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Key indicators

Single-crystal X-ray study
T = 295 K
Mean $\sigma(\text{C}-\text{C}) = 0.003 \text{ \AA}$
R factor = 0.052
wR factor = 0.135
Data-to-parameter ratio = 13.6

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

2,3-Bis[2-(trifluoromethyl)phenylimino]butane

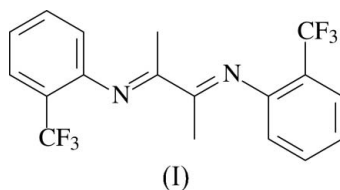
The title compound, $\text{C}_{18}\text{H}_{14}\text{F}_6\text{N}_2$, crystallizes with the $-\text{N}=\text{C}(\text{CH}_3)-\text{C}(\text{CH}_3)=\text{N}-$ diimino group around an inversion center in a *trans* configuration.

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Comment

α -Diimines are a class of ligands with a wide range of applications, especially in homogeneous catalysis, being able to chelate metal atoms forming stable five-membered rings (Van Koten & Vrieze, 1982). In addition, these compounds can present different lateral groups attached to the diazadiene backbone, allowing control over steric hindrance and electronic behaviour. Moreover, the study of α -diimine metal complexes grew considerably in the past decade as they were described as highly active polymerization catalysts (Johnson *et al.*, 1995). In this specific process, the ligand largely influences the catalytic activity and polymer structure according to its electronegativity and bulkiness, respectively (Ittel *et al.*, 2000).

The present communication describes the chief characteristics of 2,3-bis(2-trifluoromethylphenylimino)-butane, $\text{C}_{18}\text{H}_{14}\text{F}_6\text{N}_2$, (I). The compound crystallizes with the $-\text{N}=\text{C}(\text{CH}_3)-\text{C}(\text{CH}_3)=\text{N}-$ diimino group around an inversion center, in a *trans* configuration (Fig. 1).



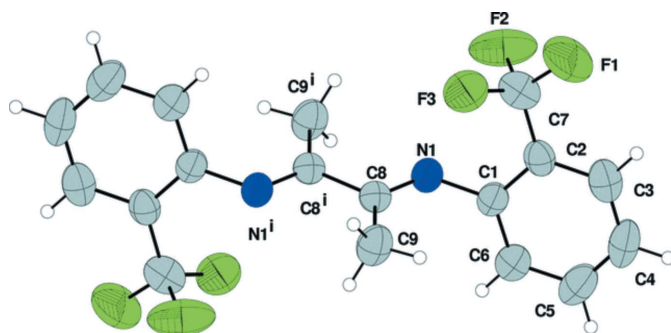
The two independent planar groups in the molecule (the central link, $-\text{N}=\text{C}(\text{CH}_3)-\text{C}(\text{CH}_3)=\text{N}-$, and the terminal aromatic ring) subtend an angle of $75.10(1)^\circ$.

Relevant bond lengths in the central core of (I) compare well with the corresponding ones in the recently reported related compound 2,3-bis(2-*tert*-butylphenylimino)butane (Ferreira *et al.*, 2006), (II): in particular, $1.423(3)/1.418(2) \text{ \AA}$ for $\text{C}-\text{N}$, $1.280(3)/1.277(2) \text{ \AA}$ for $\text{C}=\text{N}$, and $1.513(4)/1.495(3) \text{ \AA}$ for $\text{C}-\text{C}$, for (I)/(II), respectively.

The bond lengths found in (I) do not indicate a strong electron-withdrawing influence by the trifluoromethyl groups, although the $\text{F}-\text{C}-\text{F}$ bond angles are smaller than expected (Deck *et al.*, 2006). Selected geometric parameters are listed in Table 1.

Experimental

2-(Trifluoromethyl)aniline (0.6 ml, 4.8 mmol) was added slowly at room temperature to a toluene solution (15 ml) of 2,3-butanedione

**Figure 1**

The molecular structure of (I) with displacement ellipsoids at the 50% probability level. [Symmetry code: (i) $1 - x, -y, 1 - z$.]

(0.2 ml, 2.3 mmol) in the presence of a catalytic amount of acetic acid. The mixture was heated to reflux for 2 h with magnetic stirring. The solvent was partially evaporated and the crude yellow product was isolated by filtration, washed with cold methanol (3×10 ml) and dried *in vacuo*. Yellow block-shaped crystals suitable for X-ray diffraction were obtained by recrystallization from a chloroform solution (yield: 0.30 g, 35%; m.p. 432 K).

Crystal data

$C_{18}H_{14}F_6N_2$	$V = 872.7 (3) \text{ \AA}^3$
$M_r = 372.31$	$Z = 2$
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation
$a = 10.472 (2) \text{ \AA}$	$\mu = 0.13 \text{ mm}^{-1}$
$b = 7.6884 (15) \text{ \AA}$	$T = 295 \text{ K}$
$c = 10.885 (2) \text{ \AA}$	$0.30 \times 0.25 \times 0.20 \text{ mm}$
$\beta = 95.26 (3)^\circ$	

Data collection

Nonius KappaCCD diffractometer	1618 independent reflections
Absorption correction: none	838 reflections with $I > 2\sigma(I)$
5857 measured reflections	$R_{int} = 0.046$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.052$	119 parameters
$wR(F^2) = 0.135$	H-atom parameters constrained
$S = 0.99$	$\Delta\rho_{max} = 0.19 \text{ e \AA}^{-3}$
1618 reflections	$\Delta\rho_{min} = -0.20 \text{ e \AA}^{-3}$

Table 1

Selected geometric parameters (\AA , $^\circ$).

C1–C2	1.394 (3)	C7–F1	1.343 (3)
C2–C7	1.488 (4)	C7–F2	1.344 (3)
C7–F3	1.337 (3)	C8–C9	1.491 (3)
F3–C7–F1	104.9 (2)	F1–C7–F2	104.9 (2)
F3–C7–F2	105.7 (2)		

All H atoms in the structure were positioned geometrically at distances of 0.93 \AA (aromatic) and 0.96 \AA (methyl) and allowed to ride, with $U_{iso}(H) = xU_{eq}(C)$ ($x = 1.2$ and 1.5 for Csp^2 and Csp^3 , respectively).

Data collection: *COLLECT* (Hooft, 1998); cell refinement: *PhiChi* (Duisenberg *et al.*, 2000); data reduction: *DIRAX* (Duisenberg, 1992); 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: *WinGX* (Farrugia, 1999).

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