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***N*}-[(*E*)-Anthracen-9-ylmethylidene]-3,4-dimethyl-1,2-oxazol-5-amine**Abdullah M. Asiri,^{a,b} Abdulrahman O. Al-Youbi,^a
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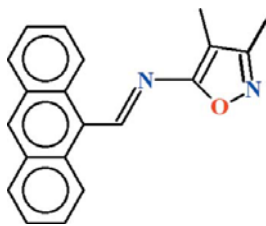
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Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å;
 R factor = 0.044; wR factor = 0.130; data-to-parameter ratio = 15.2.

In the title compound, $\text{C}_{20}\text{H}_{16}\text{N}_2\text{O}$, an intramolecular $\text{C}-\text{H}\cdots\text{N}$ forms an $S(6)$ ring motif. In the crystal, the molecules are stacked with their anthracene ring planes in sheets along [100].

Related literature

For applications of compounds containing azomethine groups, see: Khuhawar *et al.* (2004). Schiff base compounds demonstrate antibacterial (Asiri & Khan, 2010), antitumor activity (Saxena & Tandon, 1983) and anti-HIV activity (Pandeya *et al.*, 1999). For related structures, see: Asiri *et al.* (2011a,b). For graph-set notation, see: Bernstein *et al.* (1995).



Experimental

Crystal data

 $\text{C}_{20}\text{H}_{16}\text{N}_2\text{O}$
 $M_r = 300.35$
Monoclinic, $C2/c$
 $a = 22.4919$ (14) Å $b = 6.1666$ (4) Å
 $c = 22.6801$ (13) Å
 $\beta = 102.015$ (2)°
 $V = 3076.8$ (3) Å³ $Z = 8$ Mo $K\alpha$ radiation
 $\mu = 0.08$ mm⁻¹ $T = 296$ K $0.32 \times 0.24 \times 0.22$ mm

Data collection

Bruker KAPPA APEXII CCD
diffractometer
Absorption correction: multi-scan
(*SADABS*; Sheldrick, 2004)
 $T_{\min} = 0.975$, $T_{\max} = 0.980$ 12925 measured reflections
3193 independent reflections
2381 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.028$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.044$
 $wR(F^2) = 0.130$
 $S = 1.04$
3193 reflections210 parameters
H-atom parameters constrained
 $\Delta\rho_{\max} = 0.26$ e Å⁻³
 $\Delta\rho_{\min} = -0.21$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{C}2-\text{H}2\cdots\text{N}1$	0.93	2.20	2.840 (2)	125

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FK2045).

References

- Asiri, A. M. & Khan, S. A. (2010). *Molecules*, **15**, 6850–6858.
 Asiri, A. M., Khan, S. A. & Tahir, M. N. (2011a). *Acta Cryst.* **E67**, o2163.
 Asiri, A. M., Khan, S. A. & Tahir, M. N. (2011b). *Acta Cryst.* **E67**, o2305.
 Bernstein, J., Davis, R. E., Shimon, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.
 Bruker (2009). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
 Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
 Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
 Khuhawar, M. Y., Mughal, M. A. & Channar, A. H. (2004). *Eur. Polymer J.* **40**, 805–809.
 Pandeya, S. N., Sriram, D., Nath, G. & Clercq, E. De. (1999). *Pharm. Acta Helv.* **74**, 11–17.
 Saxena, A. & Tandon, J. P. (1983). *Cancer Lett.* **19**, 73–76.
 Sheldrick, G. M. (2004). *SADABS*. University of Göttingen, Germany.
 Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
 Spek, A. L. (2009). *Acta Cryst.* **D65**, 148–155.