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N,*N*′-Bis[4-(trifluoromethyl)benzylidene]-butane-1,4-diamine

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Key indicators

Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.002 Å
R factor = 0.048
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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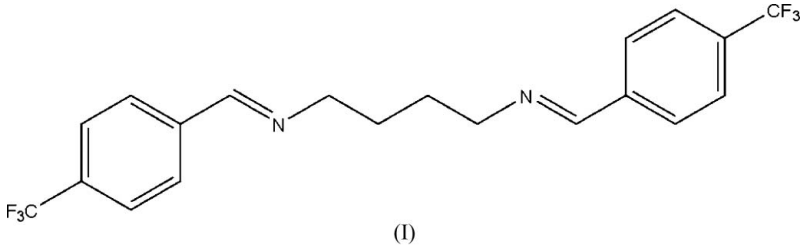
The title compound, $C_{20}H_{18}F_6N_2$, a Schiff base, was synthesized by the reaction of 1,4-diaminobutane and 4-(trifluoromethyl)benzaldehyde in chloroform solution and was crystallized from a mixture of ethanol and dichloromethane (1:1). It lies across a crystallographic inversion centre. The crystal packing is stabilized by C—H···F hydrogen bonds and π–π interactions.

Comment

Schiff bases have been used widely as ligands in the formation of transition metal complexes. Many such complexes have been structurally characterized, but only a relatively small number of free Schiff bases have been characterized (Calligaris & Randaccio, 1987). Schiff base compounds can be classified by their photochromic and thermochromic characteristics (Cohen *et al.*, 1964). Most Schiff bases possess antibacterial, anticancer and antitoxic activities (Williams, 1972). As an extension of our work (Habibi *et al.*, 2006) on the structural characterization of Schiff base compounds, the title compound, (I), is reported here.



(I)

The asymmetric unit is composed of one half-molecule of (I). there is a centre of inversion at the mid-point of the central C—C bond. The C═N unit adopts a *trans* configuration (Fig. 1). The bond lengths and angles in (I) are within expected ranges (You *et al.*, 2004, Munro & Camp, 2003). The benzene rings and the C═N imine bonds are coplanar, as indicated by the C2—N1—C3—C4 torsion angle [178.71 (13)°]. The crystals are held together by hydrogen bonds between secondary CH groups and F atoms in neighboring molecules (Fig. 2 and Table 1). The benzene rings are stacked with centroid–centroid separations of 3.820 (12) and 3.872 (11) Å, indicating π–π interactions.

Experimental

The title compound was prepared by the reaction of 1,4-diaminobutane (0.5 mmol, 44 mg) and 4-(trifluoromethyl)benzaldehyde (1 mmol, 174 mg) dissolved in chloroform (10 ml). The mixture was

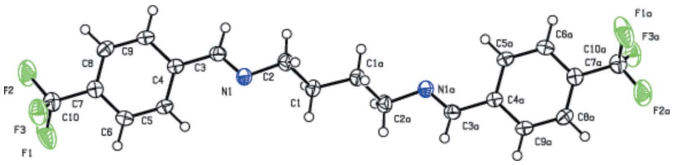


Figure 1
The molecular structure of (I), shown with 50% probability displacement ellipsoids for non-H atoms. [Symmetry code: (a) $-x$, $1-y$, $-z$.]

stirred at room temperature for 4 h. Single crystals suitable for X-ray structure analysis were obtained from an ethanol–dichloromethane (1:1) solution.

Crystal data

$C_{20}H_{18}F_6N_2$
$M_r = 400.36$
Monoclinic, $P2_1/c$
$a = 11.0107$ (16) Å
$b = 9.8541$ (14) Å
$c = 8.6457$ (13) Å
$\beta = 97.266$ (2)°
$V = 930.5$ (2) Å^3
$Z = 2$
Mo $K\alpha$ radiation
$\mu = 0.13$ mm^{-1}
$T = 150$ (2) K
0.40 × 0.40 × 0.20 mm

Data collection

Bruker SMART 1K CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
$T_{min} = 0.951$, $T_{max} = 0.975$
7930 measured reflections
2233 independent reflections
1930 reflections with $I > 2\sigma(I)$
$R_{int} = 0.021$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.048$
$wR(F^2) = 0.130$
$S = 1.06$
2233 reflections
128 parameters
H-atom parameters constrained
$\Delta\rho_{max} = 0.62$ e Å^{-3}
$\Delta\rho_{min} = -0.47$ e Å^{-3}
Absolute structure: direct methods
Flack parameter: ?
Rogers parameter: ?

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

D—H···A	D—H	H···A	D···A	D—H···A
C5—H5···N1	0.95	2.61	2.875 (2)	97
C1—H1B···F2^{i}	0.99	2.65	3.582 (2)	158

Symmetry code: (i) $-x+1, -y+1, -z+1$.

All H atoms were placed in idealized positions and constrained to ride on their parent atoms, with C—H = 0.95 or 0.99 Å and U_{iso}(H) = $1.2U_{eq}$(C).

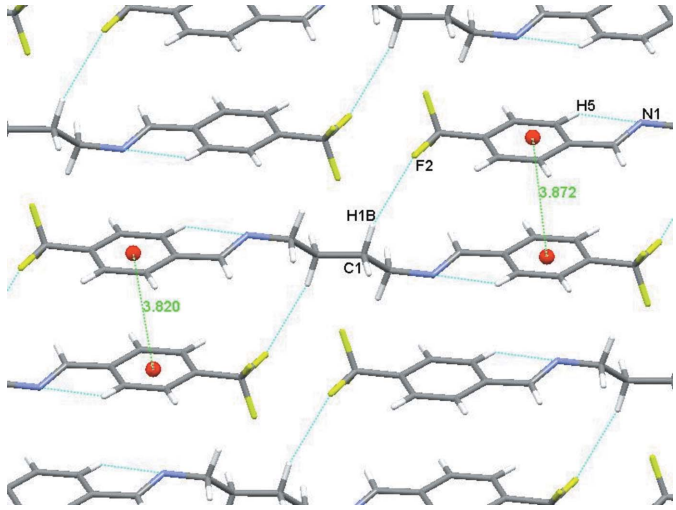


Figure 2
The packing of (I), showing one layer of molecules connected by C—H···F hydrogen bond (turquoise dotted lines) and π-π interactions (green dotted lines).

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 2001); software used to prepare material for publication: *SHELXTL* and local programs.

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