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(*Z*)-Benzyl 2-(hydroxyimino)acetoacetate

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The crystal structure of the title compound, $C_{11}H_{11}NO_4$, forms an extended interdigitated hydrogen-bonded array *via* O—H···O interactions parallel to the *c* axis. The oxime adopts a *Z* configuration.

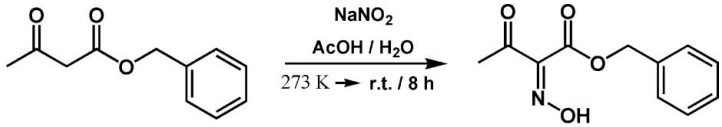
Key indicators

Single-crystal X-ray study
T = 123 K
Mean σ(C–C) = 0.003 Å
R factor = 0.036
wR factor = 0.082
Data-to-parameter ratio = 11.0

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

Comment

The synthesis of soluble multi-porphyrin architectures with specific geometries is of particular interest to our group (Bakker *et al.*, 2005). One strategy lies in the preparation of 5,15-difunctionalized porphyrins. The synthesis of the title compound, (I), is outlined in the Scheme.



(I)

The oxime adopts the *Z* configuration about the C=N bond (Fig. 1). Interestingly, the crystal structure favours what could best be described as a bifurcated intermolecular hydrogen-bonding arrangement from the hydroxyl (O4) to one molecule *via* O1 and another *via* O2 (Table 1) rather than the anticipated intramolecular arrangement, which would lead to a six-membered ring geometry. The result of this hydrogen bonding is an interdigitated structure (Fig. 2) leading to alternate phenyl ring centroid-to-centroid distances of 9.146 Å.

Experimental

The oxime (I) was prepared according to the scheme (Twyman *et al.*, 1999) and crystals suitable for X-ray analysis were grown by seeding from a neat oil sample.

Crystal data

$C_{11}H_{11}NO_4$
M_r = 221.21
Orthorhombic, $Pca2_1$
a = 10.464 (2) Å
b = 11.191 (2) Å
c = 9.1463 (18) Å
V = 1071.0 (4) Å^3
Z = 4
D_x = 1.372 Mg m^{-3}
Mo *Kα* radiation
μ = 0.11 mm^{-1}
T = 123 (2) K
Prism, colourless
0.25 × 0.13 × 0.13 mm

Data collection

Bruker X8 APEX2 CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.964, T_{max} = 0.986
22998 measured reflections
1646 independent reflections
1539 reflections with $I > 2\sigma(I)$
R_{int} = 0.029
θ_{max} = 30.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.082$
$S = 1.15$
1646 reflections
150 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0342P)^2 + 0.219P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.16$ e Å^{-3}
$\Delta\rho_{min} = -0.21$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O4—H1···O2^{i}	0.89 (3)	2.06 (3)	2.831 (2)	144 (2)
O4—H1···O1^{ii}	0.89 (3)	2.30 (3)	2.9545 (19)	130 (2)

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

The oxime H atom (H1) was located and refined. All other H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms with C—H distances in the range 0.95–1.00 Å and U_{iso}(H) = 1.2 or 1.5 times U_{eq}(C). In the absence of significant anomalous scattering, Friedel opposites were merged for the final refinement cycle.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *APEX2*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001) and *POV-RAY* (Cason, 2003); software used to prepare material for publication: *SHELXL97*.

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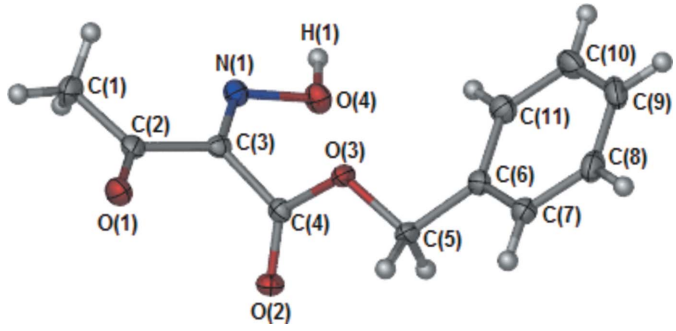

Figure 1
The molecular structure of (I) with 50% displacement ellipsoids and H atoms shown as spheres of arbitrary size.

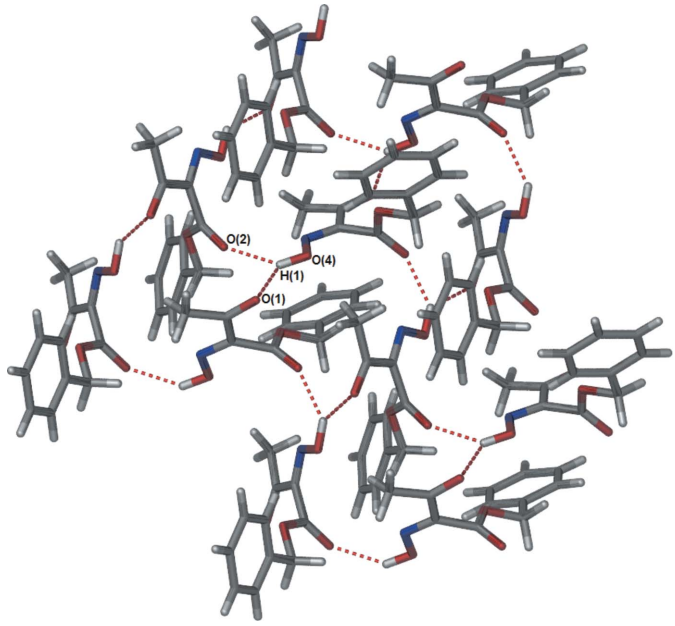

Figure 2
The packing, showing bifurcated intermolecular hydrogen bonds (dotted lines).

References

Bakker, J. M., Langford, S. J., Latter, M. J., Lee, K. A. & Woodward, C. P. (2005). *Aust. J. Chem.* **58**, 757–761.
Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
Bruker (2005). *APEX2* (Version 1.0) and *SADABS* (Version 2.03). Bruker AXS Inc., Madison, Wisconsin, USA.
Cason, C. J. (2003). *POV-RAY*. Version 3.6.0. Persistence Of Vision, Raytracer Pty Ltd, Victoria, Australia.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Twyman, L. J. & Sanders, J. K. M. (1999). *Tetrahedron Lett.* **40**, 6681–6684.