Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

N-(1,5-Dimethyl-3-oxo-2-phenyl-2,3-dihydro-1*H*-pyrazol-4-yl)acetamide–naphthalene-2,3-diol (1/1)

Abdullah M. Asiri,[a] Salman A. Khan,[a] Kong Wai Tan[b] and Seik Weng Ng[b]*

[a]Chemistry Department, Faculty of Science, King Abdul Aziz University, PO Box 80203, Jeddah 21589, Saudi Arabia, and [b]Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia
Correspondence e-mail: seikweng@um.edu.my

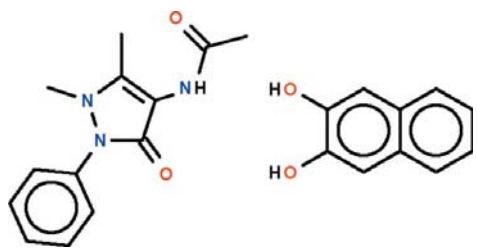
Received 16 June 2010; accepted 23 June 2010

Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; R factor = 0.052; wR factor = 0.131; data-to-parameter ratio = 16.4.

In the reaction of naphthalene-2,3-diol and 4-aminoantipyrine in the presence of acetic acid, the amine function is acetylated and the resulting acetamide co-crystallizes with the diol in the title compound, $C_{13}H_{15}N_3O_2{\cdot}C_{10}H_8O_2$, with 1:1 molar stoichiometry. The two components are linked by two O–H$\cdots$O=C hydrogen bonds. One of the hydroxy groups interacts with the pyrazolone carbonyl O atom and the other hydroxy group interacts with the amide O atom of another component, generating a chain motif. Adjacent chains are linked into a layer motif *via* N—H$\cdots$O interactions involving only the heterocyclic acetamide component.

Related literature

For the crystal structure of 4-acetamido-2,3-dimethyl-1-phenyl-5-pyrazol-3-one, see: Kuznetsov *et al.* (1999). For co-crystals of naphthalene-2,3-diol, see: Fritchie & Johnston (1975); Herbert & Truter (1980); Kuo *et al.* (1974); Nakamatsu *et al.* (2003); Wang *et al.* (2008); Wells *et al.* (1974).



Experimental

Crystal data

$C_{13}H_{15}N_3O_2{\cdot}C_{10}H_8O_2$
M_r = 405.44
Monoclinic, $P2_1/c$
a = 12.426 (1) Å
b = 14.304 (2) Å
c = 12.959 (1) Å
β = 117.845 (1)°
V = 2036.7 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 100 K
0.25 × 0.25 × 0.10 mm

Data collection

Bruker SMART APEX diffractometer
19263 measured reflections
4683 independent reflections
3189 reflections with $I > 2\sigma(I)$
R_{int} = 0.061

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.131
S = 1.02
4683 reflections
286 parameters
27 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 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$
N1—H1$\cdots$O2^{i}	0.87 (1)	2.07 (1)	2.924 (2)	169 (2)
O3—H3$\cdots$O2	0.85 (3)	1.81 (3)	2.639 (2)	163 (3)
O4—H4$\cdots$O1^{ii}	0.85 (3)	1.81 (3)	2.646 (2)	168 (3)

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $x, -y+\frac{3}{2}, z+\frac{1}{2}$.

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: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

We thank King Abdul Aziz University and the University of Malaya for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IM2213).

References

Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
Bruker (2009). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Fritchie, C. J. & Johnston, R. M. (1975). *Acta Cryst.* B**31**, 454–461.
Herbert, J. A. & Truter, M. R. (1980). *J. Chem. Soc. Perkin Trans. 2*, pp. 1253–1258.
Kuo, M. C., Dunn, J. B. R. & Fritchie, C. J. (1974). *Acta Cryst.* B**30**, 1766–1771.
Kuznetsov, M. L., Bel'skii, V. K., Dement'ev, A. I., Zaitsev, B. E., Lokshin, B. V. & Zhornik, V. G. (1999). *Russ. Chem. Bull.* **48**, 1274–1280.
Nakamatsu, S., Yoshizawa, K., Toyota, S., Toda, F. & Matijasic, I. (2003). *Org. Biomol. Chem.* **1**, 2231–2234.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Wang, Y.-T., Tang, G.-M. & Wan, W.-Z. (2008). *Acta Cryst.* E**64**, o1754.
Wells, J. L., Trus, B. L., Johnston, R. M., Marsh, R. E. & Fritchie, C. J. (1974). *Acta Cryst.* B**30**, 1127–1134.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**. Submitted.