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1,1,1,3,3,3-Hexafluoro-2-(4-nitrophenyl)-*N*-phenylisopropylamine

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.059
wR factor = 0.173
Data-to-parameter ratio = 25.2

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

There is no interaction between the amine H and any F atom in the title compound, $C_{15}H_{10}F_6N_2O_2$. Rather the amine H atom is hydrogen bonded to one of the nitro group O atoms on a neighboring molecule. This hydrogen bonding operates in the direction of the minor axis and links molecules into infinite chains.

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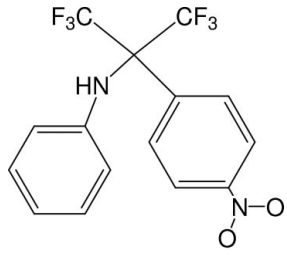
Comment

(Trifluoromethyl)trimethylsilane reacts with nitrones to afford α-(trifluoromethyl)hydroxylamines, protected as *O*-trimethylsilyl ethers. Adducts with strong electron-withdrawing groups on the α-aryl ring undergo an elimination/addition sequence to produce α,α-bis(trifluoromethyl)amines. The structure of compound, (I), produced from the *p*-nitrophenyl adduct, is reported here.



(I)

Experimental

The preparation of (I) has been reported (Nelson *et al.*, 2001). Crystals suitable for diffraction analysis were obtained from hexane.

Crystal data

$C_{15}H_{10}F_6N_2O_2$
M_r = 364.25
Monoclinic, $C2/c$
a = 16.903 (3) Å
b = 10.182 (2) Å
c = 17.971 (3) Å
β = 104.90 (1)°
V = 2989.1 (9) Å^3
Z = 8
D_x = 1.619 Mg m^{-3}
D_m: more dense than CCl_4
D_m measured by flotation
Mo $K\alpha$ radiation
Cell parameters from 13 reflections
θ = 10–12.5°
μ = 0.16 mm^{-1}
T = 293 (2) K
Cut fragment, pale yellow
0.40 × 0.35 × 0.25 mm

Data collection

Picker four-circle diffractometer
$\theta/2\theta$ scans
7110 measured reflections
3603 independent reflections
1373 reflections with $I > 2\sigma(I)$
R_{int} = 0.056
θ_{max} = 28.0°
$h = -22 \rightarrow 18$
$k = -7 \rightarrow 13$
$l = -23 \rightarrow 23$
4 standard reflections
every 150 reflections
intensity decay: <1%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.059$
$wR(F^2) = 0.173$
$S = 0.98$
3603 reflections
143 parameters
H-atom parameters constrained

$w = [\exp\{1.30(\sin\theta/\lambda)^2\}]/[\sigma^2(F_o^2) + (0.0559P)^2]$
where $P = 0.33F_o^2 + 0.67F_c^2$
$(\Delta/\sigma)_{max} = 0.010$
$\Delta\rho_{max} = 0.51$ e Å^{-3}
$\Delta\rho_{min} = -0.26$ e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.0018 (3)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1^{i}	0.86	2.42	3.234 (4)	159

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

Both phenyl rings were refined as rigid groups.

Data collection: *XSTAL* (Brown, 1985), a modification of Picker FACS–I software (Picker, 1967); cell refinement: *CELL* (Brown, 1985); data reduction: *MINCON* (Brown, 1985); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 (Farrugia, 1997).

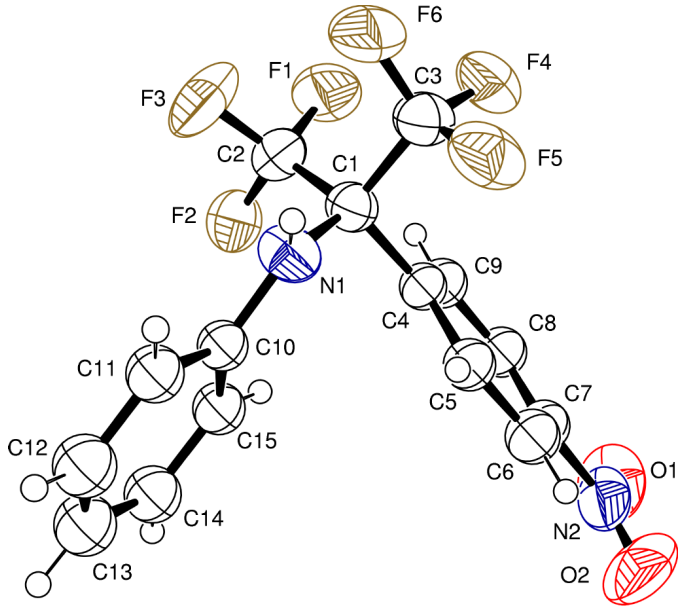


Figure 1
Displacement ellipsoid plot of the title compound with ellipsoids at the 50% probability level and H atoms omitted for clarity.

References

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