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2,5-Di-*p*-tolyl-1,3,4-oxadiazole

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.053
wR factor = 0.156
Data-to-parameter ratio = 13.0

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

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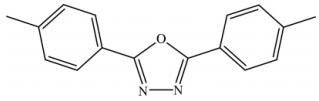
The molecule of the title compound, $C_{16}H_{14}N_2O$, consists of two equivalent parts related by a twofold axis of the space group. The O atom occupies a special position on this twofold axis.

Comment

Compounds containing a 1,3,4-oxadiazole ring as a basic building block are known as scintillator materials or as biologically active agents. Modifications of their chemical structures open up possibilities for new technical applications, for instance as potential electroluminescent materials or as active sensor materials. Also their optical properties should be taken into account, such as their potential for non-linear processes. In particular, polymers of 1,3,4-oxadiazoles show interesting properties, including high thermal resistivity, good environmental stability, doping possibility or mechanical toughness.



(I)

The molecule of the title compound, (I), consists of two equivalent parts related by a twofold axis of the space group. The O atom occupies a special position on this twofold axis. The dihedral angle between the central 1,3,4-oxadiazole ring and the ring of the *p*-tolyl group group is 8.85 (9)°, indicating a nearly planar molecule. Molecules build up layers parallel to the *ac* plane. Within the layers, molecules are held together by strong π–π electron interactions between the oxadiazole ring and the *p*-tolyl groups of neighbouring molecules related by a centre of symmetry of the space group. The shortest intermolecular distance of a benzene C atom to the oxadiazole plane is 3.465 (3) Å.

Experimental

2,5-Di-*p*-tolyl-1,3,4-oxadiazole was synthesized by direct condensation of *p*-toluic acid with hydrazine hydrate in polyphoshoric acid. 2.72 g (0.02 mol) *p*-toluic acid and 0.55 g (0.011 mol) hydrazine hydrate were stirred in 50 g polyphosphoric acid (84.6% P_2O_5 at 433 K for 3 h). After cooling, the clear solution was poured into water, filtered and the product was dried in a vacuum. The product was recrystallized three times from ethanol. The resulting crystals are colourless needles; m.p.: 449 K (literature: 448–449 K; Javaid &

Smith, 1984; Stolle & Stevens, 1904); solid ^{13}C NMR: O—C═N: 163 p.p.m.; CH_3: 22 p.p.m.

Crystal data

$C_{16}H_{14}N_2O$	D_x = 1.277 Mg m^{-3}
M_r = 250.29	Mo $K\alpha$ radiation
Monoclinic, $C2/c$	Cell parameters from 25 reflections
a = 11.404 (2) Å	θ = 12–20°
b = 11.751 (2) Å	μ = 0.08 mm^{-1}
c = 10.870 (1) Å	T = 293 (2) K
β = 116.62 (2)°	Needle, colourless
V = 1302.3 (3) Å^3	0.45 × 0.12 × 0.11 mm
Z = 4	

Data collection

Enraf–Nonius CAD-4 diffractometer	θ_{max} = 25.1°
2θ–ω scans	$h = -13 \rightarrow 12$
Absorption correction: none	$k = 0 \rightarrow 14$
1207 measured reflections	$l = -10 \rightarrow 12$
1155 independent reflections	3 standard reflections
606 reflections with $I > 2\sigma(I)$	frequency: 120 min
R_{int} = 0.030	intensity decay: 0.8%

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.1082P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.053	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2)$ = 0.156	$\Delta\rho_{max}$ = 0.27 e Å^{-3}
S = 0.91	$\Delta\rho_{min}$ = −0.19 e Å^{-3}
1155 reflections	Extinction correction: *SHELXL*97
89 parameters	Extinction coefficient: 0.005 (2)
H-atom parameters constrained	

H-atom positions were calculated corresponding to their geometrical conditions and refined using a riding model.

Data collection: *CAD*-4 *Operations Manual* (Enraf–Nonius, 1977); cell refinement: *CAD*-4 *Operations Manual*; data reduction: *PROCESS* in *MolEN* (Fair, 1990); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL-NT* (Sheldrick, 1999); software used to prepare material for publication: *SHELXL*97.

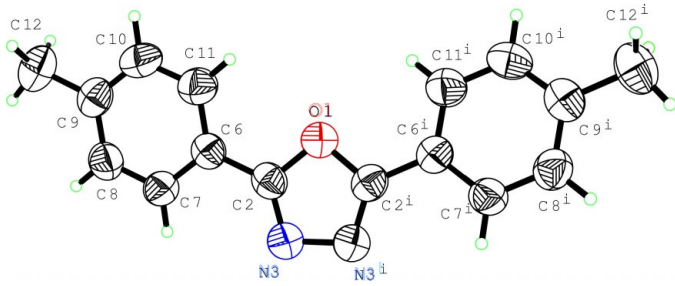


Figure 1
The molecular structure of (I), showing 50% probability displacement ellipsoids (*SHELXTL*; Sheldrick, 1999). H-atom labels have been omitted for clarity. The symmetry transformation i ($-x$, y, $\frac{1}{2} - z$) was used to generate equivalent atoms.

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