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2-[(Tri-2-pyridylmethyl)iminomethyl]phenol

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.002 Å
R factor = 0.036
wR factor = 0.102
Data-to-parameter ratio = 14.5

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

The title compound, $C_{23}H_{18}N_4O$, cyrstallizes as a discrete molecular species with an intramolecular N—H···O hydrogen bond.

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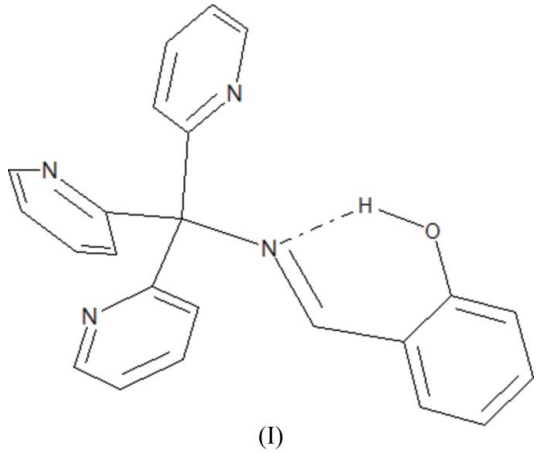
Comment

Schiff bases are of great importance in coordination chemistry and supramolecular chemistry (Martell *et al.*, 2001) and here we report the structure of the title compound, (I) (Fig. 1). The hydroxyl group forms a strong intramolecular O—H···N hydrogen bond with the Schiff base N atom (Table 1).



(I)

Experimental

The title compound was synthesized according to a method described previously (Arnold *et al.*, 1998). Yellow block-like crystals were obtained from an ethanol/water (1:1) solution. Analysis calculated for $C_{23}H_{18}N_4O$: C 75.39, N 15.29, H 4.95%; found (%): C 75.32, N 15.33, H 4.98%.

Crystal data

$C_{23}H_{18}N_4O$
M_r = 366.41
Triclinic, $P\overline{1}$
a = 8.6327 (1) Å
b = 10.6779 (2) Å
c = 10.8432 (2) Å
α = 79.001 (1)°
β = 85.057 (1)°
γ = 72.838 (1)°
V = 936.99 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 298 (2) K
0.30 × 0.20 × 0.12 mm

Data collection

Siemens SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.976, T_{max} = 0.990
4356 measured reflections
3689 independent reflections
3297 reflections with $I > 2\sigma(I)$
R_{int} = 0.018

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.036$	254 parameters
$wR(F^2) = 0.102$	H-atom parameters constrained
$S = 1.06$	$\Delta\rho_{max} = 0.18$ e Å^{-3}
3689 reflections	$\Delta\rho_{min} = -0.18$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N4	0.82	1.84	2.5638 (12)	147

All H atoms were positioned geometrically, with O—H = 0.82 and C—H = 0.93 Å, and refined as riding, with U_{iso}(H) = 1.2U_{eq}(C) or U_{iso}(H) = 1.5U_{eq}(O).

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1994); data reduction: *SAINT* and *XPREP* (Siemens, 1996); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 2000); software used to prepare material for publication: *SHELXTL*.

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References

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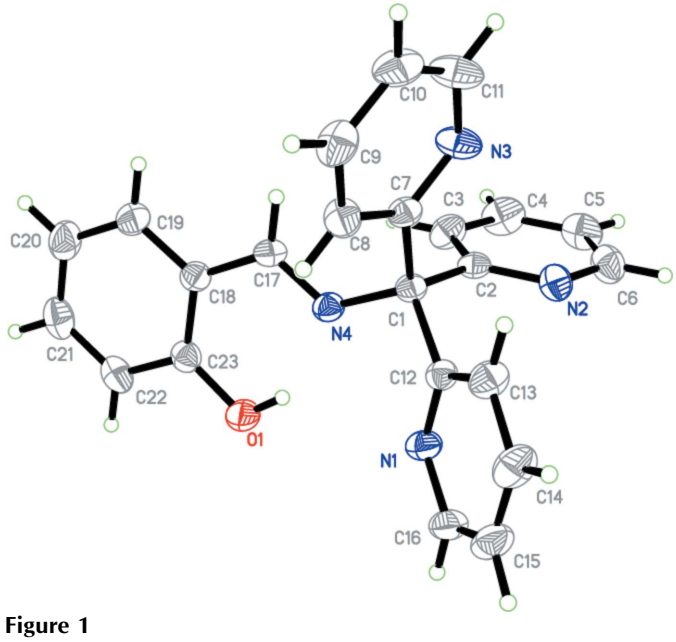

Figure 1
The molecular structure of the title compound. Displacement ellipsoids are drawn at the 30% probability level.

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