organic compounds

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4-Bromo-5-[(4-chlorobenzylidene)amino]-1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-1H-pyrazole-3-carbonitrile

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Key indicators: single-crystal X-ray study; T = 298 K; mean σ (C–C) = 0.006 Å; R factor = 0.058; wR factor = 0.186; data-to-parameter ratio = 18.1.

The title compound, C₁₈H₇BrCl₃F₃N₄, is an imine relevant to insecticides. The dihedral angles between the central pyrazole ring and the benzene ring planes are 84.3 (2) and 68.5 (2) $^{\circ}$.

Related literature

For related literature, see: Philippe (1997, 2000); Zhong et al. (2005).



Experimental

Crystal data

C₁₈H₇BrCl₃F₃N₄ V = 4009.1 (5) Å³ $M_r = 522.54$ Z = 8Orthorhombic, Pbca Mo $K\alpha$ radiation a = 10.0338 (7) Å $\mu = 2.49 \text{ mm}^{-1}$ b = 11.5819 (8) Å T = 298 (2) K c = 34.499 (3) Å $0.39 \times 0.17 \times 0.16 \text{ mm}$

Data collection

Bruker APEX area-detector 23679 measured reflections diffractometer 4736 independent reflections Absorption correction: multi-scan 3014 reflections with $I > 2\sigma(I)$ $R_{\rm int}=0.036$ (SADABS; Bruker, 2002) $T_{\min} = 0.444, \ T_{\max} = 0.691$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.058$	262 parameters
$wR(F^2) = 0.186$	H-atom parameters constrained
S = 1.04	$\Delta \rho_{\rm max} = 1.20 \text{ e } \text{\AA}^{-3}$
4736 reflections	$\Delta \rho_{\rm min} = -0.84 \ {\rm e} \ {\rm \AA}^{-3}$

Data collection: SMART (Bruker, 2002); cell refinement: SAINT (Bruker, 2002); 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, 2002); 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: TK2157).

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4-Bromo-5-[(4-chlorobenzylidene)amino]-1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-1*H*-pyrazole-3-carbonitrile

X.-C. Yu, S.-Y. Li and P. Zhong

Comment

The title compound, (I), (Fig. 1) is similar to the very effective insecticides used to treat animals such as cows and sheep (Philippe, 1997, 2000) and its structure is reported here. The molecule of (I) contains three essentially planar rings. The dihedral angles between the central pyrazole ring (C9—C11, N1, N2) and the benzene (C2—C7) and (C13—C16) ring planes are 84.3 (2)° and 68.5 (2)°, respectively.

Experimental

(2005),According to the method of Zhong et al. using 5-amino-3-cyano-1-[2,6-dichloro-4-(trifluoromethyl)phenyl]pyrazole (2.5 mmol), followed by reaction with 4-chlorobenzaldehyde (2.5 mmol) and HCl (2 ml) in anhydrous ethanol (5 ml), we obtained 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-3-cyano- 5-[(4chlorobenzylidene)amino]-1H-pyrazole, which was then reacted with N-bromosuccinimide (1.5 mmol) (Philippe, 2000) in acetonitrile (6 ml) at room temperature. After being stirred a few minutes, the reaction was monitored by TLC until the starting materials were consumed. Finally, the reaction mixture was evaporated under reduced pressure to provide the required crude product, which was then partitioned between dichloromethane and water, separating and drying the organic phase and evaporating it under reduced pressure gave the title compound in 90.8% yield. Colorless single crystals suitable for X-ray analysis were obtained by slow evaporation of an anhydrous ethanol-acetone (2:1) solution of (I), m.p. 488-489 K. IR (KBr, v cm⁻¹): 3047, 2202, 1618, 1387, 1313, 1179, 1136, 825; ¹H NMR (C₃D₆O, δ, p.p.m.): 9.39 (s, 1H), 8.14 (s, 2H), 7.90 (d, J = 8.52 Hz, 2H), 7.55 (d, J = 8.52 Hz, 2H); 13 C NMR (C₃D₆O, δ , p.p.m.): 167.4, 148.4, 140.2, 137.6, 136.4, 134.5 (q, J = 34.1 Hz), 134.3, 131.9, 130.2 (2 C), 130.1 (2 C), 127.2 (2 C), 127.1 (2 C), 121.5 (q, J = 271.1 Hz), 112.4.

Refinement

All H atoms were constrained to ride on their parent atoms, with C—H = 0.93 Å, and with $U_{iso}(H) = 1.2_{eq}(C)$. The low U_{eq} of C1 as compared to its neighbours may be attributed to the high displacement parameters for atoms F1, F2 and F3, indicating either large thermal motion or rotational disorder of the trifluoromethyl group. However, attempts to represent the CF3 group using a disorder model were unsuccessful. The maximum residual electron density peak was located 1.27 Å from the C1 and F1 atoms.

Figures



Fig. 1. The molecular structure of (I) showing the atom numbering scheme and displacement ellipsoids at 50% probability level.

4-Bromo-5-[(4-chlorobenzylidene)amino]-1-[2,6-dichloro-4- (trifluoromethyl)phenyl]-1*H*-pyrazole-3-carboni-trile

Crystal data

$C_{18}H_7BrCl_3F_3N_4$	$D_{\rm x} = 1.731 {\rm ~Mg~m^{-3}}$
$M_r = 522.54$	Melting point: 488-489 K
Orthorhombic, Pbca	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -P 2ac 2ab	Cell parameters from 4261 reflections
a = 10.0338 (7) Å	$\theta = 2.4 - 21.3^{\circ}$
<i>b</i> = 11.5819 (8) Å	$\mu = 2.49 \text{ mm}^{-1}$
c = 34.499 (3) Å	T = 298 (2) K
$V = 4009.1 (5) \text{ Å}^3$	Block, colorless
Z = 8	$0.39\times0.17\times0.16~mm$
$F_{000} = 2048$	

Data collection

Bruker APEX area-detector diffractometer	4736 independent reflections
Radiation source: fine-focus sealed tube	3014 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\rm int} = 0.036$
T = 298(2) K	$\theta_{\text{max}} = 28.3^{\circ}$
ϕ and ω scans	$\theta_{\min} = 1.2^{\circ}$
Absorption correction: multi-scan (SADABS; Bruker, 2002)	$h = -13 \rightarrow 9$
$T_{\min} = 0.444, \ T_{\max} = 0.691$	$k = -15 \rightarrow 14$
23679 measured reflections	$l = -45 \rightarrow 45$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.058$	H-atom parameters constrained
$wR(F^2) = 0.186$	$w = 1/[\sigma^2(F_0^2) + (0.0966P)^2 + 3.5182P]$ where $P = (F_0^2 + 2F_c^2)/3$

<i>S</i> = 1.04	$(\Delta/\sigma)_{max} = 0.001$
4736 reflections	$\Delta \rho_{max} = 1.20 \text{ e} \text{ Å}^{-3}$
262 parameters	$\Delta \rho_{min} = -0.84 \text{ e } \text{\AA}^{-3}$

Primary atom site location: structure-invariant direct 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 $F^2 > 2 \operatorname{sigma}(F^2)$ 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 (A^2)

	x	У	Z	$U_{\rm iso}*/U_{\rm eq}$
Br1	1.01932 (6)	0.22489 (5)	0.020072 (16)	0.0781 (2)
Cl1	0.50245 (14)	0.43701 (13)	0.08080 (3)	0.0729 (4)
Cl2	0.81344 (15)	0.17122 (15)	0.17059 (4)	0.0894 (5)
C13	1.32776 (14)	0.77979 (12)	0.17945 (4)	0.0804 (4)
F1	0.4269 (6)	0.3602 (5)	0.25418 (13)	0.150 (2)
F2	0.3552 (4)	0.4993 (4)	0.22440 (9)	0.1293 (18)
F3	0.5420 (6)	0.5033 (7)	0.25062 (15)	0.200 (4)
N1	0.7224 (3)	0.2693 (3)	0.09621 (9)	0.0474 (8)
N2	0.6684 (3)	0.1819 (3)	0.07601 (10)	0.0530 (8)
N3	0.7249 (5)	-0.0086 (4)	0.00155 (12)	0.0825 (14)
N4	0.9101 (3)	0.3884 (3)	0.10357 (9)	0.0471 (8)
C1	0.4628 (5)	0.4421 (5)	0.23040 (13)	0.0639 (13)
C2	0.5282 (4)	0.3954 (4)	0.19469 (12)	0.0484 (9)
C3	0.4871 (4)	0.4337 (4)	0.15874 (12)	0.0474 (9)
Н3	0.4178	0.4867	0.1564	0.057*
C4	0.5516 (4)	0.3913 (3)	0.12611 (11)	0.0443 (9)
C5	0.6547 (4)	0.3127 (3)	0.12953 (11)	0.0438 (9)
C6	0.6911 (4)	0.2741 (4)	0.16625 (13)	0.0527 (10)
C7	0.6291 (4)	0.3172 (4)	0.19877 (12)	0.0552 (10)
H7	0.6557	0.2934	0.2233	0.066*
C8	0.7399 (5)	0.0671 (4)	0.02214 (12)	0.0581 (11)
C9	0.7597 (4)	0.1600 (3)	0.04885 (11)	0.0474 (9)
C10	0.8695 (4)	0.2339 (3)	0.05139 (11)	0.0475 (9)
C11	0.8445 (4)	0.3047 (3)	0.08248 (11)	0.0446 (9)
C12	0.9998 (4)	0.4510 (4)	0.08793 (12)	0.0483 (9)
H12	1.0163	0.4440	0.0615	0.058*
C13	1.0769 (4)	0.5334 (3)	0.11074 (11)	0.0425 (8)

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C14	1.1751 (5)	0.5990 (4)	0.09282 (13)	0.0585 (11)
H14	1.1897	0.5908	0.0663	0.070*
C15	1.2515 (5)	0.6764 (4)	0.11383 (14)	0.0642 (12)
H15	1.3170	0.7203	0.1017	0.077*
C16	1.2289 (4)	0.6867 (3)	0.15246 (12)	0.0501 (9)
C17	1.1317 (4)	0.6240 (3)	0.17108 (12)	0.0503 (9)
H17	1.1176	0.6331	0.1975	0.060*
C18	1.0557 (4)	0.5480 (3)	0.15006 (11)	0.0468 (9)
H18	0.9892	0.5058	0.1624	0.056*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0779 (4)	0.0866 (4)	0.0696 (4)	-0.0145 (3)	0.0327 (3)	-0.0231 (3)
Cl1	0.0865 (9)	0.0873 (9)	0.0450 (6)	0.0215 (7)	0.0038 (5)	0.0120 (6)
Cl2	0.0807 (9)	0.1045 (11)	0.0831 (9)	0.0444 (9)	-0.0068 (7)	0.0048 (8)
C13	0.0756 (9)	0.0734 (9)	0.0922 (10)	-0.0251 (7)	-0.0067 (7)	-0.0206 (7)
F1	0.191 (5)	0.163 (4)	0.097 (3)	0.050 (4)	0.084 (3)	0.037 (3)
F2	0.137 (4)	0.185 (4)	0.066 (2)	0.092 (3)	0.009 (2)	-0.021 (2)
F3	0.128 (4)	0.342 (9)	0.130 (4)	-0.077 (4)	0.041 (3)	-0.163 (6)
N1	0.0422 (18)	0.0493 (19)	0.0507 (19)	-0.0050 (15)	0.0045 (14)	-0.0097 (15)
N2	0.050 (2)	0.0506 (19)	0.058 (2)	-0.0075 (16)	-0.0029 (16)	-0.0093 (17)
N3	0.107 (4)	0.076 (3)	0.065 (3)	-0.003 (3)	-0.011 (2)	-0.028 (2)
N4	0.0471 (19)	0.0453 (18)	0.0487 (18)	-0.0064 (15)	0.0043 (14)	-0.0071 (15)
C1	0.063 (3)	0.087 (4)	0.041 (2)	0.003 (3)	0.003 (2)	-0.011 (2)
C2	0.043 (2)	0.056 (2)	0.047 (2)	-0.0071 (18)	0.0034 (16)	-0.0035 (18)
C3	0.043 (2)	0.051 (2)	0.049 (2)	0.0034 (18)	0.0023 (16)	0.0014 (18)
C4	0.046 (2)	0.048 (2)	0.0394 (19)	-0.0045 (17)	-0.0002 (16)	0.0034 (16)
C5	0.040 (2)	0.044 (2)	0.046 (2)	-0.0082 (17)	0.0037 (16)	-0.0053 (17)
C6	0.043 (2)	0.056 (3)	0.059 (2)	0.0049 (19)	-0.0029 (18)	-0.001 (2)
C7	0.050 (2)	0.071 (3)	0.045 (2)	-0.001 (2)	-0.0079 (18)	0.004 (2)
C8	0.068 (3)	0.058 (3)	0.048 (2)	0.000 (2)	-0.009 (2)	-0.006 (2)
С9	0.054 (2)	0.046 (2)	0.043 (2)	0.0008 (18)	-0.0038 (18)	-0.0032 (17)
C10	0.051 (2)	0.050 (2)	0.042 (2)	-0.0013 (18)	0.0088 (17)	0.0000 (17)
C11	0.044 (2)	0.044 (2)	0.046 (2)	-0.0024 (17)	0.0006 (16)	-0.0012 (17)
C12	0.051 (2)	0.049 (2)	0.045 (2)	-0.0043 (18)	0.0032 (17)	-0.0042 (18)
C13	0.039 (2)	0.0398 (19)	0.049 (2)	0.0019 (16)	0.0013 (16)	-0.0016 (16)
C14	0.062 (3)	0.063 (3)	0.051 (2)	-0.013 (2)	0.016 (2)	-0.008 (2)
C15	0.061 (3)	0.059 (3)	0.072 (3)	-0.022 (2)	0.018 (2)	-0.006 (2)
C16	0.046 (2)	0.043 (2)	0.061 (2)	-0.0036 (18)	-0.0032 (18)	-0.0066 (19)
C17	0.057 (2)	0.044 (2)	0.049 (2)	-0.0011 (19)	0.0013 (18)	-0.0017 (18)
C18	0.046 (2)	0.045 (2)	0.049 (2)	-0.0031 (17)	0.0067 (17)	0.0029 (17)

Geometric parameters (Å, °)

Br1-C10	1.854 (4)	C4—C5	1.383 (6)
Cl1—C4	1.722 (4)	C5—C6	1.392 (6)
C12—C6	1.717 (4)	C6—C7	1.377 (6)
Cl3—C16	1.735 (4)	С7—Н7	0.9300

FI-Cl1305 (7)CS-C91431 (6) $P2-Cl$ 1273 (6)CH0-Cl11373 (5)NI-N21333 (5)C12-Cl31459 (5)NI-N21335 (5)C12-Cl31333 (5)NI-C51427 (5)Cl3-Cl41390 (6)N3-C81138 (5)Cl4-Cl51337 (6)N4-C121276 (5)Cl4-Cl51337 (6)C2-C71365 (6)Cl5-Cl61357 (6)C2-C71365 (6)Cl5-H1509300C2-C71365 (6)Cl5-Cl71376 (6)C2-C31380 (6)Cl7-Cl81372 (6)C3-C41388 (6)Cl7-H1709300C3-H309300Cl8-H1809300C3-H309300Cl8-H1809300C3-H31383 (6)Cl1-Cl-S126 (3)C0-N2-N1135 (3)N2-C9-Cl0112 4 (3)N2-N1-C5119 5 (3)N2-C9-Cl0112 4 (3)N2-N1-C5199 (3)Cl1-Cl0-SP105 7 (3)C12-N4-C11120 9 (3)Cl1-Cl0-Brl126 (3)F3-Cl-F2109 1 (6)C9-Cl0-Brl124 6 (3)F3-Cl-F11034 (6)Cl0-Cl1-N1104 7 (3)F3-Cl-F2119 (4)Cl3-Cl2-H12119 4C3-C2-Cl112 (4)N1-Cl1-N4188 1 (4)F3-Cl-C2112 (4)N1-Cl1-N4138 1 (4)F3-Cl-C2112 (4)N1-Cl2-H12119 4C3-C2-Cl112 (4)Cl3-Cl2-H12119 4C3-C2-Cl112 (4)Cl3-Cl2-H12119 4C3-C2-Cl <th></th> <th></th> <th></th> <th></th>				
F2-C11283 (6) $C9-C10$ 1.398 (6) $F3-C1$ 1.273 (6) $C10-C11$ 1.373 (5) $NI-N2$ 1.343 (5) $C12-C13$ 1.459 (5) $NI-C11$ 1.376 (5) $C12-H12$ 0.9300 $NI-C5$ 1.427 (5) $C13-C18$ 1.383 (6) $N2-C9$ 1.335 (5) $C14-C15$ 1.384 (6) $N3-C8$ 1.138 (5) $C14-C15$ 1.384 (6) $N4-C11$ 1.380 (5) $C15-C16$ 1.357 (6) $C1-C2$ 1.498 (6) $C15-H15$ 0.9300 $C2-C7$ 1.365 (6) $C16-C17$ 1.376 (6) $C2-C3$ 1.380 (6) $C17-C18$ 1.372 (6) $C3-C4$ 1.388 (6) $C17-H17$ 0.9300 $C3-H3$ 0.9300 $C18-H18$ 0.9300 $N2-NI-C11$ 113.9 (3) $N2-C9-C10$ 112.4 (3) $N2-NI-C5$ 119.5 (3) $N2-C9-C8$ 127.6 (4) $C12-N4-C11$ 120.9 (3) $C1-C10-Br1$ 129.6 (3) $C3-H3$ 0.93 (3) $C11-C10-C9$ 105.7 (3) $C3-H3$ 103.4 (6) $C10-C1-H1$ 104.7 (3) $C2-N-H1$ 103.4 (6) $C10-C1-H1$ 104.7 (3) $C3-C4-C1$ 118.0 (4) $C1-C10-Br1$ 129.6 (3) $C3-C4-C11$ 109.4 (6) $C10-C1-H1$ 104.7 (3) $C3-C4-C2$ 112.2 (4) $N1-C11-N4$ 118.1 (4) $C3-C4-C2$ 112.0 (5) $N-C12-H12$ 119.4 $C7-C2-C3$ 121.9 (4) $C13-C12-H12$ 119.4 $C3-C4-C1$ 118.7 (4) $C13-C12-H12$ 119.4 (4) $C2-C3-H3$	F1—C1	1.305 (7)	C8—C9	1.431 (6)
F3-C11273 (6)C10-C111373 (5)N1-N21.343 (5)C12-C131.499 (5)N1-C11.376 (5)C12-H120.9300N1-C51.427 (5)C13-C181.383 (5)N2-C91.335 (5)C13-C181.384 (6)N4-C121.276 (5)C14-H140.9300N4-C111.380 (5)C15-C161.357 (6)C1-C21.498 (6)C15-H150.9300C2-C71.365 (6)C16-C171.376 (6)C2-C31.380 (6)C17-C181.372 (6)C3-H30.9300C18-H180.9300N2-N1-C11113.9 (3)N2-C9-C10112.4 (3)N2-N1-C11113.9 (3)N2-C9-C10112.4 (3)N2-N1-C11113.9 (3)C1-C10-C9105.7 (3)C11-N1-C5126.6 (3)C10-C9-C8127.6 (4)C11-N1-C5126.6 (3)C10-C9-C8127.6 (4)C12-N4-C11120.9 (3)C11-C10-C9105.7 (3)C2-N2-N1103.3 (3)C11-C10-C9105.7 (3)C12-N4-C11120.9 (3)C11-C10-Brl129.6 (3)F3-C1-F1103.4 (6)C10-C11-N1104.7 (3)F3-C1-F1103.4 (6)C10-C11-N1104.7 (3)F3-C1-F1104.2 (5)C10-C11-N4138.1 (4)F3-C1-C2112.0 (4)C13-C12-H12119.4 (4)C7-C2-C3121.9 (4)C13-C12-H12119.4 (4)C7-C2-C3121.9 (4)C13-C12-H12119.4 (4)C7-C2-C3121.9 (4)C13-C14-H14119.5 (4) <tr< td=""><td>F2—C1</td><td>1.283 (6)</td><td>C9—C10</td><td>1.398 (6)</td></tr<>	F2—C1	1.283 (6)	C9—C10	1.398 (6)
N1-N2 1.343 (5) C12-C13 1.459 (5) N1-C1 1.376 (5) C12-H12 0.9300 N1-C5 1.427 (5) C13-C14 1.330 (6) N2-C9 1.335 (5) C13-C14 1.390 (6) N4-C12 1.276 (5) C14-H14 0.9300 N4-C11 1.380 (5) C15-C16 1.357 (6) C1-C2 1.498 (6) C15-H15 0.9300 C2-C7 1.365 (6) C16-C17 1.376 (6) C3-C4 1.388 (6) C17-H17 0.9300 C3-H3 0.9300 C18-H18 0.9300 N2-N1-C11 113.9 (3) N2-C9-C10 112.4 (3) N2-N1-C5 119.5 (3) N2-C9-C8 1200 (4) C11-N1-C5 126.6 (3) C10-C9-C8 127.6 (4) C9-N2-N1 103.3 (3) C11-C10-G9 105.7 (3) C12-N4-C11 120.9 (3) C11-C10-G9 105.7 (3) C12-N4-C11 103.9 (3) C11-C10-M1 104.7 (3) F3-C1-F2 109.1 (6) C9-C10-Br1 124.6 (3) F3-C1-F1 104.2 (5) C10-C11-N1	F3—C1	1.273 (6)	C10—C11	1.373 (5)
N1-C1I 1376 (5) C12-H12 0.9300 N1-C5 1.427 (5) C13-C18 1.383 (5) N2-C9 1.335 (5) C13-C14 1.390 (6) N3-C8 1.138 (5) C14-C15 1.384 (6) N4-C12 1.276 (5) C14-H14 0.9300 N4-C11 1.380 (5) C15-C16 1.357 (6) C1-C2 1.498 (6) C15-H15 0.9300 C2-C7 1.365 (6) C16-C17 1.376 (6) C3-C4 1.388 (6) C17-H17 0.9300 C3-H3 0.9300 C18-H18 0.9300 C3-H3 0.9300 C18-H18 0.9300 N2-N1-C5 126 (3) C10-C9-C8 127.6 (4) C9-N2-N1 103.3 (3) C11-C10-B71 129.6 (3) C11-N1-C5 126 (5) C10-C11-N1 104.7 (3) F3-C1-F2 109.1 (6) C9-C10-B71 124.6 (3) F3-C1-F1 103.4 (6) C10-C11-N1 104.7 (3) F3-C1-F2 109.1 (6) C9-C10-B71 129.6 (3) F3-C1-F2 109.1 (6) C9-C10-B71 129.6 (N1—N2	1.343 (5)	C12—C13	1.459 (5)
N1-CS1427 (5)C13-C181.383 (5)N2-C91.335 (5)C13-C141.390 (6)N3-C81.138 (5)C14-C151.344 (6)N4-C121.276 (5)C14-H140.9300N4-C111.380 (5)C15-C161.357 (6)C1-C21.498 (6)C15-H150.9300C2-C71.365 (6)C16-C171.376 (6)C2-C31.380 (6)C17-C181.372 (6)C3-C41.388 (6)C17-H170.9300C3-H30.9300C18-H180.9300C3-H30.9300C18-H180.9300C3-H30.9300C18-H180.9300C3-H30.9300C10-C9-C8122 (3)N2-N1-C5119 (3)N2-C9-C10112 (3)N2-N1-C5126 (3)C10-C9125 (3)C12-N4-C11120 9 (3)C11-C10-Br1129 (3)C12-N4-C11103 4 (6)C10-C11-N1104 7 (3)F3-C1-F2109 1 (6)C9-C10-Br1124 6 (3)F3-C1-F2109 1 (6)C9-C10-Br1124 6 (3)F3-C1-C2112 2 (4)N1-C11-N4185 (4)F3-C1-C2112 2 (4)N1-C11-N4185 (4)F3-C1-C2112 2 (4)N1-C12-H12119 4F3-C1-C2112 0 (5)N4-C12-C13121 2 (4)F3-C1-C2112 0 (5)N4-C12-H12119 4F3-C1-C2112 0 (4)C18-C13-C14118 6 (4)C3-C2-C1118 7 (4)C18-C13-C14118 6 (4)C3-C2-C1119 4 (3)C16-C17-H14<	N1—C11	1.376 (5)	C12—H12	0.9300
N2-C9 1.335 (5) C13-C14 1.390 (6) N3-C8 1.138 (5) C14-C15 1.384 (6) N4-C12 1.276 (5) C14-H14 0.9300 N4-C11 1.380 (5) C15-C16 1.357 (6) C1-C2 1.498 (6) C15-H15 0.9300 C2-C3 1.380 (6) C17-C18 1.372 (6) C3-C4 1.388 (6) C17-H17 0.9300 C3-H3 0.9300 C18-H18 0.9300 C3-H3 0.9300 C18-H18 0.9300 C11-N1-C5 126 (6) C10-C9-C8 120 (4) C11-N1-C5 126 (5) C10-C9-C8 120 (4) C11-N1-C5 126 (6) C10-C10-B1 129 (6) C12-N4-C11 120 (3) C11-C10-B1 129 (6) C3-C4 103 4 (6) C10-C11-N1 104 7 (3) F3-C1-F1 103 4 (6) C10-C11-N1 104 7 (3) F3-C1-F1 104 2 (5) C10-C11-N4 138 1 (4) F3-C1-C2 112 0 (4) N4-C12-C13 121 2 (4) F3-C1-C2 112 0 (4) N4-C12-C13 120 (N1—C5	1.427 (5)	C13—C18	1.383 (5)
N3-C81.138 (5)C14-C151.384 (6)N4-C121.276 (5)C14-H140.9300N4-C111.380 (5)C15-C161.357 (6)C1-C21.498 (6)C15-H150.9300C2-C71.365 (6)C16-C171.376 (6)C2-C31.380 (6)C17-C181.372 (6)C3-C41.388 (6)C17-C180.9300C3-H30.9300C18-H180.9300N2-N1-C11113.9 (3)N2-C9-C10112.4 (3)N2-N1-C5119.5 (3)N2-C9-C8120.0 (4)C11-N1-C5126.6 (3)C10-C9-C8127.6 (4)C9-N2-N1103.3 (3)C11-C10-Brl129.6 (3)C12-N4-C11120.9 (3)C11-C10-Brl129.6 (3)F3-C1-F2109.1 (6)C9-C10-Brl124.6 (3)F3-C1-F1103.4 (6)C10-C11-N4188.1 (4)F3-C1-C2115.0 (4)N4-C12-C13121.4 (6)F1-C1-C2112.0 (5)N4-C12-H12119.4C7-C2-C3121.9 (4)C13-C12-C14118.6 (4)C3-C2-C1119.4 (4)C14-C13-C12119.4 (4)C7-C2-C3120.8 (15-C14-C13120.9 (4)C4-C3-H3120.8C15-C14-C13120.9 (4)C4-C3-H3120.8C15-C14-C13120.9 (4)C4-C3-C4118.4 (4)C14-C13-C12119.6 (4)C2-C3-C4119.4 (4)C13-C12-C14118.6 (4)C3-C4-C1119.6 (3)C16-C15-C14118.6 (4)C3-C4-C1119.6 (3)C16-C15-H15120.7C	N2—C9	1.335 (5)	C13—C14	1.390 (6)
N4-C12 1.276 (5) $C14-H14$ 0.9300 $N4-C11$ 1.380 (5) $C15-C16$ 1.357 (6) $C1-C2$ 1.498 (6) $C15-C16$ 1.357 (6) $C2-C7$ 1.356 (6) $C16-C17$ 1.376 (6) $C2-C3$ 1.380 (6) $C17-C18$ 1.372 (6) $C3-C4$ 1.388 (6) $C17-H17$ 0.9300 $C3-H3$ 0.9300 $C18-H18$ 0.9300 $C3-H3$ 0.9300 $C18-H18$ 0.9300 $N2-N1-C11$ 113.9 (3) $N2-C9-C10$ 112.4 (3) $N2-N1-C5$ 126.6 (3) $C10-C9-C8$ 120.0 (4) $C11-N1-C5$ 126.6 (3) $C10-C9-C8$ 127.6 (4) $C9-N2-N1$ 103.3 (3) $C11-C10-Br1$ 129.6 (3) $F3-C1-F2$ 109.1 (6) $C9-C10-Br1$ 124.6 (3) $F3-C1-F1$ 103.4 (6) $C10-C1-N1$ 104.7 (3) $F2-C1-C2$ 112.0 (4) $N1-C11-N4$ 18.1 (4) $F3-C1-F1$ 103.4 (6) $C10-C11-N1$ 104.7 (3) $F2-C1-C2$ 112.0 (4) $N1-C12-H12$ 119.4 $F3-C1-C2$ 112.0 (4) $N1-C12-H12$ 119.4 $F1-C1-C2$ 112.0 (4) $C18-C13-C12$ 119.4 $C7-C2-C3$ 12.9 (4) $C13-C12-H12$ 119.4 $C7-C2-C1$ 118.7 (4) $C18-C13-C12$ 119.6 (4) $C2-C3-H3$ 120.8 (4) $C13-C12-H12$ 119.6 (4) $C3-C4-C1$ 119.6 (3) $C16-C15-C14$ 118.6 (4) $C3-C4-C1$ 119.6 (3) $C16-C15-H15$	N3—C8	1.138 (5)	C14—C15	1.384 (6)
N4-C111.380 (5)C15-C161.357 (6)C1-C21.498 (6)C15-H150.9300C2-C71.365 (6)C16-C171.376 (6)C2-C31.380 (6)C17-C181.372 (6)C3-C41.388 (6)C17-H170.9300C3-H30.9300C18-H180.9300N2-NI-C11113.9 (3)N2-C9-C10112.4 (3)N2-NI-C5126.6 (3)C10-C9-C8120.0 (4)C11-N1-C5126.6 (3)C10-C9-C8120.0 (4)C12-N4-C11120.9 (3)C11-C10-C9105.7 (3)C12-N4-C11120.9 (3)C11-C10-Br1124.6 (3)F3-C1-F2109.1 (6)C9-C10-Br1124.6 (3)F3-C1-F1103.4 (6)C10-C11-N1104.7 (3)F2-C1-F1104.2 (5)C10-C11-N4138.1 (4)F3-C1-C2112.0 (5)N4-C12-C13121.2 (4)F1-C1-C2112.0 (5)N4-C12-H12119.4C7-C2-C1118.7 (4)C18-C13-C12119.4C7-C2-C1118.7 (4)C18-C13-C12118.6 (4)C3-C2-C1118.4 (4)C14-C13-C12119.6 (4)C2-C3-H3120.8C15-C14-C13120.9 (4)C4-C3-H3120.8C15-C14-C13120.9 (4)C4-C3-H3120.8C15-C14-C13120.9 (4)C4-C3-H3120.8C15-C14-C13120.9 (4)C4-C3-H3120.8C15-C14-C13119.6 (3)C5-C4-C1119.6 (3)C16-C15-H15120.7C4-C5-C6119.0 (4)C15-C16-C17122.0 (4)<	N4—C12	1.276 (5)	C14—H14	0.9300
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	N4—C11	1.380 (5)	C15—C16	1.357 (6)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C1—C2	1.498 (6)	C15—H15	0.9300
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C2—C7	1.365 (6)	C16—C17	1.376 (6)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C2—C3	1.380 (6)	C17—C18	1.372 (6)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C3—C4	1.388 (6)	C17—H17	0.9300
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	С3—Н3	0.9300	C18—H18	0.9300
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	N2—N1—C11	113.9 (3)	N2—C9—C10	112.4 (3)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	N2—N1—C5	119.5 (3)	N2—C9—C8	120.0 (4)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C11—N1—C5	126.6 (3)	С10—С9—С8	127.6 (4)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C9—N2—N1	103.3 (3)	C11—C10—C9	105.7 (3)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C12—N4—C11	120.9 (3)	C11—C10—Br1	129.6 (3)
F3C1F1103.4 (6)C10C11N1104.7 (3)F2C1F1104.2 (5)C10C11N4138.1 (4)F3C1C2112.2 (4)N1C11N4116.9 (3)F2C1C2115.0 (4)N4C12C13121.2 (4)F1C1C2112.0 (5)N4C12H12119.4C7C2C3121.9 (4)C13C12H12119.4C7C2C1118.7 (4)C18C13C12121.8 (4)C2C3C1119.4 (4)C18C13C12119.6 (4)C2C3C4118.4 (4)C14C13C12119.6 (4)C2C3H3120.8C15C14C13120.9 (4)C4C3H3120.8C15C14H14119.5C5C4C3120.8 (4)C13C12H15120.7C4C5C6119.6 (3)C16C15H15120.7C4C5N1121.3 (4)C15C16C17122.0 (4)C6C5-N1119.7 (4)C15C16C13119.1 (3)C7C6C5120.4 (4)C17C16C13118.9 (3)C7C6C12120.3 (3)C18C17H17120.5C2C7C6119.5 (4)C16C17H17120.5C2C7C6119.5 (4)C16C17H17120.5C2C7H7120.3C17C18H18119.6	F3—C1—F2	109.1 (6)	C9—C10—Br1	124.6 (3)
F2C1F1 104.2 (5) $C10C11N4$ 138.1 (4)F3C1C2 112.2 (4) $N1C11N4$ 116.9 (3)F2C1C2 115.0 (4) $N4C12C13$ 121.2 (4)F1C1C2 112.0 (5) $N4C12H12$ 119.4 C7C2C3 121.9 (4) $C13C12H12$ 119.4 C7C2C1 118.7 (4) $C18C13C14$ 118.6 (4)C3C2C1 119.4 (4) $C18C13C12$ 121.8 (4)C2C3C4 118.4 (4) $C14C13C12$ 119.6 (4)C2C3C4 118.4 (4) $C14C13C12$ 119.6 (4)C2C3H3 120.8 $C15C14C13$ 120.9 (4)C4C3H3 120.8 $C15C14C13$ 120.9 (4)C4C3H3 120.8 (4) $C13C14H14$ 119.5 C5C4C11 119.6 (3) $C16C15C14$ 118.6 (4)C3C4C11 119.6 (3) $C16C15H15$ 120.7 C4C5C6 119.0 (4) $C15C16C17$ 122.0 (4)C6C5-N1 119.7 (4) $C15C16C13$ 119.1 (3)C7C6C5 120.4 (4) $C17C16C13$ 118.9 (3)C7C6C12 120.3 (3) $C18C17H17$ 120.5 C2C7C6 119.5 (4) $C16C17H17$ 120.5 C2C7C6 119.5 (4) $C16C17H17$ 120.5 C2C7H7 120.3 $C17C18H18$ 119.6 N3C8C9 178.4 (5) $C13C18H18$ 119.6	F3—C1—F1	103.4 (6)	C10-C11-N1	104.7 (3)
F3C1C2112.2 (4)N1C11N4116.9 (3)F2C1C2115.0 (4)N4C12C13121.2 (4)F1C1C2112.0 (5)N4C12H12119.4C7C2C3121.9 (4)C13C12H12119.4C7C2C1118.7 (4)C18C13C14118.6 (4)C3C2C1119.4 (4)C18C13C12121.8 (4)C2C3C4118.4 (4)C14C13C12119.6 (4)C2C3H3120.8C15C14C13120.9 (4)C4C3H3120.8C15C14H14119.5C5C4C3120.8 (4)C13C14H14119.5C5C4C11119.6 (3)C16C15C14118.6 (4)C3C4C11119.6 (3)C16C15H15120.7C4C5C6119.0 (4)C14C15H15120.7C4C5N1121.3 (4)C15C16C17122.0 (4)C6C5N1119.7 (4)C15C16C13119.1 (3)C7C6C5120.4 (4)C17C16C13118.9 (3)C7C6C5120.3 (3)C18C17H17120.5C2C7C6119.5 (4)C16C17H17120.5C2C7C6119.5 (4)C16C17H17120.5C2C7H7120.3C17C18H18119.6N3C8C9178.4 (5)C13C18H18119.6	F2—C1—F1	104.2 (5)	C10—C11—N4	138.1 (4)
F2-C1-C2115.0 (4)N4-C12-C13121.2 (4)F1-C1-C2112.0 (5)N4-C12-H12119.4C7-C2-C3121.9 (4)C13-C12-H12119.4C7-C2-C1118.7 (4)C18-C13-C14118.6 (4)C3-C2-C1119.4 (4)C18-C13-C12121.8 (4)C2-C3-C4118.4 (4)C14-C13-C12119.6 (4)C2-C3-H3120.8C15-C14-C13120.9 (4)C4-C3-H3120.8C15-C14-H14119.5C5-C4-C3120.8 (4)C13-C15-C14118.6 (4)C3-C4-C11119.6 (3)C16-C15-C14118.6 (4)C3-C4-C11119.6 (3)C16-C15-H15120.7C4-C5-C6119.0 (4)C14-C15-H15120.7C4-C5-N1121.3 (4)C15-C16-C17122.0 (4)C6-C5-N1119.7 (4)C15-C16-C13119.1 (3)C7-C6-C5120.4 (4)C17-C16-C13118.9 (3)C7-C6-C5120.4 (4)C17-C16-C13118.9 (3)C7-C6-C12120.3 (3)C18-C17-H17120.5C2-C7-C6119.5 (4)C16-C17-H17120.5C2-C7-H7120.3C17-C18-C13120.8 (4)C6-C7-H7120.3C17-C18-H18119.6	F3—C1—C2	112.2 (4)	N1—C11—N4	116.9 (3)
F1-C1-C2112.0 (5)N4-C12-H12119.4C7-C2-C3121.9 (4)C13-C12-H12119.4C7-C2-C1118.7 (4)C18-C13-C14118.6 (4)C3-C2-C1119.4 (4)C18-C13-C12121.8 (4)C2-C3-C4118.4 (4)C14-C13-C12119.6 (4)C2-C3-H3120.8C15-C14-C13120.9 (4)C4-C3-H3120.8C15-C14-H14119.5C5-C4-C3120.8 (4)C13-C14-H14119.5C5-C4-C11119.6 (3)C16-C15-C14118.6 (4)C3-C4-C11119.6 (3)C16-C15-H15120.7C4-C5-C6119.0 (4)C14-C15-H15120.7C4-C5-N1121.3 (4)C15-C16-C17122.0 (4)C6-C5-N1119.7 (4)C15-C16-C13118.9 (3)C7-C6-C5120.4 (4)C17-C16-C13118.9 (3)C7-C6-C12119.3 (3)C18-C17-H17120.5C2-C7-C6119.5 (4)C16-C17-H17120.5C2-C7-H7120.3C17-C18-C13120.8 (4)C6-C7-H7120.3C17-C18-H18119.6N3-C8-C9178.4 (5)C13-C18-H18119.6	F2—C1—C2	115.0 (4)	N4—C12—C13	121.2 (4)
C7-C2-C3121.9 (4)C13-C12-H12119.4C7-C2-C1118.7 (4)C18-C13-C14118.6 (4)C3-C2-C1119.4 (4)C18-C13-C12121.8 (4)C2-C3-C4118.4 (4)C14-C13-C12119.6 (4)C2-C3-H3120.8C15-C14-C13120.9 (4)C4-C3-H3120.8C15-C14-H14119.5C5-C4-C3120.8 (4)C13-C14-H14119.5C5-C4-C11119.6 (3)C16-C15-C14118.6 (4)C3-C4-C11119.6 (3)C16-C15-H15120.7C4-C5-C6119.0 (4)C14-C15-H15120.7C4-C5-N1121.3 (4)C15-C16-C17122.0 (4)C6-C5-N1119.7 (4)C15-C16-C13118.9 (3)C7-C6-C5120.4 (4)C17-C16-C13118.9 (3)C7-C6-C12119.3 (3)C18-C17-H17120.5C2-C7-C6119.5 (4)C16-C17-H17120.5C2-C7-C6119.5 (4)C16-C17-H17120.5C2-C7-H7120.3C17-C18-C13120.8 (4)C6-C7-H7120.3C17-C18-H18119.6N3-C8-C9178.4 (5)C13-C18-H18119.6	F1—C1—C2	112.0 (5)	N4—C12—H12	119.4
C7-C2-C1118.7 (4)C18-C13-C14118.6 (4)C3-C2-C1119.4 (4)C18-C13-C12121.8 (4)C2-C3-C4118.4 (4)C14-C13-C12119.6 (4)C2-C3-H3120.8C15-C14-C13120.9 (4)C4-C3-H3120.8C15-C14-H14119.5C5-C4-C3120.8 (4)C13-C14-H14119.5C5-C4-C11119.6 (3)C16-C15-C14118.6 (4)C3-C4-C11119.6 (3)C16-C15-H15120.7C4-C5-C6119.0 (4)C14-C15-H15120.7C4-C5-N1121.3 (4)C15-C16-C17122.0 (4)C6-C5-N1119.7 (4)C15-C16-C13119.1 (3)C7-C6-C5120.4 (4)C17-C16-C13118.9 (3)C7-C6-C12120.3 (3)C18-C17-H17120.5C2-C7-C6119.5 (4)C16-C17-H17120.5C2-C7-H7120.3C17-C18-C13120.8 (4)C6-C7-H7120.3C17-C18-H18119.6N3-C8-C9178.4 (5)C13-C18-H18119.6	C7—C2—C3	121.9 (4)	C13—C12—H12	119.4
C3-C2-C1119.4 (4)C18-C13-C12121.8 (4)C2-C3-C4118.4 (4)C14-C13-C12119.6 (4)C2-C3-H3120.8C15-C14-C13120.9 (4)C4-C3-H3120.8C15-C14-H14119.5C5-C4-C3120.8 (4)C13-C14-H14119.5C5-C4-C11119.6 (3)C16-C15-C14118.6 (4)C3-C4-C11119.6 (3)C16-C15-H15120.7C4-C5-C6119.0 (4)C14-C15-H15120.7C4-C5-N1121.3 (4)C15-C16-C17122.0 (4)C6-C5-N1119.7 (4)C15-C16-C13118.9 (3)C7-C6-C5120.4 (4)C17-C16-C13118.9 (3)C7-C6-C5120.3 (3)C18-C17-H17120.5C2-C7-C6119.5 (4)C16-C17-H17120.5C2-C7-C6119.5 (4)C16-C17-H17120.5C2-C7-H7120.3C17-C18-C13120.8 (4)C6-C7-H7120.3C17-C18-H18119.6N3-C8-C9178.4 (5)C13-C18-H18119.6	C7—C2—C1	118.7 (4)	C18—C13—C14	118.6 (4)
C2—C3—C4118.4 (4)C14—C13—C12119.6 (4)C2—C3—H3120.8C15—C14—C13120.9 (4)C4—C3—H3120.8C15—C14—H14119.5C5—C4—C3120.8 (4)C13—C14—H14119.5C5—C4—C11119.6 (3)C16—C15—C14118.6 (4)C3—C4—C11119.6 (3)C16—C15—H15120.7C4—C5—C6119.0 (4)C14—C15—H15120.7C4—C5—N1121.3 (4)C15—C16—C17122.0 (4)C6—C5—N1119.7 (4)C15—C16—C13119.1 (3)C7—C6—C5120.4 (4)C17—C16—C13118.9 (3)C7—C6—C12120.3 (3)C18—C17—C16119.1 (4)C5—C6—C12119.5 (4)C16—C17—H17120.5C2—C7—C6119.5 (4)C16—C17—H17120.5C2—C7—H7120.3C17—C18—C13120.8 (4)C6—C7—H7120.3C17—C18—H18119.6N3—C8—C9178.4 (5)C13—C18—H18119.6	C3—C2—C1	119.4 (4)	C18—C13—C12	121.8 (4)
C2-C3-H3120.8C15-C14-C13120.9 (4)C4-C3-H3120.8C15-C14-H14119.5C5-C4-C3120.8 (4)C13-C14-H14119.5C5-C4-C11119.6 (3)C16-C15-C14118.6 (4)C3-C4-C11119.6 (3)C16-C15-H15120.7C4-C5-C6119.0 (4)C14-C15-H15120.7C4-C5-N1121.3 (4)C15-C16-C17122.0 (4)C6-C5-N1119.7 (4)C15-C16-C13119.1 (3)C7-C6-C5120.4 (4)C17-C16-C13118.9 (3)C7-C6-C5120.4 (4)C17-C16-C13118.9 (3)C7-C6-C12120.3 (3)C18-C17-H17120.5C2-C7-C6119.5 (4)C16-C17-H17120.5C2-C7-H7120.3C17-C18-C13120.8 (4)C6-C7-H7120.3C17-C18-H18119.6N3-C8-C9178.4 (5)C13-C18-H18119.6	C2—C3—C4	118.4 (4)	C14—C13—C12	119.6 (4)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	С2—С3—Н3	120.8	C15—C14—C13	120.9 (4)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	С4—С3—Н3	120.8	C15—C14—H14	119.5
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C5—C4—C3	120.8 (4)	C13—C14—H14	119.5
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C5—C4—Cl1	119.6 (3)	C16—C15—C14	118.6 (4)
$\begin{array}{ccccccc} C4-C5-C6 & 119.0 (4) & C14-C15-H15 & 120.7 \\ C4-C5-N1 & 121.3 (4) & C15-C16-C17 & 122.0 (4) \\ C6-C5-N1 & 119.7 (4) & C15-C16-C13 & 119.1 (3) \\ C7-C6-C5 & 120.4 (4) & C17-C16-C13 & 118.9 (3) \\ C7-C6-C12 & 120.3 (3) & C18-C17-C16 & 119.1 (4) \\ C5-C6-C12 & 119.3 (3) & C18-C17-H17 & 120.5 \\ C2-C7-C6 & 119.5 (4) & C16-C17-H17 & 120.5 \\ C2-C7-H7 & 120.3 & C17-C18-C13 & 120.8 (4) \\ C6-C7-H7 & 120.3 & C17-C18-H18 & 119.6 \\ N3-C8-C9 & 178.4 (5) & C13-C18-H18 & 119.6 \\ \end{array}$	C3—C4—Cl1	119.6 (3)	C16—C15—H15	120.7
$\begin{array}{ccccccc} C4-C5-N1 & 121.3 \ (4) & C15-C16-C17 & 122.0 \ (4) \\ C6-C5-N1 & 119.7 \ (4) & C15-C16-C13 & 119.1 \ (3) \\ C7-C6-C5 & 120.4 \ (4) & C17-C16-C13 & 118.9 \ (3) \\ C7-C6-C12 & 120.3 \ (3) & C18-C17-C16 & 119.1 \ (4) \\ C5-C6-C12 & 119.3 \ (3) & C18-C17-H17 & 120.5 \\ C2-C7-C6 & 119.5 \ (4) & C16-C17-H17 & 120.5 \\ C2-C7-H7 & 120.3 & C17-C18-C13 & 120.8 \ (4) \\ C6-C7-H7 & 120.3 & C17-C18-H18 & 119.6 \\ N3-C8-C9 & 178.4 \ (5) & C13-C18-H18 & 119.6 \\ \end{array}$	C4—C5—C6	119.0 (4)	C14—C15—H15	120.7
C6—C5—N1119.7 (4)C15—C16—Cl3119.1 (3)C7—C6—C5120.4 (4)C17—C16—Cl3118.9 (3)C7—C6—Cl2120.3 (3)C18—C17—C16119.1 (4)C5—C6—Cl2119.3 (3)C18—C17—H17120.5C2—C7—C6119.5 (4)C16—C17—H17120.5C2—C7—H7120.3C17—C18—C13120.8 (4)C6—C7—H7120.3C17—C18—H18119.6N3—C8—C9178.4 (5)C13—C18—H18119.6	C4—C5—N1	121.3 (4)	C15—C16—C17	122.0 (4)
C7C6C5120.4 (4)C17C16C13118.9 (3)C7C6Cl2120.3 (3)C18C17C16119.1 (4)C5C6Cl2119.3 (3)C18C17H17120.5C2C7C6119.5 (4)C16C17H17120.5C2C7H7120.3C17C18C13120.8 (4)C6C7H7120.3C17C18H18119.6N3C8C9178.4 (5)C13C18H18119.6	C6—C5—N1	119.7 (4)	C15—C16—Cl3	119.1 (3)
C7C6Cl2120.3 (3)C18C17C16119.1 (4)C5C6Cl2119.3 (3)C18C17H17120.5C2C7C6119.5 (4)C16C17H17120.5C2C7H7120.3C17C18C13120.8 (4)C6C7H7120.3C17C18H18119.6N3C8C9178.4 (5)C13C18H18119.6	C7—C6—C5	120.4 (4)	C17—C16—Cl3	118.9 (3)
C5—C6—Cl2119.3 (3)C18—C17—H17120.5C2—C7—C6119.5 (4)C16—C17—H17120.5C2—C7—H7120.3C17—C18—C13120.8 (4)C6—C7—H7120.3C17—C18—H18119.6N3—C8—C9178.4 (5)C13—C18—H18119.6	C7—C6—Cl2	120.3 (3)	C18—C17—C16	119.1 (4)
C2—C7—C6119.5 (4)C16—C17—H17120.5C2—C7—H7120.3C17—C18—C13120.8 (4)C6—C7—H7120.3C17—C18—H18119.6N3—C8—C9178.4 (5)C13—C18—H18119.6	C5—C6—Cl2	119.3 (3)	C18—C17—H17	120.5
C2C7H7120.3C17C18C13120.8 (4)C6C7H7120.3C17C18H18119.6N3C8C9178.4 (5)C13C18H18119.6	C2—C7—C6	119.5 (4)	C16—C17—H17	120.5
C6—C7—H7120.3C17—C18—H18119.6N3—C8—C9178.4 (5)C13—C18—H18119.6	С2—С7—Н7	120.3	C17—C18—C13	120.8 (4)
N3—C8—C9 178.4 (5) C13—C18—H18 119.6	С6—С7—Н7	120.3	C17—C18—H18	119.6
	N3—C8—C9	178.4 (5)	C13—C18—H18	119.6

