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## Key indicators

Single-crystal X-ray study  
 $T = 298\text{ K}$   
Mean  $\sigma(\text{C}-\text{C}) = 0.005\text{ \AA}$   
 $R$  factor = 0.043  
 $wR$  factor = 0.151  
Data-to-parameter ratio = 13.9For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

## Propiophenone 2,4-dinitrophenylhydrazone

Crystals of the title compound,  $\text{C}_{15}\text{H}_{14}\text{N}_4\text{O}_4$ , were obtained from a condensation reaction between 2,4-dinitrophenylhydrazine and propiophenone. The compound crystallizes in an *E* configuration. Within the dinitrophenyl ring the distances [average  $1.417(4)\text{ \AA}$ ] of C—C bonds *ipso* to the amino group are significantly longer than the average distance of  $1.375(4)\text{ \AA}$  for the other C—C bonds in the same phenyl ring. The van der Waals contact between the methyl and nitro groups from neighboring molecules results in the deviation of the ethyl group from the phenyl plane of the propiophenone group.

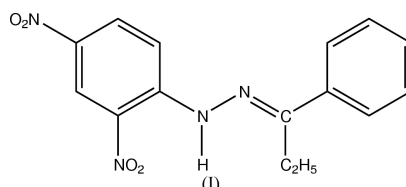
Received 19 November 2002

Accepted 25 November 2002

Online 30 November 2002

## Comment

As some phenylhydrazone derivatives have been shown to be potentially DNA damaging and mutagenic agents (Okabe *et al.*, 1993), a series of new phenylhydrazone derivatives have been synthesized in the laboratory. In order to investigate the relationship of the biological activity and the molecular structure, the X-ray structure determination of the title compound, (I), was carried out and is presented here.



The molecular structure of (I) is shown in Fig. 1. The molecule has an *E* configuration. Within the C1-phenyl ring, an appreciable difference in C—C bond distances is observed; this is consistent with the situation in acetophenone 2,4-dinitrophenylhydrazone (Shan *et al.*, 2002). The N3···O4 separation of  $2.611(3)\text{ \AA}$  and the N3—H3···O4 angle of  $128^\circ$

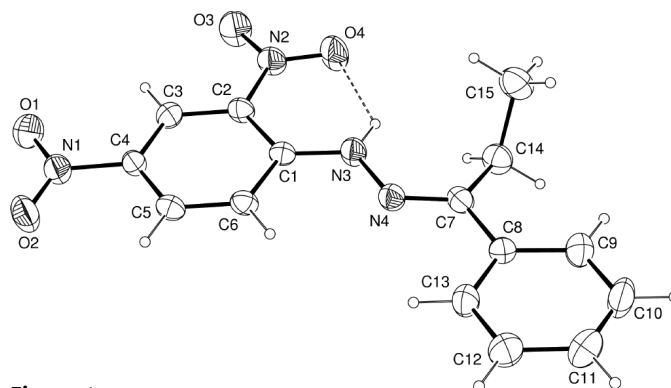
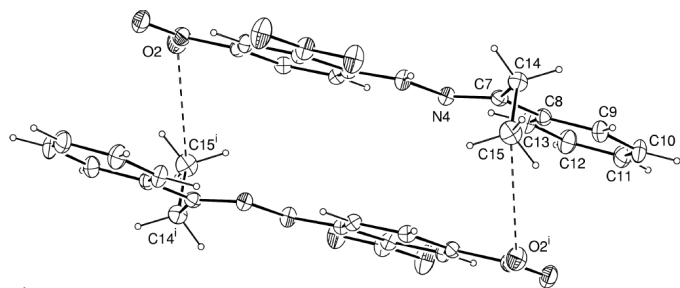


Figure 1

The structure of the title compound with 30% probability displacement ellipsoids.



**Figure 2**

A view showing the van der Waals contact between the C15-methyl and N1-nitro groups. [Symmetry code: (i)  $1 - x, 1 - y, 1 - z$ .]

suggest the existence of intramolecular hydrogen bonding between the amino and the neighboring nitro groups.

The  $C15 \cdots O2(1 - x, 1 - y, 1 - z)$  separation of  $3.418(5) \text{ \AA}$  suggests there is a van der Waals contact between the C15-methyl group and the N1-nitro group of the neighboring molecule. This may be responsible for the twist of the C14/C7/N4 plane from the C8-phenyl ring plane, indicated by the interplanar angle of  $11.2(2)^\circ$  and the atomic displacements of  $0.302(2)$  (C14) and  $-0.162(3) \text{ \AA}$  (N4) from the C8-phenyl plane, as shown in Fig. 2.

## Experimental

$H_2SO_4$  (98%, 0.5 ml) was added dropwise to an ethanol solution (20 ml) containing 2,4-dinitrophenylhydrazine (0.40 g, 0.2 mmol) at 333 K. Then propiophenone (0.27 g, 0.2 mmol) was added slowly to the above solution with continuous stirring. Red crystals of the title compound appeared immediately. The solution was cooled to room temperature and the crystals isolated. Recrystallization was performed twice, from chloroform and acetone in turn, to obtain well-shaped single crystals.

### Crystal data

$C_{15}H_{14}N_4O_4$   
 $M_r = 314.30$   
 Monoclinic,  $P2_1/c$   
 $a = 13.976(2) \text{ \AA}$   
 $b = 15.380(4) \text{ \AA}$   
 $c = 7.0465(18) \text{ \AA}$   
 $\beta = 101.38(2)^\circ$   
 $V = 1484.9(6) \text{ \AA}^3$   
 $Z = 4$

$D_x = 1.406 \text{ Mg m}^{-3}$   
 Mo  $K\alpha$  radiation  
 Cell parameters from 25 reflections  
 $\theta = 4.6\text{--}12.5^\circ$   
 $\mu = 0.11 \text{ mm}^{-1}$   
 $T = 298(2) \text{ K}$   
 Prism, red  
 $0.55 \times 0.45 \times 0.35 \text{ mm}$

### Data collection

Rigaku AFC-7S diffractometer  
 $\omega/2\theta$  scans  
 3168 measured reflections  
 2920 independent reflections  
 1124 reflections with  $I > 2\sigma(I)$   
 $R_{int} = 0.065$   
 $\theta_{max} = 26.0^\circ$

$h = -17 \rightarrow 16$   
 $k = -18 \rightarrow 0$   
 $l = 0 \rightarrow 8$   
 3 standard reflections  
 every 150 reflections  
 intensity decay: 0.3%

### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.043$   
 $wR(F^2) = 0.151$   
 $S = 0.95$   
 2920 reflections  
 210 parameters  
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0665P)^2]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{max} < 0.001$   
 $\Delta\rho_{max} = 0.19 \text{ e \AA}^{-3}$   
 $\Delta\rho_{min} = -0.17 \text{ e \AA}^{-3}$   
 Extinction correction: *SHELXL97*  
 Extinction coefficient: 0.0064 (13)

**Table 1**

Selected geometric parameters ( $\text{\AA}, ^\circ$ ).

N1—C4	1.450 (4)	N3—N4	1.379 (3)
N2—C2	1.435 (3)	N4—C7	1.289 (3)
N3—C1	1.343 (3)		
O2—N1—O1	123.3 (3)	C1—N3—N4	119.1 (2)
O3—N2—O4	121.4 (2)	C7—N4—N3	117.0 (2)

The H atoms were placed in calculated positions, with  $C-H = 0.93\text{--}0.97 \text{ \AA}$  and  $N-H = 0.86 \text{ \AA}$ . The torsion angle of the C15-methyl group was refined. All H atoms were included in the final cycles of refinement in the riding mode, with  $U_{iso}(H) = 1.2U_{eq}$  of carrier atoms.

Data collection: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation, 1992); cell refinement: *MSC/AFC Diffractometer Control Software*; data reduction: *TEXSAN* (Molecular Structure Corporation, 1985); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* (Siemens, 1994); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

The project was supported by the National Natural Science Foundation of China (No. 29973036).

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