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N,*N*′-Bis(salicylidene)-1-4-butanediamine

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Key indicators

Single-crystal X-ray study
T = 123 K
Mean σ(C–C) = 0.004 Å
R factor = 0.063
wR factor = 0.106
Data-to-parameter ratio = 9.6

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

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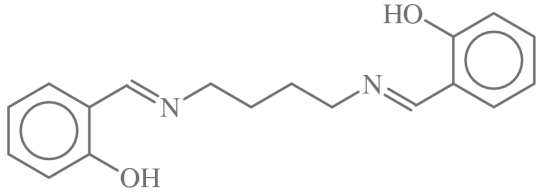
During our studies on the synthesis and structure of simple Schiff base complexes of zinc, we retrieved from the mother liquors a crystalline sample of *N*,*N*′-bis(salicylidene)-1,4-butanediamine, $C_{18}H_{20}N_2O_2$. Its structure was determined and is reported here.

Comment

During our studies on the synthesis and structure of simple Schiff base complexes of zinc, we retrieved from the mother liquors a crystalline sample of *N*,*N*′-bis(salicylidene)-1,4-butanediamine (Pfeiffer *et al.*, 1937) (m.p. 362 K). Although this compound has been known for some time, its structure remains unreported. As a consequence of our current interest in Schiff base complexes with larger diimide backbones and the fact that the analogous 1,2-ethylenediamine (Pahor *et al.*, 1978) and 1,3-propylenediamine (Elderman *et al.*, 1991) structures are known, we formed the opinion that it would be instructive to solve and report the structure of this higher homologue, (I) (Fig. 1).



(I)

Experimental

The title compound was recrystallized from dichloromethane.

Crystal data

$C_{18}H_{20}N_2O_2$
M_r = 296.36
Monoclinic, $P2_1/a$
a = 8.7330 (2) Å
b = 5.8710 (3) Å
c = 15.3070 (6) Å
β = 90.535 (1)°
V = 784.78 (5) Å^3
Z = 2
D_x = 1.254 Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 22 914 reflections
θ = 0.3–25.0°
μ = 0.08 mm^{-1}
T = 123 (2) K
Fragment, yellow
0.40 × 0.30 × 0.15 mm

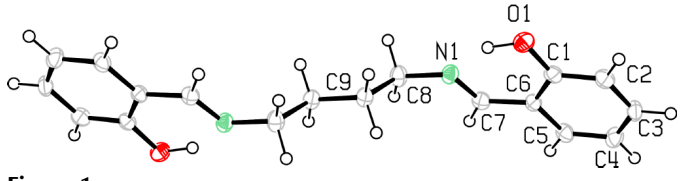


Figure 1
*ORTEP*II view of (I) with the non-H atoms drawn as 50% probability ellipsoids.

Data collection

Nonius KappaCCD diffractometer	$R_{int} = 0.069$
φ and ω scans	$\theta_{max} = 24.9^\circ$
2537 measured reflections	$h = 0 \rightarrow 10$
1358 independent reflections	$k = -6 \rightarrow 6$
910 reflections with $I > 2\sigma(I)$	$l = -17 \rightarrow 18$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0434P)^2 + 0.1547P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.063$	
$wR(F^2) = 0.135$	
$S = 1.19$	$(\Delta/\sigma)_{max} < 0.001$
1349 reflections	$\Delta\rho_{max} = 0.17$ e Å^{-3}
140 parameters	$\Delta\rho_{min} = -0.17$ e Å^{-3}
All H-atom parameters refined	

All H atoms were found in difference syntheses and refined isotropically.

Data collection: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT* (Hooft, 1988); cell refinement: *DENZO* and *COLLECT*; data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*93 (Sheldrick, 1993); molecular graphics: *ORTEP*II (Johnson, 1976); software used to prepare material for publication: *SHELXL*93.

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