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5-Methyl-2-[(*E*)-2-(5-methylbenz[*d*]oxazol-2-yl)vinyl]benz[*d*]oxazole

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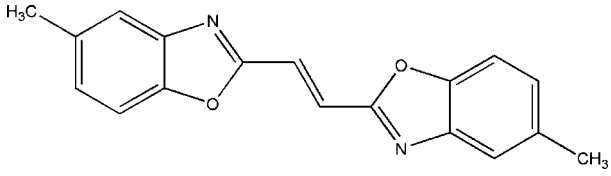
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; disorder in main residue; R factor = 0.055; wR factor = 0.155; data-to-parameter ratio = 15.3.

The title compound, $C_{18}H_{14}N_2O_2$, was prepared by recrystallization from the fluorescent brightener135. The almost perfectly planar molecule is located on a centre of inversion. The methyl H atoms are disordered equally over two positions.

Related literature

For related literature, see: Drew & Leslie (1986); Huseyin *et al.* (1998); Koyama *et al.* (2000).



Experimental

Crystal data

$C_{18}H_{14}N_2O_2$
M_r = 290.31
Monoclinic, $C2/c$
a = 22.153 (4) Å
b = 4.770 (1) Å
c = 14.053 (3) Å
β = 100.94 (3)°
V = 1458.0 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 293 (2) K
0.41 × 0.23 × 0.14 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: none
3101 measured reflections
1560 independent reflections
939 reflections with $I > 2\sigma(I)$
R_{int} = 0.037
3 standard reflections
every 200 reflections
intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.155
S = 1.04
1560 reflections
102 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *CAD-4 Software*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL/PC* (Sheldrick, 1990); software used to prepare material for publication: *SHELXTL/PC*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2434).

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supplementary materials

Acta Cryst. (2007). E**63**, o3887 [**doi:10.1107/S1600536807035362**]

5-Methyl-2-[(*E*)-2-(5-methylbenz[*d*]oxazol-2-yl)vinyl]benz[*d*]oxazole

F.-F. Jian, W. Yi, L.-M. Wang and J. Wang

Comment

Benzoxazoles are compounds having a high fluorescence and are used as optical whitening agents, photoluminescents, and active components in dye lasers (Koyama *et al.*, 2000). Benzoxazole derivatives show antiepileptic, antispasmodic and antifungal properties (Huseyin *et al.*, 1998).

In the title compund, the bond lengths and angles in the two oxazole rings and two benzene rings are normal (Drew *et al.*, 1986). C9—C9A bond distance of 1.332 (4)Å shows double bond character. The whole molecular is nearly planar. There is a π-π stacking interaction between the phenyl ring and oxazole ring at *x*,*y* + 1,*z*. The centroid-centroid distance between the six- and five-membered ring is 3.870Å and the perpendicular distance is 3.454 Å. In addition, there is a C—H···π interaction [C1—H1F$^{\cdots}$cg(C2,C3,C4,C5,C6,C7)^{i}; symmetry operator (i) *x*,*y* − 1,*z*] with a H$^{\cdots}$cg distance of 3.516 Å.

Experimental

The single crystals of the title compound were obtained by recrystalling the industrial product of the fluorescent whitener DT in ethanol and DMF 1:1 (*v*/*v*) for one week at room temperature.

Refinement

H atoms were placed in calculated positions and treated using a riding model, with C—H = 0.93–0.98 Å and with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(C) for methyl H atoms. The methyl group is disordered over two equally occupied positions.

Figures

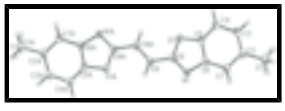


Fig. 1. The molecular structure and atom-labeling scheme for (I), with displacement ellipsoids drawn at the 30% probability level.

5-Methyl-2-[(*E*)-2-(5-methylbenz[*d*]oxazol-2-yl)vinyl]benz[*d*]oxazole

Crystal data

$C_{18}H_{14}N_2O_2$	D_x = 1.323 Mg m^{-3}
M_r = 290.31	Melting point: 182 K
Monoclinic, *C*2/*c*	Mo *K*α radiation λ = 0.71073 Å
a = 22.153 (4) Å	Cell parameters from 25 reflections
b = 4.7700 (10) Å	θ = 1.9–27.0º
c = 14.053 (3) Å	μ = 0.09 mm^{-1}

β = 100.94 (3)°	T = 293 (2) K
V = 1458.0 (5) Å^3	Needle, yellow
Z = 4	0.41 × 0.23 × 0.14 mm
F_{000} = 608	

Data collection

Bruker P4 diffractometer	R_{int} = 0.037
Radiation source: fine-focus sealed tube	θ_{max} = 27.0°
Monochromator: graphite	θ_{min} = 1.9°
T = 293(2) K	h = −27→26
ω scans	k = −5→0
Absorption correction: none	l = −16→16
3101 measured reflections	3 standard reflections
1560 independent reflections	every 200 reflections
939 reflections with $I > 2\sigma(I)$	intensity decay: none

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.055	$w = 1/[\sigma^2(F_o^2) + (0.0866P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.155	$(\Delta/\sigma)_{max} < 0.001$
S = 1.04	$\Delta\rho_{max}$ = 0.24 e Å^{-3}
1560 reflections	$\Delta\rho_{min}$ = −0.27 e Å^{-3}
102 parameters	Extinction correction: SHELXL97, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0060 (17)
Secondary atom site location: difference Fourier map	

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
O1	0.04467 (6)	0.2073 (3)	0.87972 (10)	0.0425 (5)	
N1	0.10077 (8)	0.0570 (4)	1.02211 (13)	0.0403 (5)	
C1	0.22548 (11)	−0.5999 (5)	0.8526 (2)	0.0560 (7)	
H1A	0.2142	−0.7097	0.7947	0.084*	0.50
H1B	0.2303	−0.7206	0.9082	0.084*	0.50
H1C	0.2635	−0.5049	0.8515	0.084*	0.50
H1D	0.2579	−0.5804	0.9082	0.084*	0.50
H1E	0.2417	−0.5695	0.7947	0.084*	0.50
H1F	0.2085	−0.7853	0.8514	0.084*	0.50
C2	0.17573 (10)	−0.3866 (4)	0.85785 (17)	0.0416 (6)	
C3	0.14015 (11)	−0.2845 (5)	0.77202 (18)	0.0480 (6)	
H3A	0.1475	−0.3536	0.7134	0.058*	
C4	0.09443 (11)	−0.0849 (5)	0.77017 (17)	0.0485 (6)	
H4A	0.0710	−0.0185	0.7126	0.058*	
C5	0.08615 (9)	0.0078 (5)	0.85917 (15)	0.0375 (5)	
C6	0.11992 (9)	−0.0854 (4)	0.94600 (15)	0.0360 (5)	
C7	0.16546 (10)	−0.2896 (4)	0.94564 (17)	0.0413 (6)	
H7A	0.1882	−0.3580	1.0035	0.050*	
C8	0.05734 (10)	0.2229 (5)	0.97847 (16)	0.0373 (5)	
C9	0.02220 (9)	0.4192 (4)	1.02433 (16)	0.0402 (6)	
H9A	0.0311	0.4336	1.0915	0.048*	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0460 (9)	0.0372 (9)	0.0439 (9)	0.0071 (7)	0.0077 (6)	−0.0039 (7)
N1	0.0476 (11)	0.0308 (10)	0.0438 (10)	0.0025 (9)	0.0121 (8)	−0.0008 (8)
C1	0.0577 (15)	0.0356 (13)	0.0782 (19)	0.0041 (12)	0.0220 (13)	−0.0083 (12)
C2	0.0421 (12)	0.0247 (11)	0.0610 (15)	−0.0045 (10)	0.0173 (11)	−0.0061 (10)
C3	0.0557 (14)	0.0419 (14)	0.0491 (14)	−0.0031 (12)	0.0165 (11)	−0.0142 (11)
C4	0.0519 (14)	0.0504 (15)	0.0422 (13)	0.0027 (12)	0.0060 (10)	−0.0063 (11)
C5	0.0381 (11)	0.0303 (12)	0.0454 (12)	0.0000 (10)	0.0108 (9)	−0.0053 (10)
C6	0.0419 (12)	0.0262 (11)	0.0419 (12)	−0.0035 (10)	0.0131 (9)	−0.0025 (9)
C7	0.0441 (12)	0.0286 (12)	0.0510 (14)	0.0029 (10)	0.0087 (10)	0.0029 (10)
C8	0.0417 (11)	0.0307 (11)	0.0405 (12)	−0.0031 (10)	0.0104 (9)	−0.0028 (10)
C9	0.0457 (13)	0.0313 (12)	0.0458 (13)	−0.0021 (10)	0.0144 (10)	−0.0060 (9)

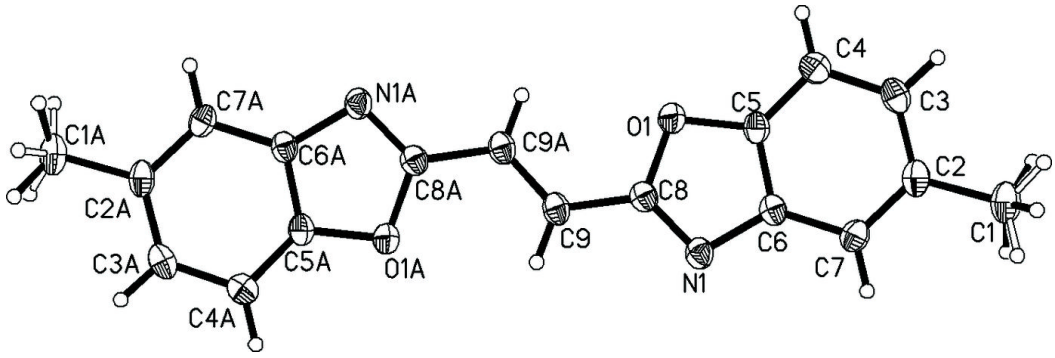
Geometric parameters (Å, °)

O1—C8	1.365 (3)	C2—C3	1.397 (3)
O1—C5	1.391 (2)	C3—C4	1.387 (3)
N1—C8	1.305 (3)	C3—H3A	0.9300
N1—C6	1.399 (3)	C4—C5	1.371 (3)
C1—C2	1.512 (3)	C4—H4A	0.9300
C1—H1A	0.9600	C5—C6	1.378 (3)

C1—H1B	0.9600	C6—C7	1.403 (3)
C1—H1C	0.9600	C7—H7A	0.9300
C1—H1D	0.9600	C8—C9	1.445 (3)
C1—H1E	0.9600	C9—C9^{i}	1.332 (4)
C1—H1F	0.9600	C9—H9A	0.9300
C2—C7	1.376 (3)		
C8—O1—C5	103.41 (16)	C7—C2—C1	121.1 (2)
C8—N1—C6	103.80 (18)	C3—C2—C1	119.3 (2)
C2—C1—H1A	109.5	C4—C3—C2	123.1 (2)
C2—C1—H1B	109.5	C4—C3—H3A	118.5
H1A—C1—H1B	109.5	C2—C3—H3A	118.5
C2—C1—H1C	109.5	C5—C4—C3	115.3 (2)
H1A—C1—H1C	109.5	C5—C4—H4A	122.3
H1B—C1—H1C	109.5	C3—C4—H4A	122.3
C2—C1—H1D	109.5	C4—C5—C6	124.0 (2)
H1A—C1—H1D	141.1	C4—C5—O1	128.2 (2)
H1B—C1—H1D	56.3	C6—C5—O1	107.82 (17)
H1C—C1—H1D	56.3	C5—C6—N1	109.12 (18)
C2—C1—H1E	109.5	C5—C6—C7	119.39 (19)
H1A—C1—H1E	56.3	N1—C6—C7	131.5 (2)
H1B—C1—H1E	141.1	C2—C7—C6	118.5 (2)
H1C—C1—H1E	56.3	C2—C7—H7A	120.7
H1D—C1—H1E	109.5	C6—C7—H7A	120.7
C2—C1—H1F	109.5	N1—C8—O1	115.84 (19)
H1A—C1—H1F	56.3	N1—C8—C9	126.5 (2)
H1B—C1—H1F	56.3	O1—C8—C9	117.67 (19)
H1C—C1—H1F	141.1	C9^{i}—C9—C8	123.6 (3)
H1D—C1—H1F	109.5	C9^{i}—C9—H9A	118.2
H1E—C1—H1F	109.5	C8—C9—H9A	118.2
C7—C2—C3	119.6 (2)		
C7—C2—C3—C4	0.6 (4)	C8—N1—C6—C7	179.4 (2)
C1—C2—C3—C4	−178.7 (2)	C3—C2—C7—C6	−1.2 (3)
C2—C3—C4—C5	0.0 (3)	C1—C2—C7—C6	178.1 (2)
C3—C4—C5—C6	0.0 (3)	C5—C6—C7—C2	1.2 (3)
C3—C4—C5—O1	179.20 (19)	N1—C6—C7—C2	−177.7 (2)
C8—O1—C5—C4	−178.4 (2)	C6—N1—C8—O1	0.2 (2)
C8—O1—C5—C6	0.9 (2)	C6—N1—C8—C9	−179.5 (2)
C4—C5—C6—N1	178.5 (2)	C5—O1—C8—N1	−0.7 (2)
O1—C5—C6—N1	−0.9 (2)	C5—O1—C8—C9	178.99 (17)
C4—C5—C6—C7	−0.7 (3)	N1—C8—C9—C9^{i}	−179.1 (3)
O1—C5—C6—C7	−179.99 (17)	O1—C8—C9—C9^{i}	1.2 (4)
C8—N1—C6—C5	0.4 (2)		

Symmetry codes: (i) −*x*, −*y*+1, −*z*+2.

Fig. 1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C3
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