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2-(4-Flouroanilino)tropone

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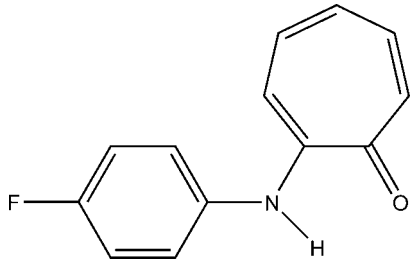
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.032; wR factor = 0.083; data-to-parameter ratio = 14.2.

The title compound, $C_{13}H_{10}FNO$, which was synthesized from the reaction of tosyloxytropone and 4-fluoroaniline, has two independent molecules of similar bond dimensions in the asymmetric unit. Adjacent molecules are linked by hydrogen bonds and C—H···F interactions.

Related literature

For general background, see: Hicks & Brookhart (2001); Kubo *et al.* (2005, 2006); Polonsky *et al.* (1981); Roesky & Burgstein (1999); Yamamoto *et al.* (2001). For related diketonato complexes, see: Janse van Rensburg & Roodt (2006); Janse van Rensburg *et al.* (2006).



Experimental

Crystal data

$C_{13}H_{10}FNO$
M_r = 215.22
Monoclinic, $P2_1/n$
a = 9.9075 (3) Å
b = 17.5746 (5) Å
c = 12.2212 (4) Å
β = 96.714 (1)°
V = 2113.37 (11) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 100 (2) K
0.19 × 0.18 × 0.18 mm

Data collection

Bruker X8 APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
T_{min} = 0.982, T_{max} = 0.983
37801 measured reflections
4116 independent reflections
3581 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.083
S = 1.05
4116 reflections
289 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N12—H12···O31^{i}	0.88	2.07	2.8891 (13)	154
N32—H32···O11^{i}	0.88	2.13	2.9524 (12)	155
C45—H45···F24	0.95	2.72	3.6058 (15)	156
C23—H23···F44^{ii}	0.95	2.57	3.4538 (16)	155

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $-x, -y+1, -z$.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT-Plus* (Bruker, 2004); data reduction: *SAINT-Plus* and *XPREP* (Bruker, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg & Putz, 2006); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG2336).

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supplementary materials

Acta Cryst. (2007). E**63**, o4353 [**doi:10.1107/S1600536807050271**]

2-(4-Flouroanilino)tropone

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Comment

In the current paper the title compound, (I), is presented as an example of a product formed during the exchange reaction of tosyloxytropone and the corresponding 4-flouroaniline. The compound is the first of a series of halogenated derivatives of tropolone type molecules, see Fig. 1. Two closely related derivatives of *N*-alkyl (Roesky & Burgstein, 1999) and *N*-aryl (Hicks & Brookhart, 2001) have been reported. The addition of a halogen moiety to the compound can drastically affect the packing of the molecule in the solid state.

Two independent molecules are present in the asymmetric unit, with the only observable difference being the rotation of the phenyl moiety compared to the tropone molecule. This is clearly illustrated by the torsional twist of the C—N—C—C (see Table 1) and the interplanar dihedral angle formed by the phenyl and seven membered tropone ring systems of 46.04 (3) and 41.45 (4) °, respectively.

Weak intra- and intermolecular interactions is observed in the solid state, see Table 2. The weak intermolecular hydrogen bonds form dimeric systems in the solid state consisting of the two independent units. The flouro moieties do have a significant effect on the packing of the molecule in the solid state, with C—F···H interactions being observed.

Experimental

The title compound was obtained during the coupling tosyloxytropone and 4-flouroaniline in a 1:1 ration in toluene. On evaporation of the solvent; crystals suitable for X-Ray crystallography was obtained.

Refinement

H atoms were positioned geometrically and refined using a riding model, with C—H = 0.95 Å and with U_{iso}(H) = 1.2 times U_{eq}(C aromatic).

Figures

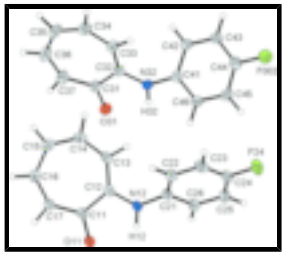


Fig. 1. : Representation of the title compound (I), showing the numbering scheme and displacement ellipsoids (50% probability).

2-(4-Flouroanilino)tropone

Crystal data

$C_{13}H_{10}FNO$	$F_{000} = 896$
$M_r = 215.22$	$D_x = 1.353$ Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -P 2yn	Cell parameters from 9979 reflections
$a = 9.9075$ (3) Å	$\theta = 2.4$–28.3º
$b = 17.5746$ (5) Å	$\mu = 0.10$ mm^{-1}
$c = 12.2212$ (4) Å	$T = 100$ (2) K
$\beta = 96.7140$ (10)º	Cuboid, yellow
$V = 2113.37$ (11) Å^3	0.19 × 0.18 × 0.18 mm
$Z = 8$	

Data collection

Bruker SMART 1K CCD area-detector diffractometer	4116 independent reflections
Radiation source: fine-focus sealed tube	3581 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.026$
Detector resolution: 512 pixels mm^{-1}	$\theta_{max} = 26.0$º
$T = 100(2)$ K	$\theta_{min} = 2.0$º
φ and ω scans	$h = -12 \rightarrow 12$
Absorption correction: multi-scan (SADABS; Bruker, 1998)	$k = -20 \rightarrow 21$
$T_{min} = 0.982$, $T_{max} = 0.983$	$l = -14 \rightarrow 14$
37801 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.032$	H-atom parameters constrained
$wR(F^2) = 0.083$	$w = 1/[\sigma^2(F_o^2) + (0.0338P)^2 + 0.8256P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.05$	$(\Delta/\sigma)_{max} = 0.001$
4116 reflections	$\Delta\rho_{max} = 0.20$ e Å^{-3}
289 parameters	$\Delta\rho_{min} = -0.20$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($Å^2$)

	x	*y*	*z*	U_{iso}*/U_{eq}
F24	0.33924 (10)	0.60818 (5)	0.00722 (6)	0.0470 (2)
F44	0.09980 (9)	0.38655 (5)	−0.11523 (7)	0.0468 (2)
O31	0.32909 (8)	0.31212 (5)	0.52144 (7)	0.0265 (2)
O11	0.50514 (8)	0.63320 (5)	0.65968 (7)	0.0294 (2)
N32	0.20137 (9)	0.33470 (6)	0.33231 (8)	0.0213 (2)
H32	0.2874	0.3423	0.3569	0.018*
N12	0.42537 (10)	0.59783 (6)	0.46111 (8)	0.0221 (2)
H12	0.5013	0.6202	0.4887	0.019*
C21	0.39972 (12)	0.59728 (6)	0.34498 (10)	0.0210 (2)
C46	0.23044 (12)	0.40892 (7)	0.17152 (10)	0.0256 (3)
H46	0.2902	0.4412	0.2168	0.031*
C41	0.16614 (11)	0.34861 (7)	0.21878 (10)	0.0208 (2)
C26	0.50927 (12)	0.59112 (7)	0.28413 (10)	0.0240 (3)
H26	0.5982	0.5839	0.3210	0.029*
C42	0.07791 (11)	0.30169 (7)	0.15148 (10)	0.0225 (3)
H42	0.0340	0.2604	0.1830	0.027*
C11	0.39801 (11)	0.59507 (7)	0.64867 (10)	0.0214 (2)
C22	0.26927 (12)	0.60873 (7)	0.29035 (10)	0.0250 (3)
H22	0.1941	0.6137	0.3315	0.030*
C15	0.13306 (12)	0.49457 (7)	0.67800 (10)	0.0260 (3)
H15	0.0593	0.4683	0.7039	0.031*
C13	0.24472 (12)	0.51698 (7)	0.50645 (10)	0.0218 (2)
H13	0.2353	0.5017	0.4314	0.026*
C31	0.20423 (12)	0.29945 (6)	0.51716 (10)	0.0222 (3)
C32	0.12203 (11)	0.31135 (6)	0.40904 (10)	0.0207 (2)
C44	0.12025 (13)	0.37460 (8)	−0.00410 (11)	0.0307 (3)
C14	0.15145 (12)	0.48383 (7)	0.56961 (10)	0.0236 (3)
H14	0.0912	0.4482	0.5313	0.028*
C16	0.21218 (12)	0.54045 (7)	0.75443 (10)	0.0252 (3)
H16	0.1821	0.5431	0.8254	0.030*
C17	0.32642 (12)	0.58199 (7)	0.74198 (10)	0.0237 (3)
H17	0.3652	0.6067	0.8074	0.028*
C25	0.48976 (14)	0.59541 (7)	0.17019 (11)	0.0296 (3)

H25	0.5643	0.5913	0.1282	0.035*
C12	0.34890 (11)	0.56856 (6)	0.53560 (9)	0.0200 (2)
C23	0.24943 (14)	0.61280 (7)	0.17668 (11)	0.0301 (3)
H23	0.1610	0.6204	0.1390	0.036*
C34	−0.11526 (12)	0.27952 (7)	0.45227 (11)	0.0290 (3)
H34	−0.2057	0.2774	0.4166	0.035*
C37	0.14884 (13)	0.27657 (7)	0.61475 (11)	0.0292 (3)
H37	0.2136	0.2740	0.6784	0.035*
C43	0.05403 (12)	0.31496 (7)	0.03915 (10)	0.0272 (3)
H43	−0.0066	0.2836	−0.0069	0.033*
C24	0.35972 (15)	0.60573 (7)	0.11933 (10)	0.0310 (3)
C45	0.20782 (13)	0.42200 (7)	0.05935 (11)	0.0309 (3)
H45	0.2518	0.4628	0.0268	0.037*
C35	−0.10052 (13)	0.25745 (7)	0.56042 (12)	0.0320 (3)
H35	−0.1802	0.2401	0.5890	0.038*
C33	−0.01810 (12)	0.30469 (7)	0.38593 (11)	0.0242 (3)
H33	−0.0538	0.3196	0.3136	0.029*
C36	0.01932 (14)	0.25768 (7)	0.63340 (12)	0.0327 (3)
H36	0.0094	0.2425	0.7066	0.039*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F24	0.0714 (6)	0.0513 (5)	0.0165 (4)	−0.0117 (5)	−0.0026 (4)	0.0076 (3)
F44	0.0561 (5)	0.0553 (6)	0.0255 (5)	−0.0206 (4)	−0.0100 (4)	0.0137 (4)
O31	0.0221 (4)	0.0298 (5)	0.0274 (5)	−0.0002 (3)	0.0023 (3)	0.0019 (4)
O11	0.0238 (4)	0.0413 (5)	0.0232 (5)	−0.0093 (4)	0.0032 (3)	−0.0070 (4)
N32	0.0170 (5)	0.0237 (5)	0.0233 (5)	−0.0024 (4)	0.0026 (4)	0.0001 (4)
N12	0.0195 (5)	0.0287 (5)	0.0178 (5)	−0.0012 (4)	0.0005 (4)	−0.0028 (4)
C21	0.0264 (6)	0.0172 (6)	0.0188 (6)	0.0018 (4)	0.0007 (5)	−0.0002 (4)
C46	0.0262 (6)	0.0231 (6)	0.0271 (7)	−0.0047 (5)	0.0015 (5)	−0.0001 (5)
C41	0.0181 (5)	0.0209 (6)	0.0237 (6)	0.0023 (4)	0.0029 (4)	0.0011 (5)
C26	0.0278 (6)	0.0216 (6)	0.0226 (7)	0.0030 (5)	0.0031 (5)	0.0010 (5)
C42	0.0180 (5)	0.0213 (6)	0.0282 (7)	−0.0003 (4)	0.0035 (5)	0.0019 (5)
C11	0.0203 (6)	0.0225 (6)	0.0208 (6)	0.0016 (5)	0.0004 (4)	−0.0020 (4)
C22	0.0263 (6)	0.0223 (6)	0.0257 (7)	0.0025 (5)	0.0000 (5)	−0.0002 (5)
C15	0.0222 (6)	0.0253 (6)	0.0302 (7)	−0.0018 (5)	0.0019 (5)	0.0057 (5)
C13	0.0234 (6)	0.0211 (6)	0.0199 (6)	0.0037 (5)	−0.0021 (5)	−0.0018 (4)
C31	0.0241 (6)	0.0161 (6)	0.0271 (7)	0.0030 (4)	0.0059 (5)	0.0002 (4)
C32	0.0225 (6)	0.0146 (5)	0.0261 (6)	0.0016 (4)	0.0072 (5)	−0.0004 (4)
C44	0.0330 (7)	0.0353 (7)	0.0218 (7)	−0.0042 (6)	−0.0044 (5)	0.0080 (5)
C14	0.0209 (6)	0.0186 (6)	0.0297 (7)	0.0015 (4)	−0.0044 (5)	0.0012 (5)
C16	0.0268 (6)	0.0272 (6)	0.0220 (6)	0.0012 (5)	0.0050 (5)	0.0031 (5)
C17	0.0266 (6)	0.0252 (6)	0.0190 (6)	0.0000 (5)	0.0016 (5)	−0.0018 (5)
C25	0.0411 (7)	0.0261 (7)	0.0230 (7)	−0.0010 (5)	0.0101 (5)	0.0006 (5)
C12	0.0192 (5)	0.0209 (6)	0.0196 (6)	0.0056 (4)	0.0010 (4)	−0.0002 (4)
C23	0.0354 (7)	0.0254 (6)	0.0265 (7)	−0.0003 (5)	−0.0087 (5)	0.0042 (5)
C34	0.0216 (6)	0.0251 (6)	0.0419 (8)	0.0019 (5)	0.0107 (5)	−0.0026 (5)

C37	0.0326 (7)	0.0276 (7)	0.0280 (7)	0.0057 (5)	0.0068 (5)	0.0067 (5)
C43	0.0230 (6)	0.0290 (6)	0.0281 (7)	−0.0041 (5)	−0.0034 (5)	0.0009 (5)
C24	0.0512 (8)	0.0248 (6)	0.0157 (6)	−0.0043 (6)	−0.0019 (6)	0.0036 (5)
C45	0.0343 (7)	0.0271 (7)	0.0306 (7)	−0.0078 (5)	0.0007 (5)	0.0078 (5)
C35	0.0285 (6)	0.0276 (7)	0.0435 (8)	0.0010 (5)	0.0190 (6)	0.0026 (6)
C33	0.0222 (6)	0.0217 (6)	0.0293 (7)	0.0031 (5)	0.0059 (5)	−0.0002 (5)
C36	0.0398 (7)	0.0273 (7)	0.0343 (8)	0.0060 (6)	0.0179 (6)	0.0081 (5)

Geometric parameters (Å, °)

F24—C24	1.3621 (15)	C13—C12	1.3886 (16)
F44—C44	1.3658 (15)	C13—C14	1.3985 (17)
O11—C11	1.2491 (14)	C13—H13	0.9500
N12—C12	1.3522 (15)	C31—C37	1.4277 (17)
N12—C21	1.4124 (15)	C31—C32	1.4837 (17)
O31—C31	1.2520 (14)	C32—C33	1.3890 (16)
N32—C32	1.3558 (15)	C44—C43	1.3746 (18)
N32—C41	1.4118 (15)	C44—C45	1.3750 (18)
N32—H32	0.8800	C14—H14	0.9500
N12—H12	0.8800	C16—C17	1.3702 (17)
C21—C26	1.3898 (17)	C16—H16	0.9500
C21—C22	1.3982 (16)	C17—H17	0.9500
C46—C45	1.3821 (18)	C25—C24	1.375 (2)
C46—C41	1.3961 (16)	C25—H25	0.9500
C46—H46	0.9500	C23—C24	1.371 (2)
C41—C42	1.3973 (16)	C23—H23	0.9500
C26—C25	1.3853 (18)	C34—C35	1.3689 (19)
C26—H26	0.9500	C34—C33	1.4007 (17)
C42—C43	1.3852 (18)	C34—H34	0.9500
C42—H42	0.9500	C37—C36	1.3701 (18)
C11—C17	1.4302 (17)	C37—H37	0.9500
C11—C12	1.4853 (16)	C43—H43	0.9500
C22—C23	1.3819 (18)	C45—H45	0.9500
C22—H22	0.9500	C35—C36	1.399 (2)
C15—C14	1.3712 (18)	C35—H35	0.9500
C15—C16	1.4020 (18)	C33—H33	0.9500
C15—H15	0.9500	C36—H36	0.9500
C12—N12—C21	128.67 (10)	C15—C14—C13	130.31 (11)
C32—N32—C41	129.45 (10)	C15—C14—H14	114.8
C32—N32—H32	115.3	C13—C14—H14	114.8
C41—N32—H32	115.3	C17—C16—C15	129.59 (12)
C12—N12—H12	115.7	C17—C16—H16	115.2
C21—N12—H12	115.7	C15—C16—H16	115.2
C26—C21—C22	119.46 (11)	C16—C17—C11	131.85 (11)
C26—C21—N12	118.57 (10)	C16—C17—H17	114.1
C22—C21—N12	121.77 (11)	C11—C17—H17	114.1
C45—C46—C41	120.51 (11)	C24—C25—C26	118.34 (12)
C45—C46—H46	119.7	C24—C25—H25	120.8
C41—C46—H46	119.7	C26—C25—H25	120.8

C46—C41—C42	119.26 (11)	N12—C12—C13	122.26 (11)
C46—C41—N32	117.76 (10)	N12—C12—C11	111.02 (10)
C42—C41—N32	122.83 (10)	C13—C12—C11	126.60 (11)
C25—C26—C21	120.51 (12)	C24—C23—C22	118.75 (12)
C25—C26—H26	119.7	C24—C23—H23	120.6
C21—C26—H26	119.7	C22—C23—H23	120.6
C43—C42—C41	120.44 (11)	C35—C34—C33	130.19 (12)
C43—C42—H42	119.8	C35—C34—H34	114.9
C41—C42—H42	119.8	C33—C34—H34	114.9
O11—C11—C17	119.65 (11)	C36—C37—C31	131.77 (13)
O11—C11—C12	116.76 (10)	C36—C37—H37	114.1
C17—C11—C12	123.53 (10)	C31—C37—H37	114.1
C23—C22—C21	120.15 (12)	C44—C43—C42	118.39 (11)
C23—C22—H22	119.9	C44—C43—H43	120.8
C21—C22—H22	119.9	C42—C43—H43	120.8
C14—C15—C16	126.56 (11)	F24—C24—C23	118.52 (12)
C14—C15—H15	116.7	F24—C24—C25	118.70 (12)
C16—C15—H15	116.7	C23—C24—C25	122.78 (12)
C12—C13—C14	130.51 (11)	C44—C45—C46	118.49 (12)
C12—C13—H13	114.7	C44—C45—H45	120.8
C14—C13—H13	114.7	C46—C45—H45	120.8
O31—C31—C37	119.31 (11)	C34—C35—C36	126.98 (12)
O31—C31—C32	116.68 (10)	C34—C35—H35	116.5
C37—C31—C32	123.99 (11)	C36—C35—H35	116.5
N32—C32—C33	122.10 (11)	C32—C33—C34	130.33 (12)
N32—C32—C31	110.88 (10)	C32—C33—H33	114.8
C33—C32—C31	126.92 (11)	C34—C33—H33	114.8
F44—C44—C43	118.53 (11)	C37—C36—C35	129.50 (13)
F44—C44—C45	118.56 (11)	C37—C36—H36	115.2
C43—C44—C45	122.90 (12)	C35—C36—H36	115.2
C12—N12—C21—C26	−145.61 (12)	C21—N12—C12—C11	−168.38 (10)
C12—N12—C21—C22	39.51 (17)	C14—C13—C12—N12	−176.39 (11)
C45—C46—C41—C42	−0.32 (18)	C14—C13—C12—C11	7.9 (2)
C45—C46—C41—N32	175.26 (11)	O11—C11—C12—N12	−5.99 (15)
C32—N32—C41—C46	143.54 (12)	C17—C11—C12—N12	171.17 (11)
C32—N32—C41—C42	−41.05 (18)	O11—C11—C12—C13	170.11 (11)
C22—C21—C26—C25	−0.71 (18)	C17—C11—C12—C13	−12.73 (18)
N12—C21—C26—C25	−175.71 (11)	C21—C22—C23—C24	−0.27 (18)
C46—C41—C42—C43	−0.23 (17)	O31—C31—C37—C36	−178.35 (13)
N32—C41—C42—C43	−175.56 (11)	C32—C31—C37—C36	3.2 (2)
C26—C21—C22—C23	0.91 (18)	F44—C44—C43—C42	178.23 (11)
N12—C21—C22—C23	175.74 (11)	C45—C44—C43—C42	−0.7 (2)
C41—N32—C32—C33	−6.94 (18)	C41—C42—C43—C44	0.72 (18)
C41—N32—C32—C31	176.37 (10)	C22—C23—C24—F24	178.64 (11)
O31—C31—C32—N32	−0.01 (14)	C22—C23—C24—C25	−0.6 (2)
C37—C31—C32—N32	178.46 (11)	C26—C25—C24—F24	−178.45 (11)
O31—C31—C32—C33	−176.51 (11)	C26—C25—C24—C23	0.79 (19)
C37—C31—C32—C33	1.97 (19)	F44—C44—C45—C46	−178.76 (12)
C16—C15—C14—C13	−3.7 (2)	C43—C44—C45—C46	0.2 (2)

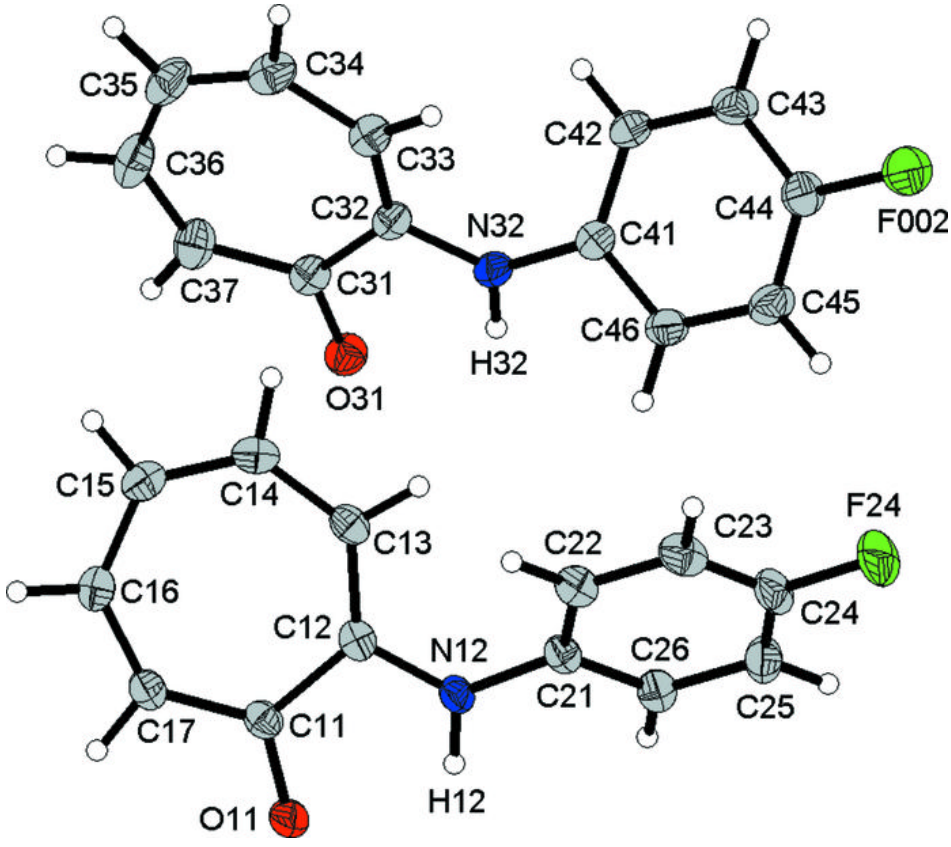
C12—C13—C14—C15	2.4 (2)	C41—C46—C45—C44	0.3 (2)
C14—C15—C16—C17	−2.9 (2)	C33—C34—C35—C36	2.6 (2)
C15—C16—C17—C11	3.2 (2)	N32—C32—C33—C34	177.67 (12)
O11—C11—C17—C16	−176.82 (13)	C31—C32—C33—C34	−6.2 (2)
C12—C11—C17—C16	6.1 (2)	C35—C34—C33—C32	3.3 (2)
C21—C26—C25—C24	−0.12 (18)	C31—C37—C36—C35	−2.1 (2)
C21—N12—C12—C13	15.32 (18)	C34—C35—C36—C37	−2.7 (2)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N12—H12···O31^{i}	0.88	2.07	2.8891 (13)	154
N32—H32···O11^{i}	0.88	2.13	2.9524 (12)	155
C45—H45···F24	0.95	2.72	3.6058 (15)	156
C23—H23···F44^{ii}	0.95	2.57	3.4538 (16)	155

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1; (ii) −*x*, −*y*+1, −*z*.

Fig. 1


C34
C35
C36
C33
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N32
C41
C42
C43
C44
F002
C37
C31
C45
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H32
C15
C14
C13
C22
C23
F24
C16
C12
N12
C26
C24
C21
C25
C17
C11
O11
H12