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N-(4-Hydroxyphenethyl)acetamide

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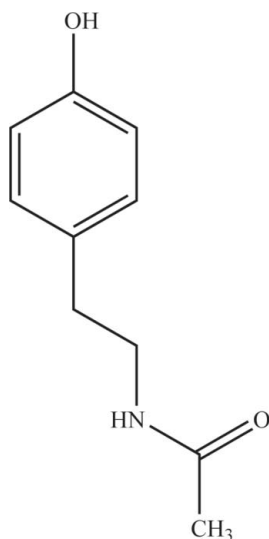
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 Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.037; wR factor = 0.100; data-to-parameter ratio = 14.4.

In the title compound, $\text{C}_{10}\text{H}_{13}\text{NO}_2$, the occurrence of intermolecular $\text{N}-\text{H}\cdots\text{O}$ and $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds between the hydroxy and acetamido groups results in the formation of tetramers with an $R_4^4(25)$ graph-set motif. These tetramers are further assembled, building up a corrugated sheet parallel to (001).

Related literature

For the biological activity of *N*-(4-hydroxyphenethyl)-acetamide, see: Garcez *et al.* (2000); Montedoro *et al.* (1993). For related structures, see: Chai *et al.* (2009); Song *et al.* (2008). For bond-length data, see: Allen *et al.* (1987). For hydrogen-bond motifs, see: Bernstein *et al.* (1995); Etter (1990)



Experimental

Crystal data

 $\text{C}_{10}\text{H}_{13}\text{NO}_2$
 $M_r = 179.21$

 Monoclinic, $P2_1/c$
 $a = 9.9206$ (13) Å
 $b = 8.7861$ (11) Å
 $c = 11.4943$ (16) Å
 $\beta = 102.9980$ (10)°
 $V = 976.2$ (2) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.09$ mm⁻¹
 $T = 298$ K
 $0.43 \times 0.38 \times 0.20$ mm

Data collection

 Bruker SMART CCD diffractometer
 Absorption correction: multi-scan (*SADABS*; Sheldrick, 2008a)
 $T_{\min} = 0.961$, $T_{\max} = 0.978$

 4753 measured reflections
 1713 independent reflections
 1196 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.027$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.037$
 $wR(F^2) = 0.100$
 $S = 1.05$
 1713 reflections

 119 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.16$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.14$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N1}-\text{H1}\cdots\text{O1}^i$	0.86	2.08	2.9048 (18)	161
$\text{O1}-\text{H1A}\cdots\text{O2}^{ii}$	0.82	1.83	2.6464 (17)	174

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008b); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008b); molecular graphics: *ORTEP-III* (Burnett & Johnson, 1996), *ORTEP-3 for Windows* (Farrugia, 1997) and *CAMERON* (Pearce *et al.*, 2000); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008b).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2469).

References

- Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
- Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.
- Bruker (1998). *SMART*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Bruker (1999). *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Burnett, M. N. & Johnson, C. K. (1996). *ORTEP-III*. Report ORNL-6895. Oak Ridge National Laboratory, Tennessee, USA.
- Chai, Y., Wan, Z.-L., Guo, H.-Y. & Liu, M.-L. (2009). *Acta Cryst. E* **65**, o282.
- Etter, M. C. (1990). *Acc. Chem. Res.* **23**, 120–126.
- Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
- Garcez, W. S., Martins, D. & Garcez, F. R. (2000). *J. Agric. Food Chem.* **48**, 3662–3665.
- Montedoro, G., Servili, M. & Baldioli, M. (1993). *J. Agric. Food Chem.* **41**, 2228–2234.
- Pearce, L., Prout, C. K. & Watkin, D. J. (2000). *CAMERON*. Chemical Crystallography Laboratory, University of Oxford, England.
- Sheldrick, G. M. (2008a). *SADABS*. University of Göttingen, Germany.
- Sheldrick, G. M. (2008b). *Acta Cryst. A* **64**, 112–122.
- Song, W.-L., Wang, D., Li, X.-H. & Wang, D.-C. (2008). *Acta Cryst. E* **64**, o785.

supporting information

Acta Cryst. (2009). E65, o1789 [doi:10.1107/S1600536809025409]

N*-(4-Hydroxyphenethyl)acetamide*Bo Wang, Yun Chai, Peizhen Tao and Mingliang Liu****S1. Comment**

N-(4-Hydroxyphenethyl)acetamide displays various biological activities (Garcez *et al.*, 2000; Montedoro *et al.*, 1993; Allen *et al.*, 1987), we report herein the crystal structure of the title compound.

In the molecule of the title compound (Fig 1), all of the bond lengths and angles are within normal ranges. the occurrence of intermolecular N–H···O and O–H···O hydrogen bonds between the hydroxy and acetamido groups results in the formation of tetramers with a $R_4^4(25)$ graph set motif (Etter, 1990; Bernstein *et al.*, 1995). These tetrameric motifs are further assemble to build up a corrugated sheet parallel to the (0 0 1) plane (Table 1, Fig. 2).

The bond lengths and bond angles agree with the values observed in related structures (Chai *et al.*, 2009; Song *et al.*, 2008).

S2. Experimental

The title compound was separated from fermentation liquor as a white solid. Single crystals suitable for X-ray analysis were obtained by slow evaporation of a methanol/water solution(2:1 v/v). ¹H NMR (DMSO-*d*₆, δ): 9.14 (1H, s, OH), 7.84 (1H, br, NH), 6.96 (2H, d, PhH₂), 6.66 (2H, d, PhH₂), 3.14–3.19 (2H, m, CH₂), 2.49–2.57 (2H, m, CH₂), 1.77 (3H, s, CH₃). MS(FAB, m/z): 180 (*M*+H)⁺.

S3. Refinement

All H atom were placed at calculated positions, with C—H = 0.96–0.97 Å and N—H = 0.86 Å, and were included in the final cycles of refinement using a riding model, with $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C}, \text{N})$ or $1.5 U_{\text{eq}}(\text{methyl C})$. The H of the methyl group were statistically disordered over two positions.

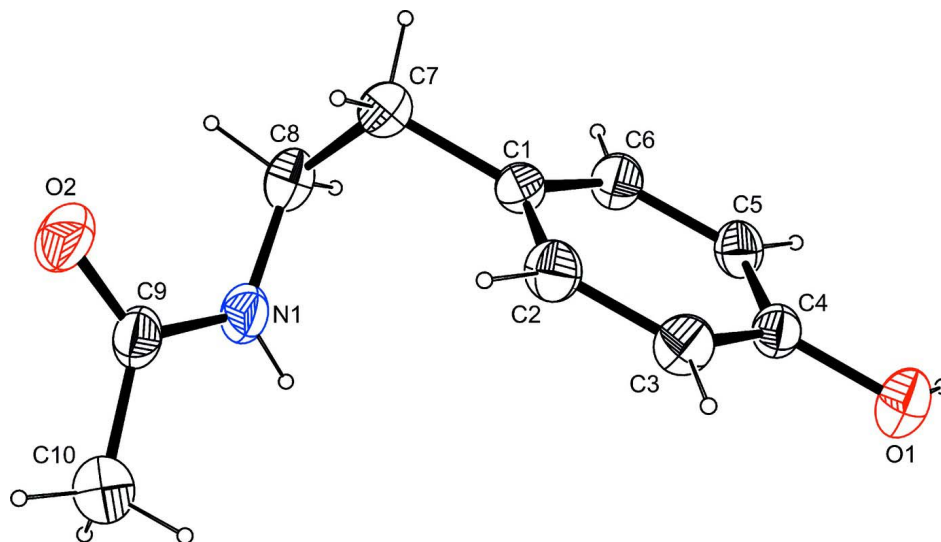


Figure 1

Molecular structure of (I) with the atom labeling scheme. Ellipsoids are drawn at the 30% probability level. H atoms are represented as small spheres of arbitrary radii.

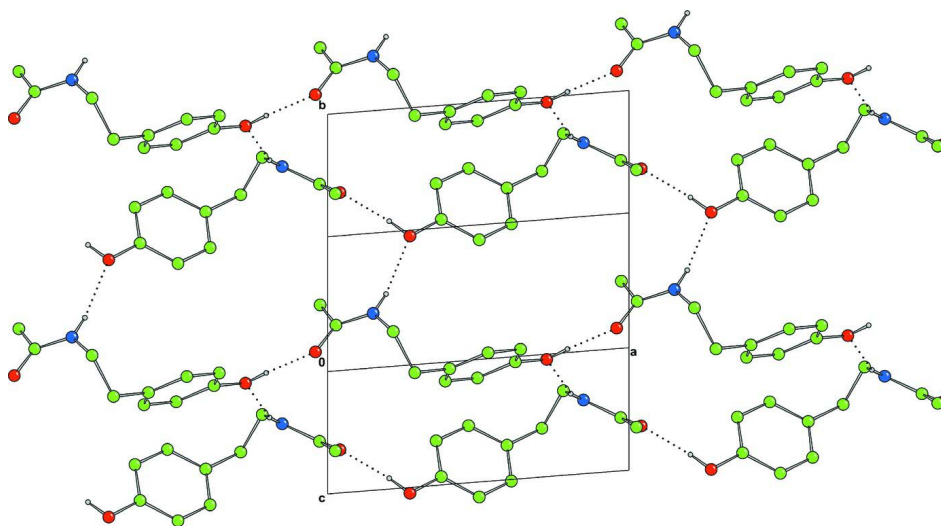


Figure 2

Partial packing view showing the corrugated sheet and the $R_4^4(25)$ graph set motif.

N-(4-Hydroxyphenethyl)acetamide

Crystal data

$C_{10}H_{13}NO_2$

$M_r = 179.21$

Monoclinic, $P2_1/c$

Hall symbol: $-P 2_1/c$

$a = 9.9206$ (13) Å

$b = 8.7861$ (11) Å

$c = 11.4943$ (16) Å

$\beta = 102.998$ (1)°

$V = 976.2$ (2) Å³

$Z = 4$

$F(000) = 384$

$D_x = 1.219$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 1622 reflections

$\theta = 3.0$ – 26.2 °

$\mu = 0.09$ mm⁻¹

$T = 298$ K $0.43 \times 0.38 \times 0.20$ mm
 Block, colorless

Data collection

Bruker SMART CCD diffractometer	4753 measured reflections
Radiation source: fine-focus sealed tube	1713 independent reflections
Graphite monochromator	1196 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{\text{int}} = 0.027$
Absorption correction: multi-scan (SADABS; Sheldrick, 2008)	$\theta_{\text{max}} = 25.0^\circ$, $\theta_{\text{min}} = 2.1^\circ$
$T_{\text{min}} = 0.961$, $T_{\text{max}} = 0.978$	$h = -7 \rightarrow 11$
	$k = -9 \rightarrow 10$
	$l = -13 \rightarrow 13$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.037$	H-atom parameters constrained
$wR(F^2) = 0.100$	$w = 1/[\sigma^2(F_o^2) + (0.0387P)^2 + 0.1837P]$
$S = 1.05$	where $P = (F_o^2 + 2F_c^2)/3$
1713 reflections	$(\Delta/\sigma)_{\text{max}} < 0.001$
119 parameters	$\Delta\rho_{\text{max}} = 0.16 \text{ e } \text{\AA}^{-3}$
0 restraints	$\Delta\rho_{\text{min}} = -0.14 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	

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 $F^2 > \sigma(F^2)$ 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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
N1	0.15094 (14)	0.38049 (16)	0.35383 (14)	0.0553 (4)	
H1	0.1936	0.4303	0.3086	0.066*	
O1	0.72697 (12)	0.10975 (15)	0.27285 (11)	0.0598 (4)	
H1A	0.7957	0.1586	0.3049	0.090*	
O2	-0.04072 (13)	0.25522 (17)	0.36772 (12)	0.0724 (4)	
C1	0.40477 (16)	0.18477 (19)	0.44391 (14)	0.0444 (4)	
C2	0.39022 (17)	0.09127 (19)	0.34533 (15)	0.0516 (5)	
H2	0.3057	0.0435	0.3162	0.062*	
C3	0.49703 (18)	0.0664 (2)	0.28865 (16)	0.0516 (5)	
H3	0.4843	0.0024	0.2226	0.062*	
C4	0.62273 (16)	0.13710 (18)	0.33044 (14)	0.0430 (4)	
C5	0.64007 (17)	0.23153 (18)	0.42830 (14)	0.0462 (4)	
H5	0.7244	0.2800	0.4568	0.055*	
C6	0.53229 (17)	0.25403 (19)	0.48397 (15)	0.0493 (4)	

H6	0.5455	0.3175	0.5503	0.059*	
C7	0.28890 (18)	0.2102 (2)	0.50690 (16)	0.0542 (5)	
H7A	0.3257	0.2034	0.5924	0.065*	
H7B	0.2210	0.1299	0.4845	0.065*	
C8	0.21757 (18)	0.3629 (2)	0.47851 (17)	0.0562 (5)	
H8A	0.1488	0.3745	0.5260	0.067*	
H8B	0.2854	0.4434	0.5012	0.067*	
C9	0.02736 (18)	0.3236 (2)	0.30588 (17)	0.0545 (5)	
C10	-0.0253 (2)	0.3440 (3)	0.17442 (18)	0.0790 (6)	
H10A	0.0416	0.3994	0.1425	0.119*	0.50
H10B	-0.1108	0.3995	0.1597	0.119*	0.50
H10C	-0.0404	0.2461	0.1366	0.119*	0.50
H10D	-0.1146	0.2973	0.1501	0.119*	0.50
H10E	0.0377	0.2972	0.1329	0.119*	0.50
H10F	-0.0326	0.4506	0.1559	0.119*	0.50

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0394 (8)	0.0592 (9)	0.0710 (10)	0.0001 (7)	0.0200 (7)	0.0143 (8)
O1	0.0472 (7)	0.0672 (9)	0.0692 (9)	-0.0047 (6)	0.0223 (6)	-0.0153 (6)
O2	0.0500 (8)	0.0981 (11)	0.0736 (9)	-0.0201 (7)	0.0232 (7)	0.0017 (8)
C1	0.0399 (9)	0.0478 (9)	0.0461 (10)	0.0014 (8)	0.0112 (7)	0.0084 (8)
C2	0.0393 (10)	0.0572 (11)	0.0565 (11)	-0.0115 (8)	0.0069 (8)	0.0006 (9)
C3	0.0503 (10)	0.0547 (11)	0.0492 (10)	-0.0075 (9)	0.0102 (8)	-0.0085 (8)
C4	0.0383 (9)	0.0445 (9)	0.0473 (10)	0.0017 (7)	0.0119 (7)	0.0022 (7)
C5	0.0348 (9)	0.0495 (10)	0.0521 (10)	-0.0034 (7)	0.0050 (7)	-0.0044 (8)
C6	0.0450 (10)	0.0542 (11)	0.0484 (10)	-0.0013 (8)	0.0096 (8)	-0.0073 (8)
C7	0.0475 (10)	0.0627 (12)	0.0545 (11)	-0.0009 (9)	0.0157 (8)	0.0079 (9)
C8	0.0439 (10)	0.0601 (12)	0.0682 (12)	-0.0054 (9)	0.0201 (9)	-0.0046 (9)
C9	0.0422 (10)	0.0601 (11)	0.0651 (12)	0.0080 (9)	0.0202 (9)	0.0039 (9)
C10	0.0602 (13)	0.1059 (18)	0.0711 (14)	0.0112 (12)	0.0150 (11)	0.0090 (13)

Geometric parameters (Å, °)

N1—C9	1.324 (2)	C5—H5	0.9300
N1—C8	1.445 (2)	C6—H6	0.9300
N1—H1	0.8600	C7—C8	1.518 (2)
O1—C4	1.3686 (19)	C7—H7A	0.9700
O1—H1A	0.8200	C7—H7B	0.9700
O2—C9	1.240 (2)	C8—H8A	0.9700
C1—C2	1.381 (2)	C8—H8B	0.9700
C1—C6	1.386 (2)	C9—C10	1.494 (3)
C1—C7	1.507 (2)	C10—H10A	0.9600
C2—C3	1.380 (2)	C10—H10B	0.9600
C2—H2	0.9300	C10—H10C	0.9600
C3—C4	1.379 (2)	C10—H10D	0.9600
C3—H3	0.9300	C10—H10E	0.9600

C4—C5	1.377 (2)	C10—H10F	0.9600
C5—C6	1.378 (2)		
C9—N1—C8	123.14 (15)	N1—C8—H8A	108.9
C9—N1—H1	118.4	C7—C8—H8A	108.9
C8—N1—H1	118.4	N1—C8—H8B	108.9
C4—O1—H1A	109.5	C7—C8—H8B	108.9
C2—C1—C6	116.94 (15)	H8A—C8—H8B	107.7
C2—C1—C7	122.18 (15)	O2—C9—N1	121.13 (17)
C6—C1—C7	120.88 (15)	O2—C9—C10	121.75 (17)
C3—C2—C1	122.12 (16)	N1—C9—C10	117.12 (17)
C3—C2—H2	118.9	C9—C10—H10A	109.5
C1—C2—H2	118.9	C9—C10—H10B	109.5
C4—C3—C2	119.64 (16)	H10A—C10—H10B	109.5
C4—C3—H3	120.2	C9—C10—H10C	109.5
C2—C3—H3	120.2	H10A—C10—H10C	109.5
O1—C4—C5	122.12 (14)	H10B—C10—H10C	109.5
O1—C4—C3	118.36 (15)	C9—C10—H10D	109.5
C5—C4—C3	119.52 (15)	H10A—C10—H10D	141.1
C4—C5—C6	119.89 (15)	H10B—C10—H10D	56.3
C4—C5—H5	120.1	H10C—C10—H10D	56.3
C6—C5—H5	120.1	C9—C10—H10E	109.5
C5—C6—C1	121.89 (16)	H10A—C10—H10E	56.3
C5—C6—H6	119.1	H10B—C10—H10E	141.1
C1—C6—H6	119.1	H10C—C10—H10E	56.3
C1—C7—C8	113.41 (14)	H10D—C10—H10E	109.5
C1—C7—H7A	108.9	C9—C10—H10F	109.5
C8—C7—H7A	108.9	H10A—C10—H10F	56.3
C1—C7—H7B	108.9	H10B—C10—H10F	56.3
C8—C7—H7B	108.9	H10C—C10—H10F	141.1
H7A—C7—H7B	107.7	H10D—C10—H10F	109.5
N1—C8—C7	113.25 (15)	H10E—C10—H10F	109.5

Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
N1—H1...O1 ⁱ	0.86	2.08	2.9048 (18)	161
O1—H1A...O2 ⁱⁱ	0.82	1.83	2.6464 (17)	174

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