Crystal Structure of *N,N'*-Bis(4-trifluoromethoxybenzylidene)ethylenediamine

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The Schiff-base compound (C₁₈H₁₄F₆N₂O₂) has been synthesized from the reaction of ethylenediamine and 4-trifluoromethoxybenzaldehyde. The crystal structure was determined by X-ray diffraction. A structure analysis showed the compound to form in a monoclinic space group, *P*2₁/*n* with *a* = 14.0414(7), *b* = 4.6641(2), *c* = 14.2275(7) Å and β = 111.8210(10)° with *Z* = 2. The crystal structure is stabilized by intermolecular C–H...F and C–H...N hydrogen bonds.

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There has been growing interest in Schiff-base ligands, mainly because of their wide application in the fields of biochemistry, synthesis and catalysis.^{1,2} This interest is still growing, and considerable research effort has been devoted to the synthesis of new ligands and their complexes.^{3,4} Schiff bases and their

biologically active complexes have often been used as chelating ligands in the coordination chemistry of transition metals as radiopharmaceuticals for cancer targeting, agrochemicals, as model systems for biological macromolecules, as catalysts and as dioxygen carriers.⁵ Although a series of Schiff base and their complexes have been studied crystallographically, there are only a very limited number of reports about free Schiff bases in the literature.^{6,7} In this research *N,N'*-bis(4-trifluoromethoxybenzylidene)ethylenediamine was prepared by the reaction of ethylenediamine (0.3 mmol, 18 mg) and 4-trifluoromethoxybenzaldehyde (0.6 mmol, 114 mg) which were

Fig. 1 Chemical diagram for the title compound.

Table 1 Crystal data and experimental details

Empirical formula	C ₁₈ H ₁₄ F ₆ N ₂ O ₂
Formula weight	404.31
Temperature (K)	120(2)
Wavelength (Å)	0.67270
Crystal system	monoclinic
Space group, <i>Z</i>	<i>P</i> 2 ₁ / <i>n</i> , 2
Unit cell dimensions	<i>a</i> = 114.0414(7) Å <i>b</i> = 4.6641(2) Å <i>c</i> = 14.2275(7) Å <i>V</i> = 865.00(7) Å ³ <i>D_x</i> = 1.552 g/cm ³
No. of reflections used	1706
$\theta_{\max}$	24.9° with synchrotron
R1(Final)	0.0391
($\Delta\rho$) _{max}	0.23 e Å ⁻³
($\Delta\rho$) _{min}	-0.17 e Å ⁻³
Measurement	Bruker APEX2 CCD diffractometer
Program system	SADABS
Structure determination	SHELEX
Refinement	full-matrix least-squares on <i>F</i> ²
CCDC ref. no.:	298116

Table 2 Atomic coordinates (Å) and equivalent isotropic displacement paramet (Å²)

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{eq}
O(1)	0.35068(8)	0.0019(3)	0.49336(8)	0.0450(3)
N(1)	0.42973(8)	0.8606(2)	0.87007(8)	0.0299(3)
F(1)	0.1782(4)	0.047(4)	0.4162(6)	0.098(5)
F(1A)	0.1944(4)	-0.1164(10)	0.4471(4)	0.0672(13)
F(2)	0.26698(7)	-0.1524(2)	0.34311(7)	0.0522(3)
F(3)	0.2835(12)	0.2723(17)	0.3732(3)	0.094(4)
F(3A)	0.2253(4)	0.2631(9)	0.3846(2)	0.0672(17)
C(1)	0.47639(11)	1.0743(3)	0.94893(10)	0.0331(3)
C(2)	0.47313(10)	0.8199(3)	0.80766(9)	0.0275(3)
C(3)	0.43689(9)	0.6076(3)	0.72544(9)	0.0255(3)
C(4)	0.33981(10)	0.4841(3)	0.69535(9)	0.0272(3)
C(5)	0.30767(10)	0.2841(3)	0.61782(9)	0.0298(3)
C(6)	0.37478(10)	0.2109(3)	0.57074(9)	0.0299(3)
C(7)	0.47133(10)	0.3272(3)	0.59887(10)	0.0310(3)
C(8)	0.50200(10)	0.5277(3)	0.67593(10)	0.0299(3)
C(9)	0.26481(11)	0.0171(3)	0.41537(10)	0.0360(3)

$$U(\text{eq}) = (1/3)\sum_i \sum_j U_{ij} a_i^* a_j^* (\mathbf{a} \cdot \mathbf{a}_j)$$

Table 3 Selected bond distances (Å) and angles (°)

C2–C3	1.4717(17)	C2–N1	1.2640(17)
O1–C6	1.4141(16)	C1–N1	1.4613(16)
C1–C1A	1.552(3)	O1–C9	1.3021(17)
		C9–F1	1.228(5)
C6–O1–C9	120.25(11)	C1–N1–C2	116.49(11)
O1–C9–F1	127.2(4)	N1–C2–C3	123.01(12)

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