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1,2-Bis[4-(trifluoromethyl)benzylidene]hydrazine

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
Disorder in main residue
R factor = 0.060
wR factor = 0.174
Data-to-parameter ratio = 12.0

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

In the title compound, $C_{16}H_{10}F_6N_2$, the dihedral angle between the two aromatic rings is 5.4 (2)°. Both trifluoromethyl groups are disordered over two positions. The crystal structure is stabilized by van der Waals interactions.

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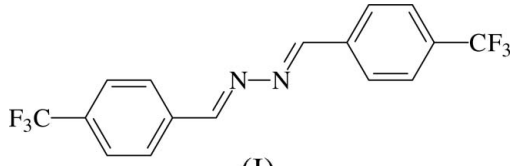
Comment

1,2-Dibenzylidenehydrazine derivatives are important starting materials for the manufacture of dyestuffs (Lienhard, 1981) and also have high potential for biological activity, possessing a wide spectrum of pesticidal activities (Werner *et al.*, 1932). The title compound, (I), was obtained during the course of our preparation of *s*-tetrazine derivatives. We report here the crystal structure of (I).



(I)

The molecular structure of (I) is illustrated in Fig. 1. All C and N atoms in the molecule are approximately coplanar, with an r.m.s deviation of 0.064 Å. The dihedral angle between the two aromatic rings is 5.4 (2)°. There are no hydrogen bonds in the crystal structure.

Experimental

Sodium borohydride (76 mg, 2 mmol) in 95% ethanol (40 ml) was added dropwise to a solution of 3,6-bis[4-(trifluoromethyl)phenyl]-1,2,4,5-tetrazine (0.74 g, 2 mmol) in chloroform (20 ml) with stirring at 263 K for 30 min, and then distilled water (200 ml) was added. The crude product obtained after drying the chloroform layer over anhydrous $MgSO_4$ for 4 h was recrystallized from absolute ethanol (yield 0.7 g). The solid product was dissolved in anhydrous ethanol and the solution evaporated gradually at room temperature to afford single crystals of (I).

Crystal data

$C_{16}H_{10}F_6N_2$
M_r = 344.26
Monoclinic, $P2_1/c$
a = 8.030 (3) Å
b = 7.903 (3) Å
c = 24.074 (9) Å
β = 100.858 (12)°
V = 1500.4 (10) Å^3
Z = 4
D_x = 1.524 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.14 mm^{-1}
T = 293 (2) K
Prism, pale yellow
0.20 × 0.18 × 0.15 mm

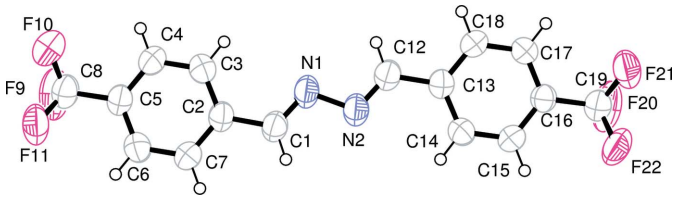


Figure 1
The molecular structure of (I), shown with 30% probability displacement ellipsoids (arbitrary spheres for H atoms). Only one disorder component for each CF_3 group is shown.

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.972, T_{max} = 0.979
7290 measured reflections
3283 independent reflections
1718 reflections with $I > 2\sigma(I)$
R_{int} = 0.075
θ_{max} = 27.1°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.060
$wR(F^2)$ = 0.174
S = 0.94
3283 reflections
273 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0881P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.050
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

The two trifluoromethyl groups (C8 and C19) are disordered over two positions with occupancies of 0.59 (3)/0.41 (3) and 0.872 (7)/0.128 (7), respectively. The C—F bond lengths were restrained to 1.32 (1) Å. The U^{ij} components of the disordered atoms were restrained to approximate isotropic behaviour. H atoms were placed in calculated positions, with C—H = 0.93 Å, and refined in riding mode, with $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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