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o-Methoxy-*N*-phenylbenzohydroxamic acid

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.047
wR factor = 0.130
Data-to-parameter ratio = 17.4

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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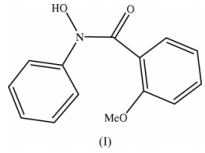
In the title compound, $C_{14}H_{13}NO_3$, the phenyl ring is *cis* to the methoxyphenyl group across the C—N bond. The crystal structure is stabilized by weak intermolecular O—H···O interactions, forming dimers that are arranged in layers parallel to the *ab* face.

Comment

Interest in hydroxamic acid derivatives lies not only in their complexation with metals as a technique for the separation of rare earth metals in particular (Kapoor *et al.*, 1975), but also in their numerous biological and medical applications.



(I)

The title compound, (I), consists of discrete molecules that have a *cis* configuration with respect to the positions of the phenyl and methoxyphenyl groups about the C7—N2 bond. The bond lengths and angles are in normal ranges (Allen *et al.*, 1987). The phenyl (C1–C6), methoxyphenyl (O3/C8–C14) [maximum deviation at O3 of 0.018 (1) Å from the mean plane] and O1/O2/N1/C6 fragments are planar. The central O1/O2/N1/C6 fragment makes dihedral angles with the phenyl and methoxyphenyl groups of 39.87 (8) and 63.75 (7)°, respectively. The phenyl and the methoxyphenyl groups are inclined at 64.53 (7) Å with respect to one another. In the

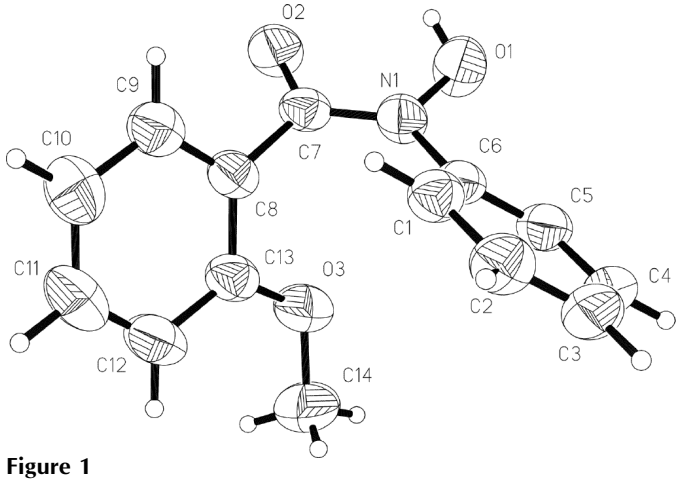


Figure 1
The molecular structure of the title compound, (I), with 50% probability displacement ellipsoids.

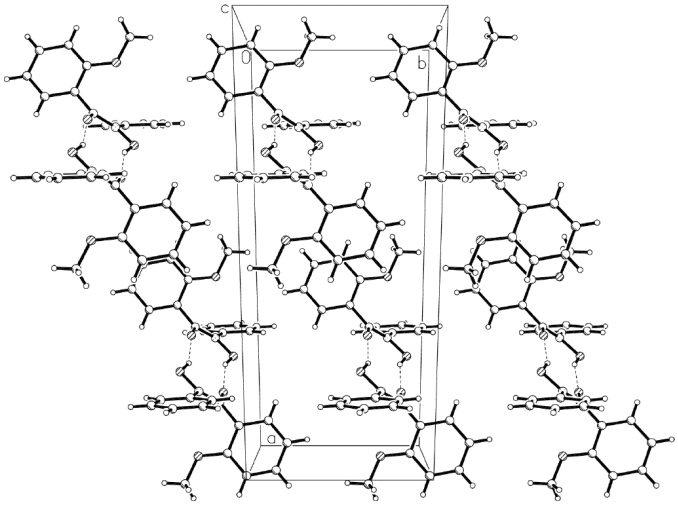


Figure 2
Packing diagram of compound (I), viewed down the *c* axis. The dashed lines denote the O—H···O hydrogen bonds.

crystal structure, the molecules are linked by intermolecular hydrogen bonding, O1—H1*A*···O2^{i} (the symmetry code is as in Table 2), to form dimers that are arranged parallel to the *ab* face (Fig. 2).

Experimental

An ether solution of *o*-methoxybenzoyl chloride (8.6 g, 50 mmol) was added dropwise to a stirred cold ethereal solution of *N*-phenylhydroxylamine (5.45 g, 50 mmol) containing sodium hydrogen carbonate (4.2 g, 50 mmol). The precipitate was filtered and washed with cold ethanol. Good quality crystals suitable for X-ray analysis were obained by recrystallization from ethyl acetate.

Crystal data

$C_{14}H_{13}NO_3$
M_r = 243.25
Monoclinic, *C*2/*c*
a = 22.451 (3) Å
b = 8.3709 (13) Å
c = 14.921 (2) Å
β = 118.531 (3)°
V = 2463.6 (6) Å^3
Z = 8
D_x = 1.312 Mg m^{-3}
Mo *K*α radiation
Cell parameters from 2709 reflections
θ = 2.1–27.5°
μ = 0.09 mm^{-1}
T = 293 (2) K
Block, colourless
0.50 × 0.32 × 0.25 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
ω scans
Absorption correction: none
8106 measured reflections
2839 independent reflections
2229 reflections with $I > 2\sigma(I)$
R_{int} = 0.033
θ_{max} = 27.5°
h = −29 → 28
k = −10 → 9
l = −19 → 19

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.130
S = 1.04
2839 reflections
163 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0593P)^2 + 0.5626P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.13 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

O1—N1	1.3931 (14)	O3—C14	1.4251 (19)
O2—C7	1.2359 (15)	N1—C7	1.3335 (17)
O3—C13	1.3554 (19)	N1—C6	1.4252 (16)
C13—O3—C14	118.22 (13)	C7—N1—C6	131.03 (10)
C7—N1—O1	116.61 (10)	O1—N1—C6	112.23 (10)

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*A*···O2^{i}	0.82	1.96	2.7200 (14)	153

Symmetry code: (i) $\frac{1}{2} - x, \frac{3}{2} - y, -z$.

After their location in a difference Fourier map, all H atoms were included in the refinement in geometrically calculated positions, and allowed to ride on the parent C or O atoms, with C—H = 0.93–0.97 Å and O—H = 0.82 Å and U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(C), and 1.5UU_{eq}(O).

Data collection: *SMART* (Seimens, 1996); cell refinement: *SAINT* (Seimens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL, PARST* (Nardelli, 1995) and *PLATON* (Spek, 1990)..

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