Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(*E*)-3-(2-Chloro-3,3,3-trifluoroprop-1-enyl)-2,2-dimethyl-*N*,*N*-diphenylcyclopropanecarboxamide

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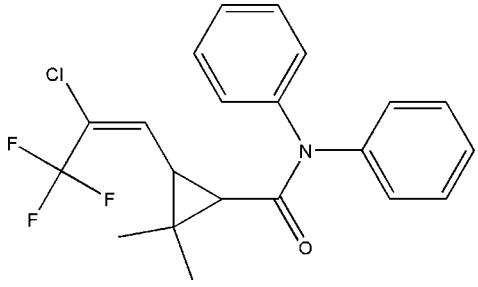
Received 8 November 2007; accepted 20 November 2007

Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.003 Å; disorder in main residue; R factor = 0.041; wR factor = 0.119; data-to-parameter ratio = 14.7.

The title compound, $C_{21}H_{19}ClF_3NO$, was synthesized from 3-[(*E*)-2-chloro-3,3,3-trifluoroprop-1-enyl]-2,2-dimethylcyclopropanecarboxylic acid and diphenylamine. The propenyl and carboxamide substituents lie on the same side of the cyclopropane ring plane, with the two methyl substituents on either side of the plane. The phenyl rings of the carboxamide are inclined at an angle of 84.6 (3)° to one another. The F atoms are disordered over two positions; the site occupancy factors are *ca* 0.6 and 0.4.

Related literature

For the preparation of the title compound, see: Liu *et al.* (2006). For the insecticidal properties of related compounds, see: Punja (1981).



Experimental

Crystal data

$C_{21}H_{19}ClF_3NO$
M_r = 393.82
Monoclinic, $P2_1/n$
a = 9.247 (6) Å
b = 21.443 (14) Å
c = 10.025 (7) Å
β = 99.068 (11)°
V = 1963 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.23 mm^{-1}
T = 294 (2) K
0.22 × 0.20 × 0.18 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.951, T_{max} = 0.960
11179 measured reflections
4030 independent reflections
2379 reflections with $I > 2\sigma(I)$
R_{int} = 0.034

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.119
S = 1.00
4030 reflections
274 parameters
60 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; 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: *SHELXTL*

This work was supported by the National Natural Science Foundation (No. 20376059)

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ2421).

References

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  doi:10.1107/S1600536807060953

supporting information

Acta Cryst. (2008). E**64**, o18 [https://doi.org/10.1107/S1600536807060953]

(*E*)-3-(2-Chloro-3,3,3-trifluoroprop-1-enyl)-2,2-dimethyl-*N*,*N*-diphenylcyclopropanecarboxamide

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S1. Comment

3-((*E*)-2-Chloro-3,3,3-trifluoroprop-1-enyl)-2,2-dimethyl cyclopropanecarboxylic acid is a very important intermediate in the preparation of tefluthrinan a useful insecticide controlling a wide range of soil insect pests in maize, sugar beet, and other crops (Punja, 1981). Diphenylamine is also a structure which has bioactivity. We reasoned that a structure containing both of these bioactive components may show enhanced insecticidal activity and prepared the title compound (I), whose structure is repoerted here Fig. 1.

The the propenyl and carboxamide substituents lie on the same side of the cyclopropane ring plane, with the two methyl substituents on either side of the plane. The benzene rings of the carboxamide are inclined at 95.4 (3)° to one another. The crystal packing of (I) is shown in Fig. 2.

S2. Experimental

The title compound was prepared according to the method of Liu *et al.* (2006). The product was recrystallized from methanol and ethyl acetate (5:1, *v*/*v*) over 3 days at ambient temperature, giving colourless single crystals of (I).

S3. Refinement

H atoms were positioned geometrically with C—H = 0.93–0.98 Å and refined using riding model with U_{iso}(H) = 1.2Ueq(carrier). The fluorine atoms of the trifluoromethyl group were disordered over two conformations. The occupancy factor for the major component refined to 0.56 (3).

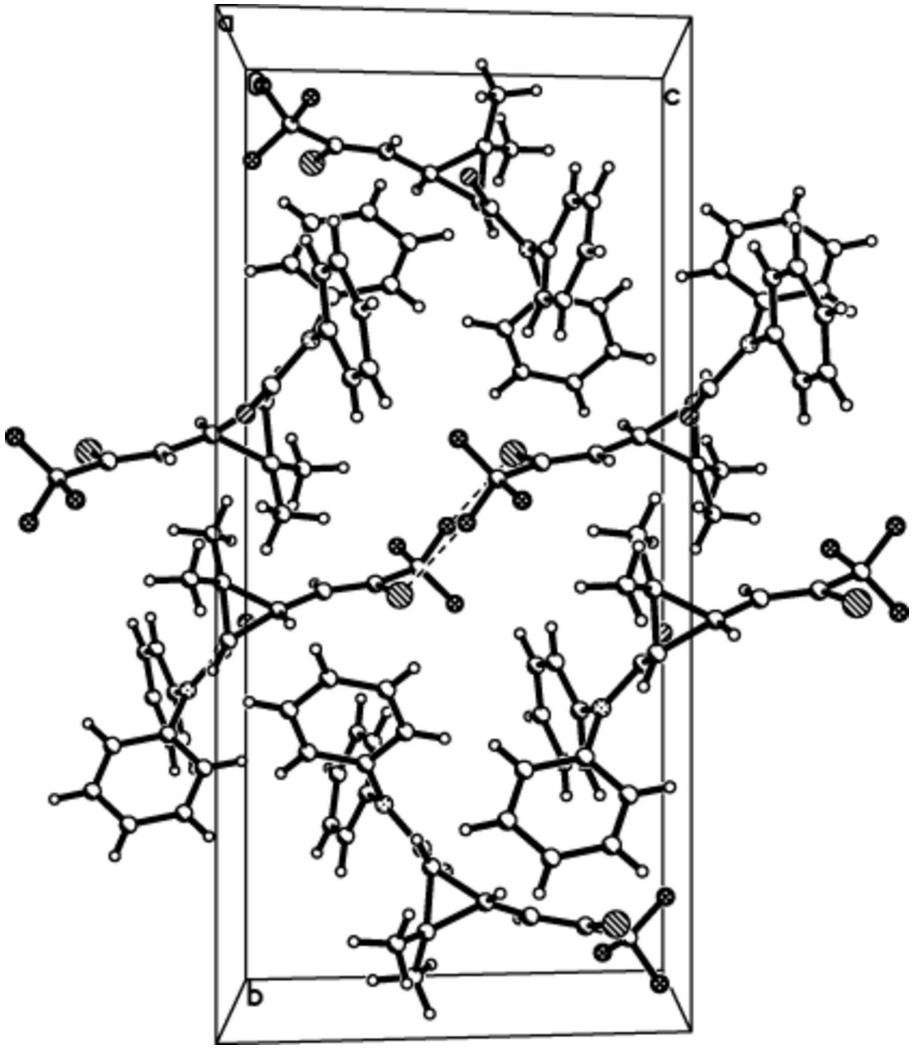

Figure 1

The molecular structure of (I), drawn with 30% probability ellipsoids. H atoms are drawn as spheres of arbitrary radius.

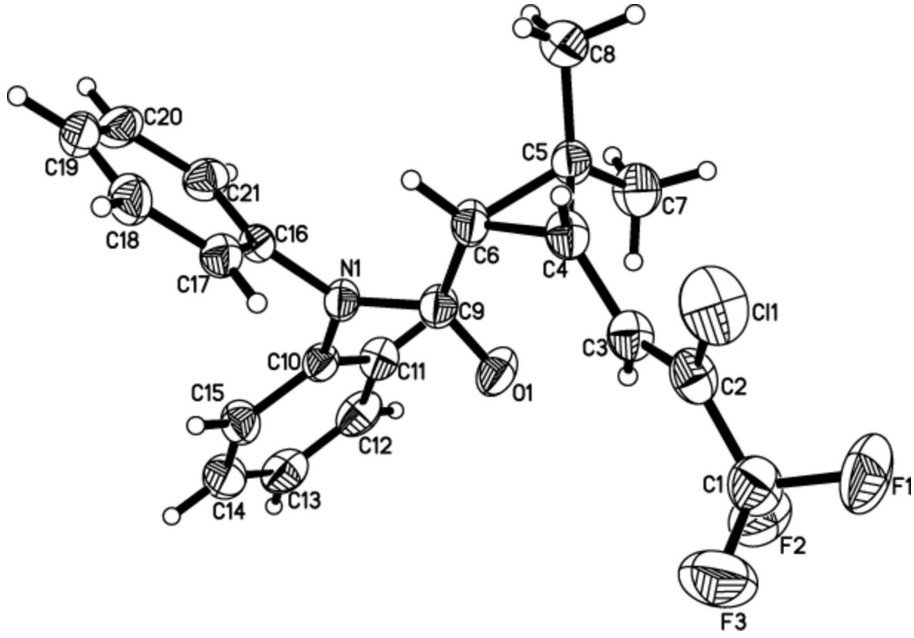

Figure 2

The crystal structure of (I), viewed along the *a* axis.

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Crystal data

$C_{21}H_{19}ClF_3NO$
$M_r = 393.82$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 9.247\ (6)$ Å
$b = 21.443\ (14)$ Å
$c = 10.025\ (7)$ Å
$\beta = 99.068\ (11)°$
$V = 1963\ (2)$ Å^3
$Z = 4$
$F(000) = 816$
$D_x = 1.333$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2995 reflections
$\theta = 2.2–24.7°$
$\mu = 0.23$ mm^{-1}
$T = 294$ K
Prism, colourles
0.22 × 0.20 × 0.18 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
$T_{min} = 0.951$, $T_{max} = 0.960$
11179 measured reflections
4030 independent reflections
2379 reflections with $I > 2\sigma(I)$
$R_{int} = 0.034$
$\theta_{max} = 26.5°$, $\theta_{min} = 1.9°$
$h = -11\rightarrow10$
$k = -20\rightarrow26$
$l = -12\rightarrow11$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.119$
$S = 1.00$
4030 reflections
274 parameters
60 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0477P)^2 + 0.4369P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.30$ e Å^{-3}
$\Delta\rho_{min} = -0.32$ e Å^{-3}

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 $F^2 > \sigma(F^2)$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Cl1	0.52632 (8)	0.07861 (4)	0.13621 (8)	0.0975 (3)	
F1	0.732 (2)	0.0017 (7)	0.0236 (16)	0.111 (4)	0.44 (3)
F2	0.9287 (12)	0.0254 (10)	0.1498 (12)	0.096 (3)	0.44 (3)
F3	0.823 (2)	0.0915 (7)	0.0041 (15)	0.122 (3)	0.44 (3)
F1′	0.7705 (16)	−0.0077 (4)	0.0400 (14)	0.103 (3)	0.56 (3)
F2′	0.9394 (7)	0.0532 (8)	0.1380 (10)	0.094 (2)	0.56 (3)
F3′	0.7669 (19)	0.0895 (6)	−0.0073 (10)	0.123 (3)	0.56 (3)
O1	1.00435 (15)	0.11409 (7)	0.53022 (16)	0.0659 (4)	
N1	0.96418 (16)	0.19188 (7)	0.67253 (17)	0.0483 (4)	
C1	0.7965 (3)	0.04904 (14)	0.0946 (3)	0.0799 (8)	
C2	0.7085 (2)	0.06733 (10)	0.1994 (2)	0.0600 (6)	
C3	0.7634 (2)	0.07596 (10)	0.3275 (2)	0.0560 (5)	
H3	0.8630	0.0683	0.3528	0.067*	
C4	0.6825 (2)	0.09642 (9)	0.4335 (2)	0.0542 (5)	
H4	0.5822	0.1103	0.4003	0.065*	
C5	0.7013 (2)	0.06512 (9)	0.5698 (2)	0.0535 (5)	
C6	0.7573 (2)	0.13142 (9)	0.5584 (2)	0.0544 (5)	
H6	0.6969	0.1637	0.5914	0.065*	
C7	0.8048 (3)	0.01108 (11)	0.5998 (3)	0.0745 (7)	
H7A	0.7580	−0.0264	0.5624	0.112*	
H7B	0.8311	0.0065	0.6958	0.112*	
H7C	0.8913	0.0186	0.5605	0.112*	
C8	0.5658 (3)	0.06042 (12)	0.6365 (3)	0.0760 (7)	
H8A	0.5011	0.0945	0.6071	0.114*	
H8B	0.5935	0.0621	0.7328	0.114*	
H8C	0.5168	0.0217	0.6117	0.114*	
C9	0.9165 (2)	0.14478 (10)	0.5816 (2)	0.0522 (5)	
C10	1.1194 (2)	0.19815 (9)	0.7161 (2)	0.0473 (5)	
C11	1.2001 (2)	0.14777 (11)	0.7713 (2)	0.0565 (5)	
H11	1.1545	0.1098	0.7811	0.068*	

C12	1.3491 (3)	0.15412 (13)	0.8119 (2)	0.0683 (7)
H12	1.4040	0.1202	0.8489	0.082*
C13	1.4170 (3)	0.21036 (14)	0.7978 (3)	0.0739 (7)
H13	1.5177	0.2142	0.8236	0.089*
C14	1.3366 (3)	0.26020 (13)	0.7462 (3)	0.0740 (7)
H14	1.3822	0.2984	0.7387	0.089*
C15	1.1871 (2)	0.25455 (10)	0.7048 (2)	0.0621 (6)
H15	1.1326	0.2888	0.6693	0.074*
C16	0.8725 (2)	0.24001 (9)	0.7137 (2)	0.0444 (5)
C17	0.7857 (2)	0.27642 (9)	0.6197 (2)	0.0521 (5)
H17	0.7830	0.2689	0.5280	0.063*
C18	0.7031 (2)	0.32397 (10)	0.6614 (3)	0.0636 (6)
H18	0.6440	0.3480	0.5974	0.076*
C19	0.7068 (2)	0.33616 (11)	0.7943 (3)	0.0666 (7)
H19	0.6507	0.3684	0.8212	0.080*
C20	0.7929 (3)	0.30110 (12)	0.8887 (3)	0.0686 (7)
H20	0.7960	0.3098	0.9800	0.082*
C21	0.8759 (2)	0.25253 (11)	0.8494 (2)	0.0588 (6)
H21	0.9337	0.2284	0.9142	0.071*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0740 (4)	0.1102 (6)	0.0929 (5)	0.0004 (4)	−0.0339 (4)	0.0028 (4)
F1	0.105 (6)	0.125 (6)	0.095 (4)	−0.004 (4)	−0.010 (4)	−0.058 (5)
F2	0.079 (3)	0.134 (7)	0.074 (3)	0.000 (4)	0.005 (3)	−0.020 (5)
F3	0.135 (7)	0.135 (5)	0.104 (5)	−0.029 (5)	0.041 (5)	0.025 (4)
F1′	0.103 (5)	0.094 (3)	0.112 (5)	−0.001 (3)	0.013 (4)	−0.025 (3)
F2′	0.081 (2)	0.128 (6)	0.076 (3)	−0.022 (3)	0.0197 (18)	−0.023 (4)
F3′	0.140 (7)	0.161 (5)	0.070 (3)	−0.007 (4)	0.021 (4)	0.033 (3)
O1	0.0450 (8)	0.0741 (10)	0.0785 (11)	0.0020 (7)	0.0097 (7)	−0.0341 (9)
N1	0.0402 (8)	0.0436 (9)	0.0607 (10)	−0.0005 (7)	0.0063 (7)	−0.0123 (8)
C1	0.090 (2)	0.089 (2)	0.0554 (16)	−0.0193 (17)	−0.0049 (15)	−0.0049 (16)
C2	0.0611 (13)	0.0561 (13)	0.0569 (14)	−0.0085 (11)	−0.0086 (11)	0.0024 (11)
C3	0.0467 (11)	0.0594 (13)	0.0579 (14)	−0.0005 (10)	−0.0041 (10)	−0.0032 (11)
C4	0.0409 (10)	0.0512 (12)	0.0669 (14)	0.0016 (9)	−0.0023 (10)	−0.0055 (11)
C5	0.0501 (12)	0.0486 (12)	0.0617 (14)	−0.0026 (10)	0.0081 (10)	−0.0088 (11)
C6	0.0424 (11)	0.0460 (12)	0.0740 (15)	0.0006 (9)	0.0068 (10)	−0.0165 (10)
C7	0.0812 (17)	0.0595 (15)	0.0812 (17)	0.0102 (13)	0.0081 (13)	0.0081 (13)
C8	0.0708 (16)	0.0765 (17)	0.0849 (18)	−0.0165 (13)	0.0252 (13)	−0.0172 (14)
C9	0.0468 (11)	0.0495 (12)	0.0599 (13)	−0.0007 (10)	0.0071 (10)	−0.0109 (11)
C10	0.0410 (10)	0.0492 (12)	0.0520 (12)	0.0002 (9)	0.0080 (9)	−0.0095 (10)
C11	0.0550 (12)	0.0571 (13)	0.0557 (13)	0.0045 (11)	0.0039 (10)	−0.0044 (11)
C12	0.0585 (14)	0.0866 (18)	0.0575 (14)	0.0222 (13)	0.0017 (11)	−0.0091 (13)
C13	0.0442 (12)	0.102 (2)	0.0748 (17)	−0.0020 (14)	0.0063 (12)	−0.0263 (15)
C14	0.0519 (14)	0.0751 (17)	0.0971 (19)	−0.0140 (13)	0.0184 (13)	−0.0202 (15)
C15	0.0514 (12)	0.0518 (13)	0.0837 (16)	−0.0025 (10)	0.0128 (11)	−0.0073 (12)
C16	0.0417 (10)	0.0407 (11)	0.0521 (12)	−0.0068 (9)	0.0111 (9)	−0.0072 (9)

C17	0.0576 (12)	0.0478 (12)	0.0521 (12)	0.0015 (10)	0.0120 (10)	0.0005 (10)
C18	0.0583 (13)	0.0469 (13)	0.0854 (18)	0.0058 (11)	0.0109 (12)	0.0011 (12)
C19	0.0548 (13)	0.0531 (14)	0.097 (2)	−0.0060 (11)	0.0264 (13)	−0.0219 (14)
C20	0.0665 (15)	0.0822 (17)	0.0622 (15)	−0.0136 (14)	0.0256 (12)	−0.0277 (13)
C21	0.0568 (13)	0.0690 (15)	0.0508 (13)	−0.0025 (11)	0.0087 (10)	−0.0044 (11)

Geometric parameters (Å, º)

Cl1—C2	1.721 (2)	C8—H8A	0.9600
F1—C1	1.324 (8)	C8—H8B	0.9600
F2—C1	1.357 (7)	C8—H8C	0.9600
F3—C1	1.334 (8)	C10—C15	1.375 (3)
F1′—C1	1.340 (7)	C10—C11	1.378 (3)
F2′—C1	1.328 (6)	C11—C12	1.381 (3)
F3′—C1	1.336 (7)	C11—H11	0.9300
O1—C9	1.221 (2)	C12—C13	1.377 (4)
N1—C9	1.385 (3)	C12—H12	0.9300
N1—C16	1.437 (2)	C13—C14	1.357 (4)
N1—C10	1.439 (2)	C13—H13	0.9300
C1—C2	1.480 (4)	C14—C15	1.385 (3)
C2—C3	1.317 (3)	C14—H14	0.9300
C3—C4	1.460 (3)	C15—H15	0.9300
C3—H3	0.9300	C16—C17	1.380 (3)
C4—C5	1.508 (3)	C16—C21	1.382 (3)
C4—C6	1.529 (3)	C17—C18	1.378 (3)
C4—H4	0.9800	C17—H17	0.9300
C5—C7	1.502 (3)	C18—C19	1.353 (3)
C5—C8	1.514 (3)	C18—H18	0.9300
C5—C6	1.523 (3)	C19—C20	1.363 (3)
C6—C9	1.481 (3)	C19—H19	0.9300
C6—H6	0.9800	C20—C21	1.387 (3)
C7—H7A	0.9600	C20—H20	0.9300
C7—H7B	0.9600	C21—H21	0.9300
C7—H7C	0.9600		

C9—N1—C16	124.86 (16)	C5—C8—H8A	109.5
C9—N1—C10	117.84 (16)	C5—C8—H8B	109.5
C16—N1—C10	116.81 (15)	H8A—C8—H8B	109.5
F1—C1—F3	105.7 (11)	C5—C8—H8C	109.5
F2′—C1—F3′	106.3 (6)	H8A—C8—H8C	109.5
F2′—C1—F1′	107.5 (6)	H8B—C8—H8C	109.5
F3′—C1—F1′	106.0 (8)	O1—C9—N1	120.42 (18)
F1—C1—F2	103.4 (8)	O1—C9—C6	122.70 (19)
F3—C1—F2	106.5 (7)	N1—C9—C6	116.76 (18)
F1—C1—C2	109.6 (8)	C15—C10—C11	119.9 (2)
F2′—C1—C2	112.3 (5)	C15—C10—N1	120.15 (18)
F3—C1—C2	118.7 (8)	C11—C10—N1	119.98 (18)
F3′—C1—C2	107.6 (7)	C10—C11—C12	119.6 (2)

F1′—C1—C2	116.6 (6)	C10—C11—H11	120.2
F2—C1—C2	111.7 (6)	C12—C11—H11	120.2
C3—C2—C1	124.0 (2)	C13—C12—C11	120.4 (2)
C3—C2—Cl1	122.9 (2)	C13—C12—H12	119.8
C1—C2—Cl1	113.06 (17)	C11—C12—H12	119.8
C2—C3—C4	126.0 (2)	C14—C13—C12	119.8 (2)
C2—C3—H3	117.0	C14—C13—H13	120.1
C4—C3—H3	117.0	C12—C13—H13	120.1
C3—C4—C5	121.75 (18)	C13—C14—C15	120.5 (2)
C3—C4—C6	121.70 (18)	C13—C14—H14	119.8
C5—C4—C6	60.22 (14)	C15—C14—H14	119.8
C3—C4—H4	114.2	C10—C15—C14	119.9 (2)
C5—C4—H4	114.2	C10—C15—H15	120.1
C6—C4—H4	114.2	C14—C15—H15	120.1
C7—C5—C4	120.27 (19)	C17—C16—C21	118.89 (19)
C7—C5—C8	113.9 (2)	C17—C16—N1	121.07 (18)
C4—C5—C8	116.37 (19)	C21—C16—N1	119.96 (18)
C7—C5—C6	121.44 (19)	C18—C17—C16	120.2 (2)
C4—C5—C6	60.57 (14)	C18—C17—H17	119.9
C8—C5—C6	114.21 (18)	C16—C17—H17	119.9
C9—C6—C5	120.64 (17)	C19—C18—C17	120.8 (2)
C9—C6—C4	122.29 (18)	C19—C18—H18	119.6
C5—C6—C4	59.21 (14)	C17—C18—H18	119.6
C9—C6—H6	114.5	C18—C19—C20	119.9 (2)
C5—C6—H6	114.5	C18—C19—H19	120.0
C4—C6—H6	114.5	C20—C19—H19	120.0
C5—C7—H7A	109.5	C19—C20—C21	120.4 (2)
C5—C7—H7B	109.5	C19—C20—H20	119.8
H7A—C7—H7B	109.5	C21—C20—H20	119.8
C5—C7—H7C	109.5	C16—C21—C20	119.8 (2)
H7A—C7—H7C	109.5	C16—C21—H21	120.1
H7B—C7—H7C	109.5	C20—C21—H21	120.1

F1—C1—C2—C3	131.3 (10)	C16—N1—C9—C6	−19.7 (3)
F2′—C1—C2—C3	−11.5 (9)	C10—N1—C9—C6	168.66 (18)
F3—C1—C2—C3	−107.2 (10)	C5—C6—C9—O1	47.4 (3)
F3′—C1—C2—C3	−128.0 (8)	C4—C6—C9—O1	−23.3 (3)
F1′—C1—C2—C3	113.2 (8)	C5—C6—C9—N1	−128.5 (2)
F2—C1—C2—C3	17.3 (11)	C4—C6—C9—N1	160.74 (19)
F1—C1—C2—Cl1	−50.5 (10)	C9—N1—C10—C15	126.5 (2)
F2′—C1—C2—Cl1	166.7 (8)	C16—N1—C10—C15	−45.8 (3)
F3—C1—C2—Cl1	70.9 (10)	C9—N1—C10—C11	−54.5 (3)
F3′—C1—C2—Cl1	50.2 (8)	C16—N1—C10—C11	133.2 (2)
F1′—C1—C2—Cl1	−68.6 (8)	C15—C10—C11—C12	−1.5 (3)
F2—C1—C2—Cl1	−164.5 (11)	N1—C10—C11—C12	179.52 (19)
C1—C2—C3—C4	177.4 (2)	C10—C11—C12—C13	0.2 (3)
Cl1—C2—C3—C4	−0.7 (3)	C11—C12—C13—C14	1.3 (4)
C2—C3—C4—C5	134.6 (2)	C12—C13—C14—C15	−1.4 (4)

C2—C3—C4—C6	−153.1 (2)	C11—C10—C15—C14	1.3 (3)
C3—C4—C5—C7	−0.4 (3)	N1—C10—C15—C14	−179.7 (2)
C6—C4—C5—C7	−111.4 (2)	C13—C14—C15—C10	0.2 (4)
C3—C4—C5—C8	−144.8 (2)	C9—N1—C16—C17	−53.0 (3)
C6—C4—C5—C8	104.2 (2)	C10—N1—C16—C17	118.7 (2)
C3—C4—C5—C6	111.0 (2)	C9—N1—C16—C21	130.3 (2)
C7—C5—C6—C9	−2.2 (3)	C10—N1—C16—C21	−58.1 (2)
C4—C5—C6—C9	−111.7 (2)	C21—C16—C17—C18	−0.6 (3)
C8—C5—C6—C9	140.5 (2)	N1—C16—C17—C18	−177.38 (17)
C7—C5—C6—C4	109.5 (2)	C16—C17—C18—C19	0.7 (3)
C8—C5—C6—C4	−107.8 (2)	C17—C18—C19—C20	−0.1 (3)
C3—C4—C6—C9	−2.1 (3)	C18—C19—C20—C21	−0.6 (3)
C5—C4—C6—C9	109.0 (2)	C17—C16—C21—C20	−0.1 (3)
C3—C4—C6—C5	−111.1 (2)	N1—C16—C21—C20	176.72 (18)
C16—N1—C9—O1	164.25 (19)	C19—C20—C21—C16	0.7 (3)
C10—N1—C9—O1	−7.4 (3)		