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(E)-3-(2-Chloro-3,3,3-trifluoroprop-1-enyl)-N-(9,10-dioxo-9,10-dihydroanthracen-1-yl)-2,2-dimethylcyclopropanecarboxamide

Fan-Yong Yan* and Dong-Qing Liu

School of Materials and Chemical Engineering, Tianjin Polytechnic University, Tianjin 300160, People's Republic of China

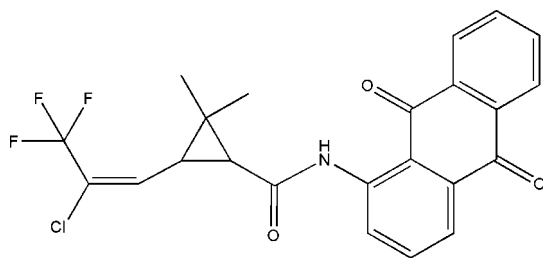
Correspondence e-mail: yfany@163.com

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Key indicators: single-crystal X-ray study; $T = 113$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.047; wR factor = 0.120; data-to-parameter ratio = 16.1.

In the title compound, $\text{C}_{23}\text{H}_{17}\text{ClF}_3\text{NO}_3$, the dihedral angle between the dihydroanthracene and cyclopropane ring systems is $58.5(4)^\circ$. The amino H atom forms an intramolecular hydrogen bond to a carbonyl O atom of the dioxodihydroanthracene moiety. The crystal packing is further stabilized by an intermolecular $\text{C}-\text{H}\cdots\text{F}$ contact.

Related literature

For related literature, see: Liu *et al.* (2006); Punja (1981).

Experimental

Crystal data

$\text{C}_{23}\text{H}_{17}\text{ClF}_3\text{NO}_3$
 $M_r = 447.83$
 Triclinic, $P\bar{1}$

$a = 8.1270(10)$ Å
 $b = 8.1518(9)$ Å
 $c = 15.821(2)$ Å

$\alpha = 79.518(8)^\circ$
 $\beta = 88.256(9)^\circ$
 $\gamma = 72.328(8)^\circ$
 $V = 981.7(2)$ Å³
 $Z = 2$

Mo $K\alpha$ radiation
 $\mu = 0.25$ mm⁻¹
 $T = 113(2)$ K
 $0.26 \times 0.24 \times 0.10$ mm

Data collection

Rigaku Saturn diffractometer
 Absorption correction: multi-scan
 (Jacobson, 1998)
 $T_{\min} = 0.924$, $T_{\max} = 0.975$

7669 measured reflections
 4630 independent reflections
 3258 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.034$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.047$
 $wR(F^2) = 0.120$
 $S = 1.01$
 4630 reflections
 287 parameters

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\max} = 0.34$ e Å⁻³
 $\Delta\rho_{\min} = -0.34$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{N1}-\text{H1}\cdots\text{O2}$	0.94 (3)	1.89 (2)	2.639 (2)	134.7 (18)
$\text{C5}-\text{H5A}\cdots\text{F1}^i$	0.98	2.49	3.412 (3)	158

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

Data collection: *CrystalClear* (Rigaku/MSC, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *CrystalStructure* (Rigaku/MSC, 2005).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2502).

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supplementary materials

Acta Cryst. (2007). E63, o4201 [doi:10.1107/S160053680704408X]

(*E*)-3-(2-Chloro-3,3,3-trifluoroprop-1-enyl)-*N*-(9,10-dioxo-9,10-dihydroanthracen-1-yl)-2,2-dimethylcyclopropanecarboxamide

F.-Y. Yan and D.-Q. Liu

Comment

3-((*E*)-2-Chloro-3,3,3-trifluoroprop-1-enyl)-2,2-dimethyl cyclopropanecarboxylic acid is a very important intermediate for tefluthrin, an important insecticide controlling a wide range of soil insect pests in maize, sugar beet, and other crops (Punja, 1981). The title compound may have some insecticide activity. The present X-ray crystal structure analysis was undertaken in order to study the stereochemistry and crystal packing of the title compound.

The dihedral angles between the dihydroanthracen moiety and the cyclopropane group is 58.5 (4)°. The fluoro in CF₃ and methyl hydrogen in another molecule are linked by an intermolecular C—H···F hydrogen bond. The carbonyl atom O2 forms an intramolecular hydrogen bond to atom N1.

Experimental

The title compound was prepared according to the method of Liu *et al.* (2006). 3-((*E*)-2-Chloro-3,3,3-trifluoroprop-1-enyl)-2,2-dimethylcyclopropanecarboxylic acid 0.97 g (4.0 mmol) was dispersed in SOCl₂ (15 ml), and a drop of anhydrous DMF was added. The mixture was heated to reflux for 4 h. SOCl₂ was removed by rotoevaporation. The crude the product could be directly dissolved in anhydrous toluene, mixed with aminopyridine (0.90 g, 4.1 mmol). Then, triethylamine was dropped into the solution. After 12 h stirring at room temperature, the reaction mixture was poured into hexane. The red precipitate was filtrated off and recrystallized from acetone and a small amount of water (50:1) over 3 d at ambient temperature.

Refinement

H atoms were positioned geometrically with C—H = 0.93–0.98 Å and refined using riding model with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. The amino H atom of was located in a difference map and freely refined.

Figures

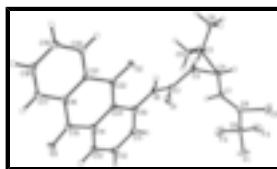


Fig. 1. The molecular structure of the title compound, drawn with 30% probability ellipsoids. H atoms are drawn as spheres of arbitrary radius.

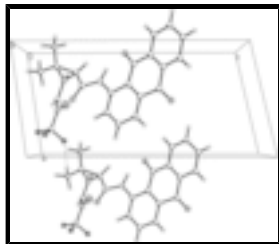


Fig. 2. The crystal packing of the title compound, viewed along *a* axis. The C—H...F contact is shown as a dashed line.

(*E*)-3-(2-Chloro-3,3,3-trifluoroprop-1-enyl)-N-(9,10-dioxo-9,10-dihydroanthracen-1-yl)-2,2-dimethylcyclopropanecarboxamide

Crystal data

$C_{23}H_{17}ClF_3NO_3$	$Z = 2$
$M_r = 447.83$	$F_{000} = 460$
Triclinic, $P\bar{1}$	$D_x = 1.515 \text{ Mg m}^{-3}$
$a = 8.1270 (10) \text{ \AA}$	Mo $K\alpha$ radiation
$b = 8.1518 (9) \text{ \AA}$	$\lambda = 0.71070 \text{ \AA}$
$c = 15.821 (2) \text{ \AA}$	Cell parameters from 2347 reflections
$\alpha = 79.518 (8)^\circ$	$\theta = 2.6\text{--}27.9^\circ$
$\beta = 88.256 (9)^\circ$	$\mu = 0.25 \text{ mm}^{-1}$
$\gamma = 72.328 (8)^\circ$	$T = 113 (2) \text{ K}$
$V = 981.7 (2) \text{ \AA}^3$	Platelet, yellow
	$0.26 \times 0.24 \times 0.10 \text{ mm}$

Data collection

Rigaku Saturn diffractometer	3258 reflections with $I > 2\sigma(I)$
Radiation source: rotating anode	$R_{\text{int}} = 0.034$
Monochromator: confocal	$\theta_{\text{max}} = 27.9^\circ$
$T = 113(2) \text{ K}$	$\theta_{\text{min}} = 2.6^\circ$
ω scans	$h = -10 \rightarrow 10$
Absorption correction: multi-scan (Jacobson, 1998)	$k = -10 \rightarrow 10$
$T_{\text{min}} = 0.924$, $T_{\text{max}} = 0.975$	$l = -20 \rightarrow 17$
7669 measured reflections	Standard reflections: ?
4630 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.047$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.120$	$w = 1/[\sigma^2(F_o^2) + (0.0616P)^2]$
	where $P = (F_o^2 + 2F_c^2)/3$

$S = 1.01$ $(\Delta/\sigma)_{\max} < 0.001$
 4630 reflections $\Delta\rho_{\max} = 0.34 \text{ e } \text{\AA}^{-3}$
 287 parameters $\Delta\rho_{\min} = -0.34 \text{ e } \text{\AA}^{-3}$
 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 $F^2 > 2\sigma(F^2)$ 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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
C11	-0.15058 (7)	0.51727 (7)	0.13945 (4)	0.03385 (16)
F1	-0.10806 (19)	0.87745 (17)	0.10610 (8)	0.0423 (4)
F2	0.12094 (18)	0.81308 (18)	0.03437 (10)	0.0489 (4)
F3	-0.1147 (2)	0.79087 (17)	-0.01174 (8)	0.0429 (4)
O1	0.4957 (2)	0.4919 (2)	0.20203 (8)	0.0300 (4)
O2	0.67461 (17)	0.07963 (17)	0.47055 (8)	0.0214 (3)
O3	0.8801 (2)	0.52026 (19)	0.62598 (9)	0.0310 (4)
N1	0.5423 (2)	0.3304 (2)	0.33821 (10)	0.0196 (3)
C1	0.4817 (2)	0.3672 (3)	0.25405 (11)	0.0199 (4)
C2	0.3993 (2)	0.2382 (2)	0.23394 (11)	0.0184 (4)
H2	0.3866	0.1502	0.2846	0.022*
C3	0.4193 (3)	0.1739 (3)	0.14854 (11)	0.0210 (4)
C4	0.2483 (2)	0.2995 (2)	0.16698 (11)	0.0180 (4)
H4	0.1536	0.2452	0.1816	0.022*
C5	0.5315 (3)	0.2333 (3)	0.07951 (12)	0.0289 (5)
H5A	0.6506	0.1558	0.0889	0.043*
H5B	0.5288	0.3534	0.0818	0.043*
H5C	0.4882	0.2293	0.0230	0.043*
C6	0.4225 (3)	-0.0144 (3)	0.15474 (13)	0.0291 (5)
H6A	0.5402	-0.0918	0.1694	0.044*
H6B	0.3853	-0.0310	0.0994	0.044*
H6C	0.3441	-0.0423	0.1995	0.044*
C7	0.1912 (2)	0.4809 (2)	0.12117 (11)	0.0178 (4)
H7	0.2787	0.5321	0.1006	0.021*
C8	0.0293 (2)	0.5801 (3)	0.10575 (11)	0.0187 (4)
C9	-0.0175 (3)	0.7647 (3)	0.05808 (12)	0.0211 (4)
C10	0.6061 (2)	0.4383 (3)	0.37939 (11)	0.0186 (4)

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C11	0.5739 (3)	0.6158 (3)	0.34485 (12)	0.0229 (4)
H11	0.5138	0.6631	0.2911	0.027*
C12	0.6285 (3)	0.7231 (3)	0.38801 (13)	0.0242 (4)
H12	0.6057	0.8435	0.3637	0.029*
C13	0.7166 (3)	0.6567 (3)	0.46663 (12)	0.0232 (4)
H13	0.7531	0.7317	0.4961	0.028*
C14	0.7510 (2)	0.4816 (2)	0.50191 (12)	0.0181 (4)
C15	0.8468 (2)	0.4175 (3)	0.58665 (12)	0.0207 (4)
C16	0.9029 (2)	0.2269 (3)	0.61968 (11)	0.0187 (4)
C17	1.0105 (3)	0.1594 (3)	0.69284 (12)	0.0229 (4)
H17	1.0448	0.2362	0.7221	0.027*
C18	1.0673 (3)	-0.0194 (3)	0.72283 (12)	0.0248 (4)
H18	1.1417	-0.0652	0.7723	0.030*
C19	1.0158 (3)	-0.1321 (3)	0.68083 (11)	0.0217 (4)
H19	1.0564	-0.2549	0.7011	0.026*
C20	0.9051 (2)	-0.0654 (3)	0.60921 (11)	0.0192 (4)
H20	0.8673	-0.1424	0.5817	0.023*
C21	0.8494 (2)	0.1138 (2)	0.57768 (11)	0.0170 (4)
C22	0.7344 (2)	0.1811 (2)	0.49952 (11)	0.0166 (4)
C23	0.6969 (2)	0.3674 (2)	0.45955 (11)	0.0178 (4)
H1	0.543 (3)	0.224 (3)	0.3731 (14)	0.033 (6)*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C11	0.0159 (2)	0.0332 (3)	0.0444 (3)	-0.0065 (2)	-0.0019 (2)	0.0122 (2)
F1	0.0587 (10)	0.0220 (7)	0.0316 (7)	0.0105 (7)	0.0018 (6)	-0.0075 (6)
F2	0.0305 (8)	0.0247 (7)	0.0816 (10)	-0.0090 (6)	0.0053 (7)	0.0159 (7)
F3	0.0691 (11)	0.0251 (7)	0.0297 (6)	-0.0104 (7)	-0.0262 (7)	0.0051 (6)
O1	0.0368 (9)	0.0360 (9)	0.0218 (7)	-0.0221 (8)	-0.0028 (6)	0.0030 (7)
O2	0.0242 (7)	0.0145 (7)	0.0259 (7)	-0.0061 (6)	-0.0047 (5)	-0.0034 (6)
O3	0.0389 (9)	0.0224 (8)	0.0351 (8)	-0.0101 (7)	-0.0090 (7)	-0.0108 (7)
N1	0.0218 (8)	0.0160 (8)	0.0198 (8)	-0.0049 (7)	-0.0036 (6)	-0.0014 (7)
C1	0.0154 (9)	0.0233 (11)	0.0198 (9)	-0.0047 (8)	-0.0012 (7)	-0.0026 (8)
C2	0.0183 (9)	0.0181 (10)	0.0164 (8)	-0.0042 (8)	-0.0022 (7)	0.0010 (8)
C3	0.0205 (10)	0.0178 (10)	0.0197 (9)	0.0019 (8)	-0.0038 (7)	-0.0032 (8)
C4	0.0151 (9)	0.0149 (10)	0.0210 (8)	-0.0016 (8)	-0.0033 (7)	-0.0003 (8)
C5	0.0228 (11)	0.0300 (12)	0.0256 (10)	0.0041 (9)	0.0036 (8)	-0.0050 (10)
C6	0.0365 (12)	0.0161 (11)	0.0287 (10)	0.0012 (9)	-0.0059 (9)	-0.0039 (9)
C7	0.0166 (9)	0.0180 (10)	0.0192 (8)	-0.0054 (8)	0.0017 (7)	-0.0043 (8)
C8	0.0184 (9)	0.0207 (10)	0.0168 (8)	-0.0067 (8)	0.0007 (7)	-0.0017 (8)
C9	0.0221 (10)	0.0178 (10)	0.0218 (9)	-0.0026 (8)	-0.0012 (7)	-0.0051 (8)
C10	0.0174 (9)	0.0171 (10)	0.0220 (9)	-0.0057 (8)	0.0027 (7)	-0.0045 (8)
C11	0.0232 (10)	0.0187 (10)	0.0238 (9)	-0.0034 (8)	-0.0006 (8)	-0.0012 (8)
C12	0.0284 (11)	0.0129 (10)	0.0288 (10)	-0.0049 (9)	0.0031 (8)	-0.0003 (8)
C13	0.0264 (11)	0.0184 (10)	0.0275 (10)	-0.0091 (9)	0.0018 (8)	-0.0072 (9)
C14	0.0182 (9)	0.0156 (10)	0.0213 (9)	-0.0054 (8)	0.0024 (7)	-0.0051 (8)
C15	0.0201 (10)	0.0194 (10)	0.0245 (9)	-0.0070 (8)	0.0014 (7)	-0.0075 (8)

C16	0.0179 (9)	0.0192 (10)	0.0193 (9)	-0.0050 (8)	0.0010 (7)	-0.0055 (8)
C17	0.0241 (10)	0.0247 (11)	0.0209 (9)	-0.0075 (9)	-0.0025 (8)	-0.0062 (9)
C18	0.0246 (10)	0.0275 (12)	0.0183 (9)	-0.0041 (9)	-0.0039 (7)	0.0004 (9)
C19	0.0220 (10)	0.0190 (10)	0.0204 (9)	-0.0027 (8)	0.0023 (7)	-0.0004 (8)
C20	0.0199 (9)	0.0174 (10)	0.0198 (9)	-0.0050 (8)	0.0026 (7)	-0.0032 (8)
C21	0.0150 (9)	0.0172 (10)	0.0179 (8)	-0.0036 (8)	0.0028 (7)	-0.0036 (8)
C22	0.0172 (9)	0.0152 (10)	0.0183 (8)	-0.0050 (8)	0.0022 (7)	-0.0052 (8)
C23	0.0161 (9)	0.0165 (10)	0.0205 (9)	-0.0042 (8)	0.0019 (7)	-0.0043 (8)

Geometric parameters (Å, °)

C11—C8	1.7295 (19)	C7—H7	0.9500
F1—C9	1.331 (2)	C8—C9	1.495 (3)
F2—C9	1.324 (2)	C10—C11	1.398 (3)
F3—C9	1.325 (2)	C10—C23	1.421 (2)
O1—C1	1.218 (2)	C11—C12	1.378 (2)
O2—C22	1.2353 (19)	C11—H11	0.9500
O3—C15	1.224 (2)	C12—C13	1.388 (3)
N1—C1	1.382 (2)	C12—H12	0.9500
N1—C10	1.405 (2)	C13—C14	1.379 (3)
N1—H1	0.94 (3)	C13—H13	0.9500
C1—C2	1.489 (2)	C14—C23	1.416 (2)
C2—C3	1.523 (2)	C14—C15	1.496 (3)
C2—C4	1.547 (2)	C15—C16	1.478 (3)
C2—H2	1.0000	C16—C17	1.394 (2)
C3—C5	1.508 (3)	C16—C21	1.402 (2)
C3—C6	1.512 (3)	C17—C18	1.384 (3)
C3—C4	1.512 (3)	C17—H17	0.9500
C4—C7	1.463 (3)	C18—C19	1.390 (3)
C4—H4	1.0000	C18—H18	0.9500
C5—H5A	0.9800	C19—C20	1.389 (2)
C5—H5B	0.9800	C19—H19	0.9500
C5—H5C	0.9800	C20—C21	1.391 (3)
C6—H6A	0.9800	C20—H20	0.9500
C6—H6B	0.9800	C21—C22	1.489 (2)
C6—H6C	0.9800	C22—C23	1.476 (3)
C7—C8	1.321 (3)		
C1—N1—C10	126.38 (17)	F2—C9—C8	111.90 (16)
C1—N1—H1	119.3 (12)	F3—C9—C8	112.83 (14)
C10—N1—H1	114.3 (12)	F1—C9—C8	111.76 (16)
O1—C1—N1	123.11 (16)	C11—C10—N1	120.95 (17)
O1—C1—C2	123.92 (15)	C11—C10—C23	119.70 (16)
N1—C1—C2	112.97 (17)	N1—C10—C23	119.27 (17)
C1—C2—C3	123.23 (16)	C12—C11—C10	120.66 (17)
C1—C2—C4	119.42 (16)	C12—C11—H11	119.7
C3—C2—C4	58.98 (11)	C10—C11—H11	119.7
C1—C2—H2	114.6	C11—C12—C13	120.57 (18)
C3—C2—H2	114.6	C11—C12—H12	119.7
C4—C2—H2	114.6	C13—C12—H12	119.7

supplementary materials

C5—C3—C6	114.14 (17)	C14—C13—C12	119.96 (16)
C5—C3—C4	119.85 (17)	C14—C13—H13	120.0
C6—C3—C4	115.70 (17)	C12—C13—H13	120.0
C5—C3—C2	121.19 (16)	C13—C14—C23	121.12 (16)
C6—C3—C2	114.75 (16)	C13—C14—C15	117.53 (15)
C4—C3—C2	61.29 (12)	C23—C14—C15	121.34 (17)
C7—C4—C3	121.31 (16)	O3—C15—C16	121.59 (17)
C7—C4—C2	120.40 (14)	O3—C15—C14	120.61 (18)
C3—C4—C2	59.72 (12)	C16—C15—C14	117.78 (14)
C7—C4—H4	114.8	C17—C16—C21	119.91 (18)
C3—C4—H4	114.8	C17—C16—C15	119.68 (16)
C2—C4—H4	114.8	C21—C16—C15	120.41 (16)
C3—C5—H5A	109.5	C18—C17—C16	120.01 (16)
C3—C5—H5B	109.5	C18—C17—H17	120.0
H5A—C5—H5B	109.5	C16—C17—H17	120.0
C3—C5—H5C	109.5	C17—C18—C19	120.22 (17)
H5A—C5—H5C	109.5	C17—C18—H18	119.9
H5B—C5—H5C	109.5	C19—C18—H18	119.9
C3—C6—H6A	109.5	C20—C19—C18	120.09 (19)
C3—C6—H6B	109.5	C20—C19—H19	120.0
H6A—C6—H6B	109.5	C18—C19—H19	120.0
C3—C6—H6C	109.5	C19—C20—C21	120.19 (16)
H6A—C6—H6C	109.5	C19—C20—H20	119.9
H6B—C6—H6C	109.5	C21—C20—H20	119.9
C8—C7—C4	126.07 (17)	C20—C21—C16	119.56 (16)
C8—C7—H7	117.0	C20—C21—C22	119.03 (15)
C4—C7—H7	117.0	C16—C21—C22	121.41 (17)
C7—C8—C9	122.53 (17)	O2—C22—C23	122.63 (16)
C7—C8—C11	125.14 (16)	O2—C22—C21	119.02 (16)
C9—C8—C11	112.31 (14)	C23—C22—C21	118.35 (14)
F2—C9—F3	107.74 (17)	C14—C23—C10	117.99 (17)
F2—C9—F1	106.43 (15)	C14—C23—C22	119.72 (16)
F3—C9—F1	105.76 (16)	C10—C23—C22	122.29 (15)
C10—N1—C1—O1	8.9 (3)	C12—C13—C14—C15	179.79 (18)
C10—N1—C1—C2	-171.50 (18)	C13—C14—C15—O3	5.9 (3)
O1—C1—C2—C3	37.9 (3)	C23—C14—C15—O3	-173.82 (19)
N1—C1—C2—C3	-141.67 (18)	C13—C14—C15—C16	-172.65 (18)
O1—C1—C2—C4	-32.4 (3)	C23—C14—C15—C16	7.6 (3)
N1—C1—C2—C4	148.07 (17)	O3—C15—C16—C17	-6.4 (3)
C1—C2—C3—C5	2.4 (3)	C14—C15—C16—C17	172.18 (17)
C4—C2—C3—C5	109.4 (2)	O3—C15—C16—C21	173.94 (19)
C1—C2—C3—C6	146.10 (19)	C14—C15—C16—C21	-7.5 (3)
C4—C2—C3—C6	-106.97 (19)	C21—C16—C17—C18	1.4 (3)
C1—C2—C3—C4	-106.9 (2)	C15—C16—C17—C18	-178.27 (18)
C5—C3—C4—C7	-2.2 (2)	C16—C17—C18—C19	-0.8 (3)
C6—C3—C4—C7	-145.25 (16)	C17—C18—C19—C20	-0.9 (3)
C2—C3—C4—C7	109.31 (17)	C18—C19—C20—C21	1.9 (3)
C5—C3—C4—C2	-111.49 (18)	C19—C20—C21—C16	-1.3 (3)
C6—C3—C4—C2	105.44 (18)	C19—C20—C21—C22	178.45 (17)

C1—C2—C4—C7	2.5 (3)	C17—C16—C21—C20	-0.4 (3)
C3—C2—C4—C7	-110.8 (2)	C15—C16—C21—C20	179.28 (17)
C1—C2—C4—C3	113.3 (2)	C17—C16—C21—C22	179.90 (17)
C3—C4—C7—C8	152.17 (17)	C15—C16—C21—C22	-0.4 (3)
C2—C4—C7—C8	-136.94 (19)	C20—C21—C22—O2	8.5 (3)
C4—C7—C8—C9	-179.86 (16)	C16—C21—C22—O2	-171.75 (18)
C4—C7—C8—C11	1.9 (3)	C20—C21—C22—C23	-171.26 (17)
C7—C8—C9—F2	0.0 (2)	C16—C21—C22—C23	8.5 (3)
C11—C8—C9—F2	178.45 (13)	C13—C14—C23—C10	0.1 (3)
C7—C8—C9—F3	121.71 (19)	C15—C14—C23—C10	179.84 (16)
C11—C8—C9—F3	-59.84 (19)	C13—C14—C23—C22	-179.41 (17)
C7—C8—C9—F1	-119.26 (19)	C15—C14—C23—C22	0.3 (3)
C11—C8—C9—F1	59.20 (17)	C11—C10—C23—C14	0.3 (3)
C1—N1—C10—C11	16.6 (3)	N1—C10—C23—C14	-176.43 (17)
C1—N1—C10—C23	-166.71 (18)	C11—C10—C23—C22	179.80 (18)
N1—C10—C11—C12	176.31 (18)	N1—C10—C23—C22	3.1 (3)
C23—C10—C11—C12	-0.4 (3)	O2—C22—C23—C14	171.94 (18)
C10—C11—C12—C13	0.0 (3)	C21—C22—C23—C14	-8.3 (3)
C11—C12—C13—C14	0.4 (3)	O2—C22—C23—C10	-7.5 (3)
C12—C13—C14—C23	-0.5 (3)	C21—C22—C23—C10	172.25 (16)

Hydrogen-bond geometry (\AA , $^\circ$)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
N1—H1 \cdots O2	0.94 (3)	1.89 (2)	2.639 (2)	134.7 (18)
C5—H5A \cdots F1 ⁱ	0.98	2.49	3.412 (3)	158

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

Fig. 1

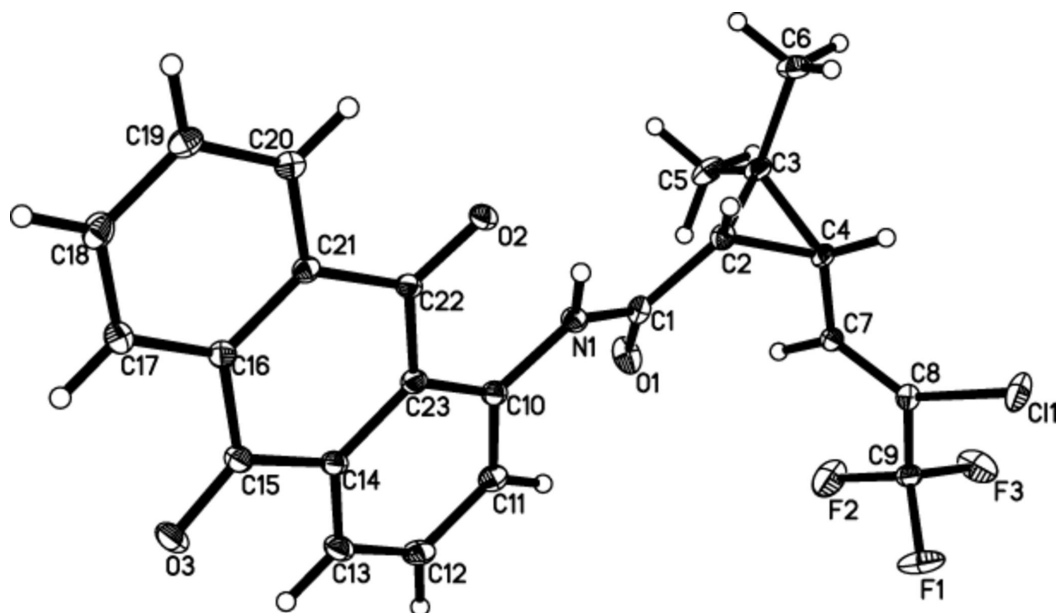


Fig. 2

