2—C3—C4	105·6 (3)	O5—C4—C3	108·1 (3)
O5—C4—C5	109·9 (3)	C3—C4—C5	105·9 (3)
C4—C5—C6	108·4 (3)	C4—C5—C12	100·1 (3)
C6—C5—C12	105·9 (3)	C4—C5—C14	113·5 (3)
C6—C5—C14	113·9 (3)	C12—C5—C14	113·9 (3)
C5—C6—C7	111·6 (3)	C5—C6—C11	110·1 (3)
C7—C6—C11	107·0 (3)	C5—C6—C15	112·3 (3)
C7—C6—C15	110·3 (3)	C11—C6—C15	105·3 (3)
C6—C7—C8	115·6 (3)	O8—C8—C7	108·3 (4)
O8—C8—C9	107·9 (3)	C7—C8—C9	115·2 (4)
C8—C9—C10	121·6 (4)	C8—C9—C16	116·5 (5)
C10—C9—C16	121·8 (5)	C9—C10—C11	124·9 (4)
O1—C11—C6	112·1 (3)	C1—C11—C10	104·3 (3)
C6—C11—C10	114·4 (4)	O2—C12—C2	113·7 (3)
O2—C12—C5	118·0 (3)	C2—C12—C5	103·8 (3)
O2—C12—C13	60·1 (2)	C2—C12—C13	125·5 (4)
C5—C12—C13	127·7 (4)	O2—C13—C12	59·8 (3)
O3—C15—C6	108·3 (3)	O3—C17—O4	122·9 (5)
O3—C17—C18	110·8 (5)	O4—C17—C18	126·2 (5)
O5—C19—O6	121·8 (4)	O5—C19—C20	112·7 (4)
O6—C19—C20	125·5 (5)	O8—C21—O9	121·5 (6)
O8—C21—C22	113·9 (5)	O9—C21—C22	124·3 (6)
C21—C22—C23	116·3 (6)	C22—C23—C24	115·8 (5)
C22—C23—C25	118·8 (6)	C24—C23—C25	109·5 (6)
C2*A*—O1*A*—C11*A*	115·4 (3)	C12*A*—O2*A*—C13*A*	59·9 (3)
C15*A*—O3*A*—C17*A*	115·0 (3)	C4*A*—O5*A*—C19*A*	117·7 (4)
C8*A*—O8*A*—C21*A*	119·2 (4)	O1*A*—C2*A*—C3*A*	113·4 (4)
O1*A*—C2*A*—C12*A*	109·8 (3)	C3*A*—C2*A*—C12*A*	101·2 (4)
O7*A*—C3*A*—C2*A*	112·4 (4)	O7*A*—C3*A*—C4*A*	112·3 (4)
C2*A*—C3*A*—C4*A*	105·3 (3)	O5*A*—C4*A*—C3*A*	107·9 (3)
O5*A*—C4*A*—C5*A*	111·9 (3)	C3*A*—C4*A*—C5*A*	105·9 (3)
C4*A*—C5*A*—C6*A*	107·8 (3)	C4*A*—C5*A*—C12*A*	100·6 (3)
C6*A*—C5*A*—C12*A*	106·5 (3)	C4*A*—C5*A*—C14*A*	113·7 (4)
C6*A*—C5*A*—C14*A*	114·1 (4)	C12*A*—C5*A*—C14*A*	113·0 (4)
C5*A*—C6*A*—C7*A*	112·1 (3)	C5*A*—C6*A*—C11*A*	108·9 (3)
C7*A*—C6*A*—C11*A*	107·7 (3)	C5*A*—C6*A*—C15*A*	111·9 (3)
C7*A*—C6*A*—C15*A*	110·0 (3)	C11*A*—C6*A*—C15*A*	106·0 (3)
C6*A*—C7*A*—C8*A*	114·5 (4)	O8*A*—C8*A*—C7*A*	113·2 (4)
O8*A*—C8*A*—C9*A*	104·6 (4)	C7*A*—C8*A*—C9*A*	113·8 (4)
C8*A*—C9*A*—C10*A*	121·4 (4)	C8*A*—C9*A*—C16*A*	114·9 (4)
C10*A*—C9*A*—C16*A*	123·6 (5)	C9*A*—C10*A*—C11*A*	125·4 (5)
O1*A*—C11*A*—C6*A*	113·5 (3)	O1*A*—C11*A*—C10*A*	104·4 (3)
C6*A*—C11*A*—C10*A*	114·3 (4)	O2*A*—C12*A*—C2*A*	114·3 (4)
O2*A*—C12*A*—C5*A*	117·3 (4)	C2*A*—C12*A*—C5*A*	103·4 (4)
O2*A*—C12*A*—C13*A*	59·8 (3)	C2*A*—C12*A*—C13*A*	125·7 (4)

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† Lists of structure factors, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52312 (34 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 2 (*cont.*)

C5*A*—C12*A*—C13*A*	128·1 (4)	O2*A*—C13*A*—C12*A*	60·3 (3)
O3*A*—C15*A*—C6*A*	108·9 (3)	O3*A*—C17*A*—O4*A*	124·6 (4)
O3*A*—C17*A*—C18*A*	110·3 (5)	O4*A*—C17*A*—C18*A*	125·1 (5)
O5*A*—C19*A*—O6*A*	122·2 (5)	O5*A*—C19*A*—C20*A*	111·1 (5)
O6*A*—C19*A*—C20*A*	126·7 (6)	O8*A*—C21*A*—O9*A*	120·2 (6)
O8*A*—C21*A*—C22*A*	111·8 (6)	O9*A*—C21*A*—C22*A*	128·0 (6)
C21*A*—C22*A*—C23*A*	115·3 (6)	C22*A*—C23*A*—C24*A*	113·4 (7)
C22*A*—C23*A*—C25*A*	113·5 (8)	C24*A*—C23*A*—C25*A*	104·1 (7)

in other mycotoxins: isororidin E (Flippen-Anderson & Gilardi, 1986), mycotoxin A and B, (Jarvis, Cömezoğlu, Lee, Flippen-Anderson, Gilardi & George, 1986) and verrucarin A (McPhail & Sim, 1966). The major feature of the packing is the presence of three-centered intermolecular hydrogen bonding in which O7 acts as a donor to both O1*A* ($x - 1, y, z$) and O7*A* ($x - 1, y, z$). Hydrogen bonding also occurs when O7*A* acts as a donor to O2 ($x + 0{\cdot}5,\ 1{\cdot}5 - y,\ 2 - z$). The respective hydrogen bond parameters for H···O, O···O, and ∠O—H···O are 2·30 (4), 2·20 (4), 1·88 (4) Å; 2·97 (1), 2·89 (1), 2·74 (1) Å; and 134 (3), 136 (3) and 159 (3)° respectively. No other contacts less than van der Waals distances occur.

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Structure of Ethyl (2,4,6-Trinitrophenyl)carbamate

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Abstract. $C_9H_8N_4O_8$, $M_r = 300{\cdot}21$, monoclinic, $P2_1$, $a = 4{\cdot}978\,(2)$, $b = 6{\cdot}974\,(2)$, $c = 17{\cdot}991\,(6)$ Å, $\beta = 94{\cdot}69\,(3)°$, $V = 622{\cdot}7\,(3)$ Å^3, $Z = 2$, $D_x = 1{\cdot}60$ Mg m^{-3}, $\lambda(\text{Mo } K\alpha) = 0{\cdot}71073$ Å, $\mu = 0{\cdot}134$ mm^{-1}, $F(000) = 308$, $T = 225$ K, final $R = 0{\cdot}058$, $wR = 0{\cdot}063$ for 769 independent reflections. This trinitroaromatic compound forms an *intermolecular* hydrogen bond rather than a possible *intramolecular* hydrogen bond which would constrain one nitro group to be coplanar with the phenyl ring. The molecules form a hydrogen-bonded chain along the *a* axis.

Introduction. The crystal structure of the title compound was determined as part of an ongoing study of structure–reactivity relationships in polynitroaromatic compounds. Such compounds find application as propellants and explosives. A combination of quantum-mechanical (INDO) calculations and structural parameters (C—NO_2 distances) has been used (Delpuech & Cherville, 1979) to correlate sensitivity of explosives. Hence, structural data are needed to test the validity of this and other structure–reactivity correlations.

Experimental. A clear, colorless 0·03 × 0·22 × 0·48 mm data crystal from material supplied by Dr Paul Bolduc, Eglin Air Force Base. Automated Nicolet *R*3*m* diffractometer with incident beam monochromator. 25 centered reflections within $21 \le 2\theta \le 30°$ used for determining lattice parameters. $[\sin(\theta)/\lambda]_{\max} = 0{\cdot}54$ Å^{-1}, range of *hkl*: $0 \le h \le 5$, $-7 \le k \le 0$, $-19 \le l \le 19$. Standards $\bar{1}\bar{1}0$, $\bar{1}\bar{3}0$, 006 monitored every 100 reflections showed no decrease in intensity. θ–2θ mode, θ scan width 0·9°, θ scan rate a function of count rate, 3° min^{-1} minimum, 15°

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