organic papers

[3,5-Bis(trifluoromethyl)phenyl]{(E)-2-[(E)-3,5-bis(trifluoromethyl)phenylimino]-1-methylpropylidene}amine

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Key indicators

Single-crystal X-ray study
$T = 150$ K
Mean σ(C–C) = 0.002 Å
Disorder in main residue
R factor = 0.059
wR factor = 0.192
Data-to-parameter ratio = 21.9

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

At 150 K, the two imine groups of the title compound, $C_{20}H_{12}F_{12}N_2$, are mutually *trans*. The molecule has crystallographic inversion symmetry.

Comment

The title compound, (I), is of interest as a bidentate ligand for catalytically active platinum(II) compounds (Johansson *et al.*, 1999), in which the imine groups are mutually *cis*.

(I)
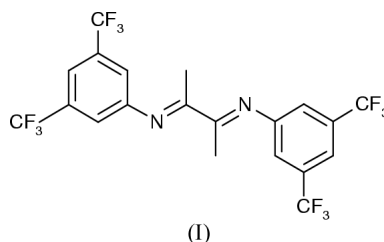
The molecule of (I) is centrosymmetric in the crystal structure. Thus the central diimine group is *trans* and planar. The dihedral angle between the least-squares planes of this group and the benzene ring is 77.25 (12)°. Atom C3 lies 0.0291 (16) Å out of the least-squares plane of the diimine group and N1 lies 0.1344 (13) Å out of the plane of the benzene ring. Thus, there is a slight pyramidalization of *ipso*-C atom C3, which lies 0.0471 (14) Å above the plane of its bonded neighbouring atoms (N1, C4 and C8).

Experimental

The title compound was prepared by the method of Johansson *et al.* (1999). Suitable crystals were grown from chloroform by slow evaporation.
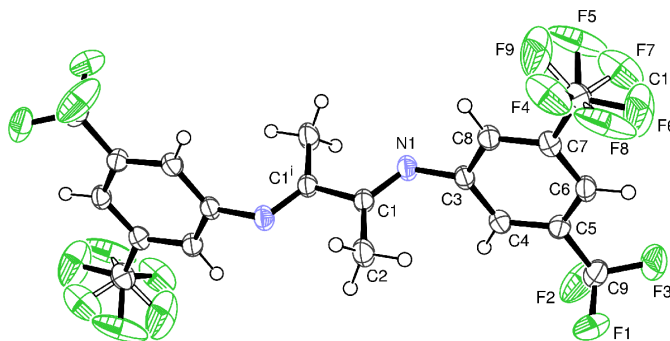
Figure 1
View of the molecule of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are represented by circles of arbitrary size. Symmetry code (i) is as in Table 1. Both disorder components are shown.

Crystal data

$C_{20}H_{12}F_{12}N_2$
$M_r = 508.32$
Triclinic, $P\bar{1}$
$a = 8.1406 (12)$ Å
$b = 8.2225 (12)$ Å
$c = 8.7087 (13)$ Å
$\alpha = 82.044 (12)°$
$\beta = 71.590 (11)°$
$\gamma = 68.264 (11)°$
$V = 513.62 (13)$ Å^3

$Z = 1$
$D_x = 1.643$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 8717
  reflections
$\theta = 2.5$–$32.3°$
$\mu = 0.17$ mm^{-1}
$T = 150 (2)$ K
Lath, colourless
$0.60 \times 0.30 \times 0.10$ mm

Data collection

Stoe IPDS-II diffractometer
ω scans
Absorption correction: none
10945 measured reflections
3638 independent reflections
2477 reflections with $I > 2\sigma(I)$

$R_{int} = 0.036$
$\theta_{max} = 32.3°$
$h = -12 \rightarrow 12$
$k = -12 \rightarrow 12$
$l = -13 \rightarrow 13$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.059$
$wR(F^2) = 0.192$
$S = 1.15$
3638 reflections
166 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.1038P)^2$
  $+ 0.0549P]$
  where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.62$ e Å^{-3}
$\Delta\rho_{min} = -0.45$ e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.065 (17)

Table 1
Selected geometric parameters (Å, °).

N1—C1	1.2731 (19)	C1—C2	1.497 (2)
N1—C3	1.4079 (18)	C1—C1^i	1.505 (3)
C1—N1—C3	121.92 (13)	C2—C1—C1^i	117.77 (15)
N1—C1—C2	126.47 (13)	C8—C3—N1	119.56 (13)
N1—C1—C1^i	115.74 (16)	C4—C3—N1	120.81 (13)
C3—N1—C1—C2	2.5 (2)	C1—N1—C3—C8	−107.89 (17)
C3—N1—C1—C1^i	−179.06 (14)	C1—N1—C3—C4	78.82 (19)

Symmetry code: (i) $-x, 2 - y, 1 - z$.

All H atoms were initially located in a difference Fourier map. The methyl H atoms were constrained to an ideal geometry, with C—H distances of 0.98 Å, but each group was allowed to rotate freely about its X—C bond. All other H atoms were placed in geometrically idealized positions, with C—H distances of 0.95 Å. $U_{iso}(H)$ values were set at $1.2U_{eq}(C)$ for all H atoms. The C10 CF$_3$ group was disordered over two sites with relative occupancies of 0.887 (2):0.113 (2).
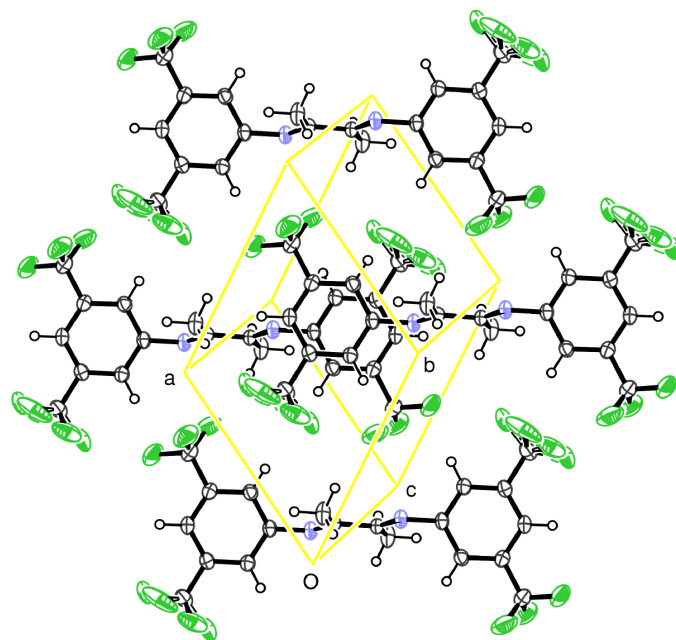

Figure 2
The molecular packing of (I).

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-RED* (Stoe & Cie, 2001); program(s) used to solve structure: *X-STEP*32 (Stoe & Cie, 2001) and *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *WinGX* (Farrugia, 1999) and *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 *for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX*.

References

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