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An unexpected *N*-substituted oxindole: 5-methyl-1-(3,3,5-trimethyl-2-*p*-tolyl-1,2-oxazolidin-5-yl)-1*H*-indol-3(2*H*)-one

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Key indicators

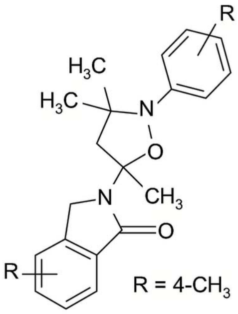
Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.003 Å
R factor = 0.054
wR factor = 0.145
Data-to-parameter ratio = 18.3

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

There are two independent molecules in the asymmetric unit of the title *N*-substituted oxindole, $C_{22}H_{26}N_2O_2$, which was obtained unexpectedly. The heterocyclic rings in both molecules adopt *N*-envelope conformations and the isoindole ring systems are essentially planar.

Comment

The background to this study is set out in the preceding paper (Parvez et al., 2007). In this paper, we report the structure of the *N*-substituted oxindol (4*b*).



(4*b*)

There are two independent molecules in the asymmetric unit of (4*b*) (Figs. 1 and 2); each molecule is composed of a ketonic *p*-methylisoindole group and a trimethyl- and *p*-methylphenyl-substituted isoxazolidine unit. The heterocyclic rings in both molecules adopt envelope conformations, with N1 and N1′ lying 0.736 (3) and 0.715 (2) Å, repectively, out of the planes formed by the other ring atoms. The *p*-methylisoindole units in the two molecules of (4*b*) are also planar, the maximum deviations of atoms from their mean planes being 0.0622 (13) and 0.0814 (14) for N2 and C13′, respectively, while the ketonic O2 and O2′ atoms are 0.132 (2) and 0.254 (2) Å, respectively, out of the ring planes. There are some minor but significant conformational differences in the two molecules of (4*b*), *e.g.* the deviations of pairs of atoms C1/C1′ and C13/C13′ from their respective isoindole ring systems are 0.084 (3), 0.141 (3) and 0.0370 (14), 0.0814 (14) Å, respectively. The structure is devoid of any classical hydrogen bonds. The crystal structure of (4*a*) is reported in the preceding paper (Parvez *et al.*, 2007).

Experimental

The preparation of (4*b*) has been reported previously (Mehrdad *et al.*, 2007). Single crystals of (4*b*) were obtained by slow evaporation from petroleum ether (b.p. 310–330 K) in an ice box.

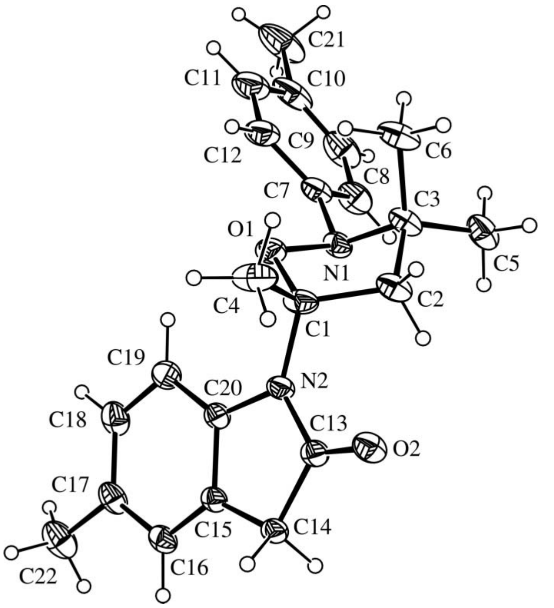


Figure 1
The structure of one of the molecules of (4*b*), with displacement ellipsoids drawn at the 30% probability level.

Crystal data

$C_{22}H_{26}N_2O_2$
$M_r = 350.45$
Monoclinic, $P2_1/c$
$a = 19.390\ (3)$ Å
$b = 14.037\ (3)$ Å
$c = 14.266\ (5)$ Å
$\beta = 96.057\ (8)^\circ$
$V = 3861.2\ (17)$ Å^3
$Z = 8$
$D_x = 1.206$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.08$ mm^{-1}
$T = 173$ (2) K
Block, colorless
0.24 × 0.22 × 0.18 mm

Data collection

Nonius KappaCCD diffractometer
ω and φ scans
Absorption correction: multi-scan (*SORTAV*; Blessing, 1997)
$T_{\min} = 0.982$, $T_{\max} = 0.986$
32322 measured reflections
8752 independent reflections
3897 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.143$
$\theta_{\max} = 27.4^\circ$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.054$
$wR(F^2) = 0.145$
$S = 0.99$
8752 reflections
479 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.06P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.28$ e Å^{-3}
$\Delta\rho_{\min} = -0.32$ e Å^{-3}

H atoms were located in difference Fourier syntheses and were included in the refinement at geometrically idealized positions, with C—H = 0.95, 0.98 and 0.99 Å and $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$.

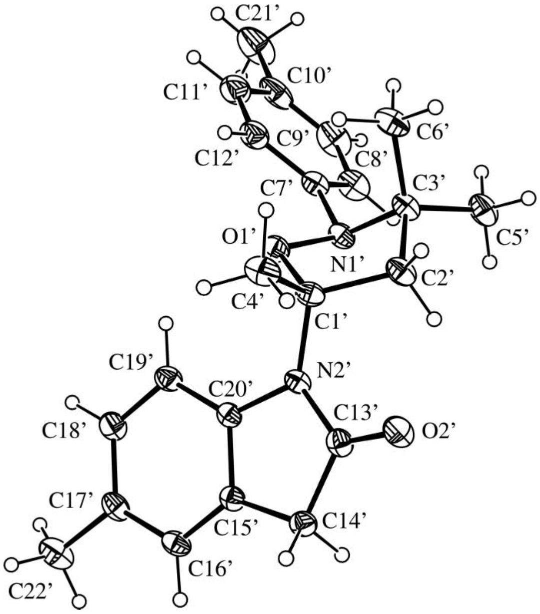


Figure 2
The structure of the other molecule of (4*b*), with displacement ellipsoids drawn at the 30% probability level.

Data collection: *COLLECT* (Hooft, 1998); cell refinement: *DENZO* (Otwinowski & Minor, 1997); data reduction: *SCALEPACK* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SAPI91* (Fan, 1991); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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