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N′-[(*E*)-2-Hydroxybenzylidene]-2-(6-methoxynaphthalen-2-yl)propanohydrazide: a redetermination

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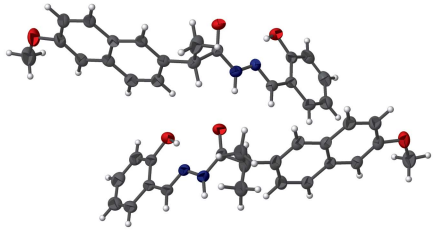
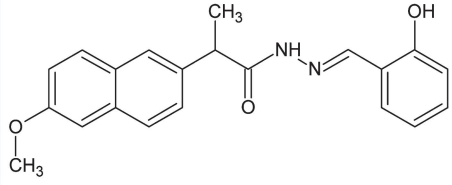
The structure of the title compound, $C_{21}H_{20}N_2O_3$, was originally determined at ambient temperature [Wu *et al.* (2007). *Inorg. Chim. Acta*, **360**, 3069–3074]. In this determination, with data collected at 150 K, the asymmetric unit comprises two independent molecules (1 and 2) that differ considerably in their conformations. In particular, the methyl group at the mid-point of molecule 2 is disordered over two sites. This was modelled with restraints so that the geometries of the two components are comparable and the disorder components refined to an occupancy ratio of 0.750 (6):0.250 (6). Intramolecular O—H···N and intermolecular N—H···O hydrogen bonds stabilize the structure with significant additional input from C—H···π interactions.

3D view



Chemical scheme



Structure description

Non-steroidal anti-inflammatory drugs (NSAIDs) are among the most widely used therapeutic agents. They are very effective in the alleviation of pain, fever and inflammation (Meek *et al.*, 2010; Batlouni, 2010). Naproxen, (+)-(*S*)-2-(6-methoxynaphthalen-2-yl)propanoic acid, is often used for the treatment of acute and chronic inflammation conditions, musculoskeletal disorders, primary dysmenorrhoea, fever and also in the management of mild pain (Capone *et al.*, 2007; Assali *et al.*, 2014). The structure of the title compound, in which the 6-methoxynaphthalene moiety is closely related to the naproxen molecule, has been determined previously at ambient temperature (Wu *et al.*, 2007) but this article did not address the possibility of pseudo-symmetry in the structure,

Table 1
Hydrogen-bond geometry (Å, °).

*Cg*1 is the centroid of the hydroxyphenyl ring (C1–C6) of molecule 1; *Cg*4 and *Cg*6 are the centroids of the hydroxyphenyl ring (C22–C27) and the benzene ring (C34–C39) of the naphthalene group of molecule 2, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*O*···N1	0.87	1.81	2.606 (3)	151
N2—H2*N*···O5^{i}	0.91	1.99	2.776 (3)	143
O4—H4*O*···N3	0.87	1.83	2.630 (3)	152
N4—H4*N*···O2	0.91	1.87	2.724 (3)	154
C6—H6···*Cg*6^{i}	0.95	2.97	3.734 (4)	139
C21—H21*A*···*Cg*1^{ii}	0.98	2.66	3.476 (4)	141
C42—H42*A*···*Cg*4^{iii}	0.98	2.62	3.403 (5)	137

Symmetry codes: (i) $x+1, y, z$; (ii) $x, y, z+1$; (iii) $x, y, z-1$.

the disorder in one of the unique molecules or the presence of significant C—H···π interactions in the crystal structure.

Although complicated by pseudosymmetry, it is felt that the correct crystal system is monoclinic with a β angle very close to 90° rather than orthorhombic on the basis of lower merging *R* values for equivalent reflections and a more satisfactory refinement. Moreover, with two molecules in the asymmetric unit, refinement shows that the C10 methyl group in molecule 1 is disordered over two sites with a 0.750 (6):0.250 (6) occupancy ratio while molecule 2 is completely ordered so that the two molecules are not identical. In molecule 1, the dihedral angle between the phenyl and naphthyl groups is 79.90 (8)° while in molecule 2 it is 82.66 (8)°. The two naphthyl groups are inclined at an angle of 38.51 (8)°. The conformations of both molecules are partially determined by intramolecular O—H···N hydrogen bonds while the two molecules in the asymmetric unit are associated through an N4—H4*N*···O2 hydrogen bond (Table 1 and Fig. 1). The crystal structure is further stabilized by three C—H···π hydrogen bonds (Table 1). C21—H21*A*···*Cg*1 interactions link type 1 molecules into chains along *c*, while C42—H42*A*···*Cg*4 contacts form parallel chains in an obverse fashion, Fig. 2 (*Cg*1 and *Cg*4 are the centroids of the hydroxyphenyl rings of molecules 1 and 2, respectively). The chains are linked by the N4—H4*N*···O2 hydrogen bonds and these pairs of chains are further interconnected by N2—H2*N*···O5 hydrogen bonds, supported by C6—H6···*Cg*6 contacts, forming sheets of molecules in the *ac* plane (*Cg*6 is the centroid of the C35–C39 ring in molecule 2).

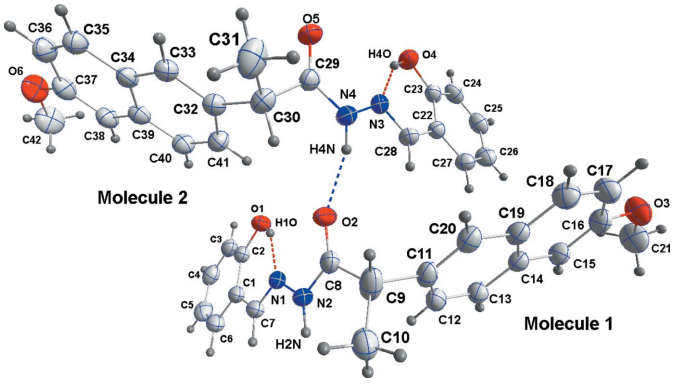


Figure 1
The asymmetric unit with the atom-labeling scheme and 50% probability ellipsoids. Only the major component of the disorder in the C10 methyl group is shown. O—H···N and N—H···O hydrogen bonds are shown, respectively, as red and blue dashed lines.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{21}H_{20}N_2O_3$
M_r	348.39
Crystal system, space group	Monoclinic, $P2_1$
Temperature (K)	150
a, *b*, *c* (Å)	9.5461 (5), 11.8724 (6), 15.9962 (8)
β (°)	90.104 (2)
V (Å^3)	1812.93 (16)
Z	4
Radiation type	Cu *K*α
μ (mm^{-1})	0.70
Crystal size (mm)	0.25 × 0.18 × 0.04
Data collection	
Diffractometer	Bruker D8 VENTURE PHOTON 100 CMOS
Absorption correction	Multi-scan (*SADABS*; Bruker, 2016)
T_{min}, T_{max}	0.86, 0.97
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	14005, 6487, 5685
R_{int}	0.035
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.619
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.042, 0.109, 1.03
No. of reflections	6487
No. of parameters	479
No. of restraints	2
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.31, −0.22
Absolute structure	Flack *x* determined using 2150 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	0.21 (19)

Computer programs: *APEX3* and *SAINT* (Bruker, 2016), , *SHELXTL* (Sheldrick, 2008), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*), *DIAMOND* (Brandenburg & Putz, 2012) and *Mercury* (Macrae *et al.*, 2008).

Synthesis and crystallization

A mixture of 1 mmol (244 mg) of 2-(6-methoxynaphthalen-2-yl)propanehydrazide and 1 mmol (122 mg) of salicaldehyde with a few drops of glacial acetic acid was refluxed in 20 ml of

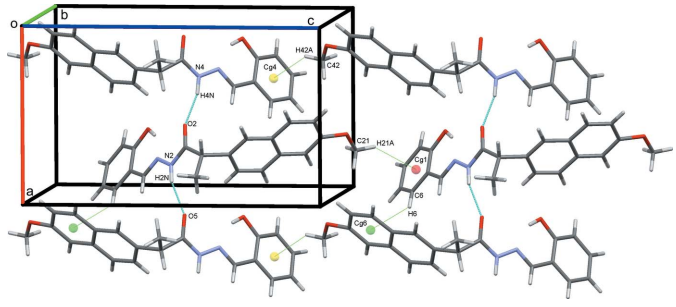


Figure 2
Sheets of molecules in the *ac* plane formed by N—H···O hydrogen bonds (blue dashed lines)and C—H···π contacts (green dotted lines). Ring centroids are shown as coloured spheres.

absolute ethanol for 6 h. The mixture was cooled and the excess solvent evaporated. The solid was filtered off, dried and recrystallized from ethanol to afford yellow crystals of quality suitable for X-ray diffraction with m.p 442–445 K.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. In the final stages of the refinement, it became evident that C10 was disordered over two sets of sites. This was modelled with restraints to ensure that the geometries of the two components were comparable and the occupancy factors refined to a ratio of 0.750 (6):0.250 (6).

Acknowledgements

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full crystallographic data

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Crystal data

$C_{21}H_{20}N_2O_3$
M_r = 348.39
Monoclinic, $P2_1$
a = 9.5461 (5) Å
b = 11.8724 (6) Å
c = 15.9962 (8) Å
β = 90.104 (2)°
V = 1812.93 (16) Å^3
Z = 4
$F(000)$ = 736
D_x = 1.276 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 9655 reflections
θ = 4.6–72.4°
μ = 0.70 mm^{-1}
T = 150 K
Plate, yellow
0.25 × 0.18 × 0.04 mm

Data collection

Bruker D8 VENTURE PHOTON 100 CMOS diffractometer
Radiation source: INCOATEC IμS micro–focus source
Mirror monochromator
Detector resolution: 10.4167 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2016)
T_{min} = 0.86, T_{max} = 0.97
14005 measured reflections
6487 independent reflections
5685 reflections with $I > 2\sigma(I)$
R_{int} = 0.035
θ_{max} = 72.5°, θ_{min} = 4.6°
h = −11→11
k = −14→14
l = −19→18

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.109
S = 1.03
6487 reflections
479 parameters
2 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0576P)^2 + 0.2712P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}
Extinction correction: *SHELXL 2014/7* (Sheldrick, 2015a), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0036 (5)
Absolute structure: Flack x determined using 2150 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: 0.21 (19)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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. H-atoms attached to carbon were placed in calculated positions (C—H = 0.95 - 1.00 Å) while those attached to nitrogen and oxygen were placed in locations derived from a difference map and their parameters adjusted to give N—H = 0.91 and O—H = 0.87 Å. All were included as riding contributions with isotropic displacement parameters 1.2 - 1.5 times those of the attached atoms. In the final stges of the refinement, it became evident that C10 was disordered over two sites. This was modeled with restraints that the geometries of the two components be comparable and refined to a 3:1 ratio.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
O1	0.6485 (2)	0.6624 (2)	0.34737 (14)	0.0461 (6)	
H1O	0.6721	0.6019	0.3747	0.069*	
O2	0.5976 (2)	0.4145 (2)	0.49980 (14)	0.0457 (6)	
O3	0.6524 (3)	0.5185 (2)	1.03109 (14)	0.0501 (6)	
N1	0.7942 (2)	0.4900 (2)	0.39852 (15)	0.0355 (6)	
N2	0.8194 (2)	0.4042 (2)	0.45369 (16)	0.0384 (6)	
H2N	0.9073	0.3751	0.4579	0.046*	
C1	0.8776 (3)	0.6135 (3)	0.29323 (19)	0.0367 (7)	
C2	0.7594 (3)	0.6842 (3)	0.29667 (19)	0.0382 (7)	
C3	0.7558 (4)	0.7815 (3)	0.2483 (2)	0.0463 (8)	
H3	0.6785	0.8315	0.2528	0.056*	
C4	0.8636 (4)	0.8061 (3)	0.1937 (2)	0.0505 (9)	
H4	0.8591	0.8721	0.1603	0.061*	
C5	0.9788 (4)	0.7345 (3)	0.1876 (2)	0.0501 (9)	
H5	1.0521	0.7506	0.1493	0.060*	
C6	0.9854 (3)	0.6404 (3)	0.2372 (2)	0.0440 (8)	
H6	1.0648	0.5924	0.2336	0.053*	
C7	0.8931 (3)	0.5174 (3)	0.34828 (19)	0.0369 (7)	
H7	0.9770	0.4744	0.3472	0.044*	
C8	0.7144 (3)	0.3729 (3)	0.50537 (18)	0.0378 (7)	
C9	0.7485 (5)	0.2842 (3)	0.5710 (2)	0.0533 (10)	0.750 (6)
H9	0.6630	0.2356	0.5724	0.064*	0.750 (6)
C10	0.8613 (5)	0.2058 (4)	0.5588 (3)	0.0446 (10)	0.750 (6)
H10A	0.8490	0.1672	0.5052	0.067*	0.750 (6)
H10B	0.8612	0.1503	0.6042	0.067*	0.750 (6)
H10C	0.9506	0.2465	0.5589	0.067*	0.750 (6)
C9A	0.7485 (5)	0.2842 (3)	0.5710 (2)	0.0533 (10)	0.250 (6)
H9A	0.8508	0.2720	0.5611	0.064*	0.250 (6)
C10A	0.6945 (14)	0.1744 (7)	0.5570 (8)	0.0446 (10)	0.250 (6)
H10D	0.5936	0.1739	0.5681	0.067*	0.250 (6)
H10E	0.7414	0.1209	0.5943	0.067*	0.250 (6)

H10F	0.7112	0.1526	0.4988	0.067*	0.250 (6)
C11	0.7502 (3)	0.3408 (3)	0.65668 (18)	0.0384 (7)	
C12	0.8507 (3)	0.4254 (3)	0.6747 (2)	0.0407 (7)	
H12	0.9166	0.4460	0.6329	0.049*	
C13	0.8551 (3)	0.4779 (3)	0.75069 (18)	0.0371 (7)	
H13	0.9227	0.5351	0.7606	0.045*	
C14	0.7602 (3)	0.4481 (3)	0.81483 (18)	0.0329 (6)	
C15	0.7607 (3)	0.5016 (3)	0.89421 (18)	0.0363 (7)	
H15	0.8275	0.5587	0.9061	0.044*	
C16	0.6650 (3)	0.4711 (3)	0.95362 (19)	0.0386 (7)	
C17	0.5681 (3)	0.3831 (3)	0.9375 (2)	0.0425 (7)	
H17	0.5037	0.3610	0.9796	0.051*	
C18	0.5668 (3)	0.3303 (3)	0.86249 (19)	0.0403 (7)	
H18	0.5015	0.2714	0.8528	0.048*	
C19	0.6611 (3)	0.3614 (3)	0.79797 (18)	0.0341 (6)	
C20	0.6579 (3)	0.3106 (3)	0.71823 (19)	0.0385 (7)	
H20	0.5901	0.2541	0.7069	0.046*	
C21	0.7521 (5)	0.6018 (4)	1.0534 (2)	0.0591 (10)	
H21A	0.7346	0.6270	1.1108	0.089*	
H21B	0.7440	0.6660	1.0152	0.089*	
H21C	0.8466	0.5700	1.0496	0.089*	
O4	0.1372 (2)	0.6691 (2)	0.66597 (14)	0.0467 (6)	
H4O	0.1615	0.6097	0.6376	0.070*	
O5	0.1009 (2)	0.4092 (2)	0.49733 (14)	0.0434 (5)	
O6	0.1563 (3)	0.5107 (2)	−0.03381 (15)	0.0565 (7)	
N3	0.2906 (2)	0.5061 (2)	0.60278 (14)	0.0346 (5)	
N4	0.3235 (2)	0.4228 (2)	0.54634 (16)	0.0367 (6)	
H4N	0.4157	0.4041	0.5432	0.044*	
C22	0.3748 (3)	0.6290 (3)	0.70936 (18)	0.0325 (6)	
C23	0.2518 (3)	0.6945 (3)	0.71272 (19)	0.0362 (7)	
C24	0.2460 (4)	0.7886 (3)	0.7648 (2)	0.0443 (8)	
H24	0.1652	0.8355	0.7645	0.053*	
C25	0.3570 (4)	0.8139 (3)	0.8167 (2)	0.0474 (8)	
H25	0.3518	0.8777	0.8525	0.057*	
C26	0.4768 (4)	0.7467 (3)	0.8173 (2)	0.0460 (8)	
H26	0.5518	0.7629	0.8545	0.055*	
C27	0.4853 (3)	0.6567 (3)	0.76323 (19)	0.0385 (7)	
H27	0.5681	0.6123	0.7625	0.046*	
C28	0.3916 (3)	0.5368 (3)	0.65108 (18)	0.0347 (6)	
H28	0.4787	0.4983	0.6484	0.042*	
C29	0.2252 (3)	0.3820 (3)	0.49370 (18)	0.0347 (7)	
C30	0.2816 (3)	0.2981 (3)	0.42970 (19)	0.0371 (7)	
H30	0.3825	0.2840	0.4430	0.044*	
C31	0.2038 (4)	0.1867 (3)	0.4377 (2)	0.0518 (9)	
H31A	0.2411	0.1327	0.3971	0.078*	
H31B	0.1038	0.1987	0.4269	0.078*	
H31C	0.2163	0.1568	0.4944	0.078*	
C32	0.2738 (3)	0.3507 (3)	0.34317 (19)	0.0334 (6)	

C33	0.1834 (3)	0.3126 (3)	0.28257 (18)	0.0333 (6)
H33	0.1216	0.2521	0.2950	0.040*
C34	0.1805 (3)	0.3619 (3)	0.20190 (18)	0.0323 (6)
C35	0.0885 (3)	0.3238 (3)	0.13800 (19)	0.0370 (7)
H35	0.0285	0.2616	0.1488	0.044*
C36	0.0841 (3)	0.3740 (3)	0.06201 (19)	0.0418 (7)
H36	0.0216	0.3469	0.0204	0.050*
C37	0.1726 (4)	0.4669 (3)	0.0444 (2)	0.0422 (7)
C38	0.2655 (3)	0.5054 (3)	0.10334 (19)	0.0389 (7)
H38	0.3265	0.5662	0.0906	0.047*
C39	0.2705 (3)	0.4542 (2)	0.18322 (19)	0.0334 (6)
C40	0.3638 (3)	0.4918 (3)	0.2469 (2)	0.0397 (7)
H40	0.4259	0.5525	0.2359	0.048*
C41	0.3649 (3)	0.4413 (3)	0.3238 (2)	0.0398 (7)
H41	0.4283	0.4676	0.3653	0.048*
C42	0.2464 (5)	0.6007 (4)	−0.0567 (3)	0.0649 (11)
H42A	0.2295	0.6211	−0.1152	0.097*
H42B	0.3441	0.5772	−0.0498	0.097*
H42C	0.2278	0.6659	−0.0209	0.097*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0351 (11)	0.0595 (15)	0.0438 (13)	0.0128 (11)	0.0022 (9)	−0.0024 (12)
O2	0.0295 (10)	0.0650 (16)	0.0425 (12)	0.0093 (11)	0.0011 (8)	0.0095 (11)
O3	0.0633 (15)	0.0544 (14)	0.0327 (11)	−0.0122 (13)	0.0029 (10)	−0.0091 (11)
N1	0.0301 (11)	0.0451 (14)	0.0311 (12)	0.0039 (11)	−0.0035 (9)	−0.0094 (11)
N2	0.0315 (12)	0.0493 (15)	0.0343 (13)	0.0133 (12)	−0.0042 (10)	−0.0042 (12)
C1	0.0293 (14)	0.0461 (18)	0.0347 (16)	0.0018 (13)	−0.0016 (11)	−0.0108 (13)
C2	0.0329 (15)	0.0471 (18)	0.0346 (16)	0.0024 (14)	−0.0037 (12)	−0.0097 (14)
C3	0.0465 (18)	0.0475 (19)	0.0447 (19)	0.0064 (16)	−0.0087 (14)	−0.0106 (16)
C4	0.057 (2)	0.0446 (19)	0.050 (2)	−0.0071 (17)	−0.0119 (16)	−0.0052 (17)
C5	0.0445 (18)	0.055 (2)	0.050 (2)	−0.0134 (17)	0.0008 (15)	−0.0055 (18)
C6	0.0346 (16)	0.052 (2)	0.0448 (18)	0.0006 (15)	0.0018 (13)	−0.0091 (16)
C7	0.0284 (13)	0.0462 (18)	0.0361 (15)	0.0048 (13)	−0.0010 (11)	−0.0102 (14)
C8	0.0395 (16)	0.0458 (18)	0.0281 (14)	0.0067 (14)	−0.0044 (11)	−0.0067 (13)
C9	0.079 (3)	0.047 (2)	0.0339 (18)	0.0216 (19)	−0.0079 (16)	−0.0057 (15)
C10	0.051 (2)	0.046 (2)	0.037 (2)	0.002 (2)	0.0006 (17)	−0.0022 (18)
C9A	0.079 (3)	0.047 (2)	0.0339 (18)	0.0216 (19)	−0.0079 (16)	−0.0057 (15)
C10A	0.051 (2)	0.046 (2)	0.037 (2)	0.002 (2)	0.0006 (17)	−0.0022 (18)
C11	0.0490 (17)	0.0365 (16)	0.0298 (15)	0.0121 (14)	−0.0055 (12)	−0.0014 (13)
C12	0.0442 (16)	0.0463 (18)	0.0318 (15)	0.0101 (15)	0.0023 (12)	0.0063 (14)
C13	0.0383 (15)	0.0389 (16)	0.0341 (16)	0.0006 (13)	−0.0021 (12)	0.0023 (13)
C14	0.0333 (14)	0.0342 (15)	0.0313 (15)	0.0034 (12)	−0.0049 (11)	0.0022 (12)
C15	0.0391 (15)	0.0364 (16)	0.0333 (15)	−0.0017 (13)	−0.0052 (12)	−0.0011 (13)
C16	0.0468 (17)	0.0391 (17)	0.0299 (15)	0.0009 (14)	−0.0044 (12)	−0.0015 (13)
C17	0.0428 (16)	0.0486 (19)	0.0361 (16)	−0.0081 (15)	0.0005 (12)	0.0009 (15)
C18	0.0412 (16)	0.0415 (17)	0.0383 (16)	−0.0072 (14)	−0.0040 (12)	0.0003 (14)

C19	0.0367 (14)	0.0342 (15)	0.0313 (14)	0.0039 (12)	−0.0063 (11)	−0.0015 (13)
C20	0.0438 (16)	0.0361 (16)	0.0357 (16)	0.0046 (14)	−0.0084 (12)	−0.0002 (14)
C21	0.074 (3)	0.059 (2)	0.044 (2)	−0.015 (2)	−0.0021 (18)	−0.0171 (19)
O4	0.0355 (11)	0.0608 (15)	0.0438 (13)	0.0142 (11)	−0.0031 (9)	0.0045 (12)
O5	0.0269 (10)	0.0599 (15)	0.0435 (12)	0.0003 (10)	−0.0034 (8)	0.0008 (11)
O6	0.0744 (17)	0.0602 (16)	0.0350 (12)	−0.0096 (14)	0.0013 (11)	0.0130 (12)
N3	0.0322 (12)	0.0441 (14)	0.0274 (12)	−0.0001 (11)	0.0007 (9)	0.0000 (11)
N4	0.0293 (11)	0.0452 (15)	0.0355 (13)	0.0012 (11)	−0.0020 (9)	−0.0049 (12)
C22	0.0299 (14)	0.0357 (15)	0.0320 (15)	−0.0001 (12)	0.0012 (11)	0.0040 (12)
C23	0.0341 (15)	0.0418 (17)	0.0326 (16)	0.0050 (13)	0.0042 (11)	0.0108 (13)
C24	0.0498 (18)	0.0384 (17)	0.0447 (19)	0.0088 (15)	0.0134 (14)	0.0079 (15)
C25	0.059 (2)	0.0383 (18)	0.0445 (18)	−0.0058 (16)	0.0128 (15)	−0.0007 (15)
C26	0.0453 (18)	0.0480 (19)	0.0447 (19)	−0.0107 (16)	0.0022 (14)	−0.0035 (16)
C27	0.0314 (14)	0.0425 (17)	0.0417 (17)	−0.0012 (13)	−0.0007 (12)	0.0008 (14)
C28	0.0287 (13)	0.0421 (17)	0.0333 (15)	0.0028 (13)	−0.0009 (11)	0.0004 (13)
C29	0.0327 (14)	0.0422 (17)	0.0293 (14)	−0.0040 (13)	−0.0038 (11)	0.0052 (13)
C30	0.0354 (15)	0.0381 (16)	0.0376 (16)	−0.0006 (13)	−0.0058 (12)	−0.0002 (13)
C31	0.073 (2)	0.0419 (19)	0.0410 (19)	−0.0109 (18)	−0.0129 (16)	0.0098 (15)
C32	0.0312 (14)	0.0331 (15)	0.0358 (15)	−0.0004 (12)	0.0015 (11)	0.0005 (13)
C33	0.0305 (13)	0.0355 (16)	0.0339 (15)	−0.0021 (12)	0.0017 (11)	−0.0011 (13)
C34	0.0306 (13)	0.0348 (15)	0.0316 (14)	0.0006 (12)	0.0043 (11)	−0.0008 (12)
C35	0.0363 (15)	0.0400 (17)	0.0347 (15)	−0.0052 (14)	0.0014 (11)	−0.0001 (14)
C36	0.0442 (16)	0.0484 (19)	0.0329 (15)	−0.0044 (15)	−0.0009 (12)	0.0004 (14)
C37	0.0493 (18)	0.0444 (18)	0.0328 (16)	0.0028 (15)	0.0082 (13)	0.0058 (14)
C38	0.0408 (16)	0.0368 (16)	0.0390 (16)	−0.0021 (14)	0.0081 (12)	0.0028 (14)
C39	0.0330 (14)	0.0284 (14)	0.0387 (16)	0.0007 (12)	0.0072 (12)	−0.0002 (12)
C40	0.0387 (15)	0.0359 (16)	0.0444 (18)	−0.0073 (14)	0.0051 (13)	−0.0010 (14)
C41	0.0385 (16)	0.0412 (17)	0.0399 (16)	−0.0070 (14)	−0.0010 (13)	−0.0063 (14)
C42	0.084 (3)	0.060 (3)	0.050 (2)	−0.012 (2)	0.008 (2)	0.025 (2)

Geometric parameters (Å, º)

O1—C2	1.360 (4)	C21—H21A	0.9800
O1—H1O	0.8700	C21—H21B	0.9800
O2—C8	1.223 (4)	C21—H21C	0.9800
O3—C16	1.367 (4)	O4—C23	1.358 (4)
O3—C21	1.417 (5)	O4—H4O	0.8701
N1—C7	1.283 (4)	O5—C29	1.231 (4)
N1—N2	1.369 (4)	O6—C37	1.363 (4)
N2—C8	1.352 (4)	O6—C42	1.420 (5)
N2—H2N	0.9100	N3—C28	1.287 (4)
C1—C6	1.402 (5)	N3—N4	1.375 (4)
C1—C2	1.407 (4)	N4—C29	1.349 (4)
C1—C7	1.449 (5)	N4—H4N	0.9100
C2—C3	1.390 (5)	C22—C27	1.400 (4)
C3—C4	1.382 (6)	C22—C23	1.410 (4)
C3—H3	0.9500	C22—C28	1.447 (4)
C4—C5	1.394 (6)	C23—C24	1.396 (5)

C4—H4	0.9500	C24—C25	1.378 (5)
C5—C6	1.372 (5)	C24—H24	0.9500
C5—H5	0.9500	C25—C26	1.395 (5)
C6—H6	0.9500	C25—H25	0.9500
C7—H7	0.9500	C26—C27	1.377 (5)
C8—C9A	1.523 (5)	C26—H26	0.9500
C8—C9	1.523 (5)	C27—H27	0.9500
C9—C10	1.436 (6)	C28—H28	0.9500
C9—C11	1.526 (4)	C29—C30	1.528 (5)
C9—H9	1.0000	C30—C32	1.520 (4)
C10—H10A	0.9800	C30—C31	1.523 (5)
C10—H10B	0.9800	C30—H30	1.0000
C10—H10C	0.9800	C31—H31A	0.9800
C9A—C10A	1.419 (7)	C31—H31B	0.9800
C9A—C11	1.526 (4)	C31—H31C	0.9800
C9A—H9A	1.0000	C32—C33	1.374 (4)
C10A—H10D	0.9800	C32—C41	1.418 (4)
C10A—H10E	0.9800	C33—C34	1.417 (4)
C10A—H10F	0.9800	C33—H33	0.9500
C11—C20	1.370 (5)	C34—C35	1.421 (4)
C11—C12	1.418 (5)	C34—C39	1.425 (4)
C12—C13	1.367 (4)	C35—C36	1.354 (4)
C12—H12	0.9500	C35—H35	0.9500
C13—C14	1.415 (4)	C36—C37	1.418 (5)
C13—H13	0.9500	C36—H36	0.9500
C14—C15	1.420 (4)	C37—C38	1.372 (5)
C14—C19	1.424 (4)	C38—C39	1.415 (4)
C15—C16	1.368 (5)	C38—H38	0.9500
C15—H15	0.9500	C39—C40	1.423 (4)
C16—C17	1.419 (5)	C40—C41	1.368 (5)
C17—C18	1.353 (5)	C40—H40	0.9500
C17—H17	0.9500	C41—H41	0.9500
C18—C19	1.419 (4)	C42—H42A	0.9800
C18—H18	0.9500	C42—H42B	0.9800
C19—C20	1.411 (4)	C42—H42C	0.9800
C20—H20	0.9500		

C2—O1—H1O	104.9	C11—C20—H20	119.2
C16—O3—C21	117.1 (3)	C19—C20—H20	119.2
C7—N1—N2	117.7 (2)	O3—C21—H21A	109.5
C8—N2—N1	118.0 (2)	O3—C21—H21B	109.5
C8—N2—H2N	122.3	H21A—C21—H21B	109.5
N1—N2—H2N	119.4	O3—C21—H21C	109.5
C6—C1—C2	118.6 (3)	H21A—C21—H21C	109.5
C6—C1—C7	119.5 (3)	H21B—C21—H21C	109.5
C2—C1—C7	121.8 (3)	C23—O4—H4O	104.6
O1—C2—C3	118.1 (3)	C37—O6—C42	117.1 (3)
O1—C2—C1	122.3 (3)	C28—N3—N4	115.2 (2)

C3—C2—C1	119.6 (3)	C29—N4—N3	120.6 (2)
C4—C3—C2	120.6 (3)	C29—N4—H4N	123.4
C4—C3—H3	119.7	N3—N4—H4N	115.7
C2—C3—H3	119.7	C27—C22—C23	118.3 (3)
C3—C4—C5	120.3 (4)	C27—C22—C28	119.4 (3)
C3—C4—H4	119.8	C23—C22—C28	122.4 (3)
C5—C4—H4	119.8	O4—C23—C24	118.3 (3)
C6—C5—C4	119.4 (3)	O4—C23—C22	121.8 (3)
C6—C5—H5	120.3	C24—C23—C22	119.9 (3)
C4—C5—H5	120.3	C25—C24—C23	120.2 (3)
C5—C6—C1	121.5 (3)	C25—C24—H24	119.9
C5—C6—H6	119.3	C23—C24—H24	119.9
C1—C6—H6	119.3	C24—C25—C26	120.6 (3)
N1—C7—C1	120.4 (3)	C24—C25—H25	119.7
N1—C7—H7	119.8	C26—C25—H25	119.7
C1—C7—H7	119.8	C27—C26—C25	119.3 (3)
O2—C8—N2	121.4 (3)	C27—C26—H26	120.4
O2—C8—C9A	121.5 (3)	C25—C26—H26	120.4
N2—C8—C9A	117.0 (3)	C26—C27—C22	121.6 (3)
O2—C8—C9	121.5 (3)	C26—C27—H27	119.2
N2—C8—C9	117.0 (3)	C22—C27—H27	119.2
C10—C9—C8	120.9 (3)	N3—C28—C22	121.2 (3)
C10—C9—C11	113.6 (3)	N3—C28—H28	119.4
C8—C9—C11	108.4 (3)	C22—C28—H28	119.4
C10—C9—H9	104.0	O5—C29—N4	123.0 (3)
C8—C9—H9	104.0	O5—C29—C30	122.9 (3)
C11—C9—H9	104.0	N4—C29—C30	114.0 (2)
C9—C10—H10A	109.5	C32—C30—C31	114.2 (3)
C9—C10—H10B	109.5	C32—C30—C29	109.0 (3)
H10A—C10—H10B	109.5	C31—C30—C29	109.7 (3)
C9—C10—H10C	109.5	C32—C30—H30	107.9
H10A—C10—H10C	109.5	C31—C30—H30	107.9
H10B—C10—H10C	109.5	C29—C30—H30	107.9
C10A—C9A—C8	116.7 (6)	C30—C31—H31A	109.5
C10A—C9A—C11	123.4 (6)	C30—C31—H31B	109.5
C8—C9A—C11	108.4 (3)	H31A—C31—H31B	109.5
C10A—C9A—H9A	101.4	C30—C31—H31C	109.5
C8—C9A—H9A	101.4	H31A—C31—H31C	109.5
C11—C9A—H9A	101.4	H31B—C31—H31C	109.5
C9A—C10A—H10D	109.5	C33—C32—C41	118.7 (3)
C9A—C10A—H10E	109.5	C33—C32—C30	122.5 (3)
H10D—C10A—H10E	109.5	C41—C32—C30	118.8 (3)
C9A—C10A—H10F	109.5	C32—C33—C34	121.2 (3)
H10D—C10A—H10F	109.5	C32—C33—H33	119.4
H10E—C10A—H10F	109.5	C34—C33—H33	119.4
C20—C11—C12	118.4 (3)	C33—C34—C35	122.3 (3)
C20—C11—C9	121.6 (3)	C33—C34—C39	119.9 (3)
C12—C11—C9	120.0 (3)	C35—C34—C39	117.8 (3)

C20—C11—C9A	121.6 (3)	C36—C35—C34	121.6 (3)
C12—C11—C9A	120.0 (3)	C36—C35—H35	119.2
C13—C12—C11	121.5 (3)	C34—C35—H35	119.2
C13—C12—H12	119.2	C35—C36—C37	120.2 (3)
C11—C12—H12	119.2	C35—C36—H36	119.9
C12—C13—C14	120.8 (3)	C37—C36—H36	119.9
C12—C13—H13	119.6	O6—C37—C38	125.2 (3)
C14—C13—H13	119.6	O6—C37—C36	114.3 (3)
C13—C14—C15	122.4 (3)	C38—C37—C36	120.5 (3)
C13—C14—C19	118.0 (3)	C37—C38—C39	119.9 (3)
C15—C14—C19	119.6 (3)	C37—C38—H38	120.0
C16—C15—C14	120.1 (3)	C39—C38—H38	120.0
C16—C15—H15	119.9	C38—C39—C40	122.1 (3)
C14—C15—H15	119.9	C38—C39—C34	120.0 (3)
O3—C16—C15	125.5 (3)	C40—C39—C34	117.9 (3)
O3—C16—C17	114.2 (3)	C41—C40—C39	120.7 (3)
C15—C16—C17	120.3 (3)	C41—C40—H40	119.7
C18—C17—C16	120.5 (3)	C39—C40—H40	119.7
C18—C17—H17	119.8	C40—C41—C32	121.7 (3)
C16—C17—H17	119.8	C40—C41—H41	119.2
C17—C18—C19	121.3 (3)	C32—C41—H41	119.2
C17—C18—H18	119.3	O6—C42—H42A	109.5
C19—C18—H18	119.3	O6—C42—H42B	109.5
C20—C19—C18	122.3 (3)	H42A—C42—H42B	109.5
C20—C19—C14	119.5 (3)	O6—C42—H42C	109.5
C18—C19—C14	118.2 (3)	H42A—C42—H42C	109.5
C11—C20—C19	121.7 (3)	H42B—C42—H42C	109.5

C7—N1—N2—C8	−178.3 (3)	C12—C11—C20—C19	0.0 (4)
C6—C1—C2—O1	178.0 (3)	C9—C11—C20—C19	178.7 (3)
C7—C1—C2—O1	−4.8 (4)	C9A—C11—C20—C19	178.7 (3)
C6—C1—C2—C3	−3.5 (4)	C18—C19—C20—C11	−179.6 (3)
C7—C1—C2—C3	173.7 (3)	C14—C19—C20—C11	1.5 (4)
O1—C2—C3—C4	−178.0 (3)	C28—N3—N4—C29	178.5 (3)
C1—C2—C3—C4	3.5 (5)	C27—C22—C23—O4	−176.2 (3)
C2—C3—C4—C5	−1.1 (5)	C28—C22—C23—O4	5.4 (5)
C3—C4—C5—C6	−1.2 (5)	C27—C22—C23—C24	4.1 (4)
C4—C5—C6—C1	1.1 (5)	C28—C22—C23—C24	−174.2 (3)
C2—C1—C6—C5	1.2 (5)	O4—C23—C24—C25	176.4 (3)
C7—C1—C6—C5	−176.0 (3)	C22—C23—C24—C25	−3.9 (5)
N2—N1—C7—C1	−174.8 (3)	C23—C24—C25—C26	0.7 (5)
C6—C1—C7—N1	−178.4 (3)	C24—C25—C26—C27	2.2 (5)
C2—C1—C7—N1	4.5 (4)	C25—C26—C27—C22	−1.9 (5)
N1—N2—C8—O2	4.7 (4)	C23—C22—C27—C26	−1.3 (5)
N1—N2—C8—C9A	−175.0 (3)	C28—C22—C27—C26	177.1 (3)
N1—N2—C8—C9	−175.0 (3)	N4—N3—C28—C22	175.6 (3)
O2—C8—C9—C10	155.7 (4)	C27—C22—C28—N3	177.4 (3)
N2—C8—C9—C10	−24.6 (5)	C23—C22—C28—N3	−4.3 (5)

O2—C8—C9—C11	−70.5 (4)	N3—N4—C29—O5	−6.0 (5)
N2—C8—C9—C11	109.2 (3)	N3—N4—C29—C30	174.6 (3)
O2—C8—C9A—C10A	74.2 (8)	O5—C29—C30—C32	68.8 (4)
N2—C8—C9A—C10A	−106.1 (7)	N4—C29—C30—C32	−111.8 (3)
O2—C8—C9A—C11	−70.5 (4)	O5—C29—C30—C31	−57.0 (4)
N2—C8—C9A—C11	109.2 (3)	N4—C29—C30—C31	122.4 (3)
C10—C9—C11—C20	−104.9 (4)	C31—C30—C32—C33	11.7 (5)
C8—C9—C11—C20	117.6 (4)	C29—C30—C32—C33	−111.4 (3)
C10—C9—C11—C12	73.8 (4)	C31—C30—C32—C41	−167.2 (3)
C8—C9—C11—C12	−63.7 (4)	C29—C30—C32—C41	69.6 (3)
C10A—C9A—C11—C20	−24.2 (8)	C41—C32—C33—C34	0.3 (5)
C8—C9A—C11—C20	117.6 (4)	C30—C32—C33—C34	−178.7 (3)
C10A—C9A—C11—C12	154.5 (7)	C32—C33—C34—C35	179.7 (3)
C8—C9A—C11—C12	−63.7 (4)	C32—C33—C34—C39	−1.4 (4)
C20—C11—C12—C13	−1.3 (5)	C33—C34—C35—C36	178.0 (3)
C9—C11—C12—C13	180.0 (3)	C39—C34—C35—C36	−0.9 (5)
C9A—C11—C12—C13	180.0 (3)	C34—C35—C36—C37	0.0 (5)
C11—C12—C13—C14	1.0 (5)	C42—O6—C37—C38	2.4 (5)
C12—C13—C14—C15	−179.3 (3)	C42—O6—C37—C36	−177.2 (3)
C12—C13—C14—C19	0.5 (4)	C35—C36—C37—O6	−179.0 (3)
C13—C14—C15—C16	178.8 (3)	C35—C36—C37—C38	1.4 (5)
C19—C14—C15—C16	−1.0 (4)	O6—C37—C38—C39	178.6 (3)
C21—O3—C16—C15	−3.9 (5)	C36—C37—C38—C39	−1.8 (5)
C21—O3—C16—C17	175.9 (3)	C37—C38—C39—C40	−179.3 (3)
C14—C15—C16—O3	−178.0 (3)	C37—C38—C39—C34	0.9 (5)
C14—C15—C16—C17	2.3 (5)	C33—C34—C39—C38	−178.5 (3)
O3—C16—C17—C18	178.5 (3)	C35—C34—C39—C38	0.4 (4)
C15—C16—C17—C18	−1.7 (5)	C33—C34—C39—C40	1.7 (4)
C16—C17—C18—C19	−0.3 (5)	C35—C34—C39—C40	−179.4 (3)
C17—C18—C19—C20	−177.4 (3)	C38—C39—C40—C41	179.3 (3)
C17—C18—C19—C14	1.5 (5)	C34—C39—C40—C41	−0.9 (5)
C13—C14—C19—C20	−1.7 (4)	C39—C40—C41—C32	−0.2 (5)
C15—C14—C19—C20	178.1 (3)	C33—C32—C41—C40	0.5 (5)
C13—C14—C19—C18	179.3 (3)	C30—C32—C41—C40	179.6 (3)
C15—C14—C19—C18	−0.9 (4)		

Hydrogen-bond geometry (Å, º)

Cg1 is the centroid of the hydroxyphenyl ring (C1–C6) of molecule 1; Cg4 and Cg6 are the centroids of the hydroxyphenyl ring (C22–C27) and the benzene ring (C34–C39) of the naphthalene group of molecule 2, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*O*···N1	0.87	1.81	2.606 (3)	151
N2—H2*N*···O5^{i}	0.91	1.99	2.776 (3)	143
O4—H4*O*···N3	0.87	1.83	2.630 (3)	152
N4—H4*N*···O2	0.91	1.87	2.724 (3)	154
C6—H6···*Cg*6^{i}	0.95	2.97	3.734 (4)	139

C21—H21*A*···*Cg*1^{ii}	0.98	2.66	3.476 (4)	141
C42—H42*A*···*Cg*4^{iii}	0.98	2.62	3.403 (5)	137

Symmetry codes: (i) *x*+1, *y*, *z*; (ii) *x*, *y*, *z*+1; (iii) *x*, *y*, *z*−1.