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5-{[4-(Dimethylamino)phenyl]ethynyl}pyrimidine–1,2,3,5-tetrafluoro-4,6-diiodobenzene (1/2)

Eric Bosch[a]* and Nathan P. Bowling[b]

[a]Chemistry and Biochemistry Department, Missouri State University, Springfield MO 65897, USA, and [b]Department of Chemistry, University of Wisconsin-Stevens Point, 2101 Fourth Avenue, Stevens Point, WI 54481, USA. *Correspondence e-mail: ericbosch@missouristate.edu

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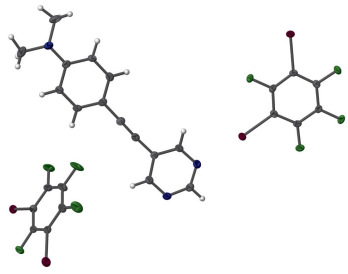
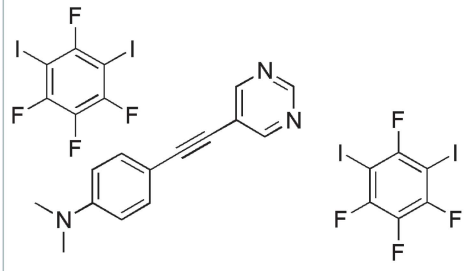
Structural data: full structural data are available from iucrdata.iucr.org

The treatment of 5-{[4-(dimethylamino)phenyl]ethynyl}pyrimidine with a threefold excess of 1,2,3,5-tetrafluoro-4,6-diiodobenzene in dichloromethane solution led to the formation of the unexpected 1:2 title co-crystal, $C_{14}H_{13}N_3{\cdot}2CF_4I_2$. In the extended structure, two unique C—I···N halogen bonds from one of the 1,2,3,5-tetrafluoro-4,6-diiodobenzene molecules to the pyrimidine N atoms of the 5-{[4-(dimethylamino)phenyl]ethynyl}pyrimidine molecule generate [110] chains and layers of these chains are π-stacked along the *a*-axis direction. The second 1,2,3,5-tetrafluoro-4,6-diiodobenzene molecule resides in channels formed parallel to the *a*-axis direction between stacks of 5-{[4-(dimethylamino)phenyl]ethynyl}pyrimidine molecules and interacts with them *via* C—I···π(alkyne) contacts.

3D view



Chemical scheme



Structure description

Halogen bonding is now a widely studied and accepted non-covalent interaction wherein a halogen atom, most commonly iodine, interacts with a Lewis base as halogen-bond acceptor (Cavallo *et al.*, 2016). This interaction has predictable geometry and has accordingly been incorporated in strategies for the self-assembly of multicomponent molecular solids (Mir *et al.*, 2019). Among the most studied ditopic halogen-bond donors are the three isomeric diiodotetrafluorobenzenes as the halogen-bond donor ability is increased by substitution of iodobenzenes with electronegative fluorine atoms (Roper *et al.*, 2010). Herein we report a rare example of inclusion of a 1,2,3,5-tetrafluoro-4,6-diiodobenzene molecule in a co-crystal in which one of the 1,2,3,5-tetrafluoro-4,6-diiodobenzene molecules does not interact with the primary Lewis base.

In the 1:2 co-crystal (Fig. 1) formed between 5-{[4-(dimethylamino)phenyl]ethynyl}-pyrimidine, $C_{14}H_{13}N_3$ (APEP) and 1,2,3,5-tetrafluoro-4,6-diiodobenzene, $C_6F_4I_2$

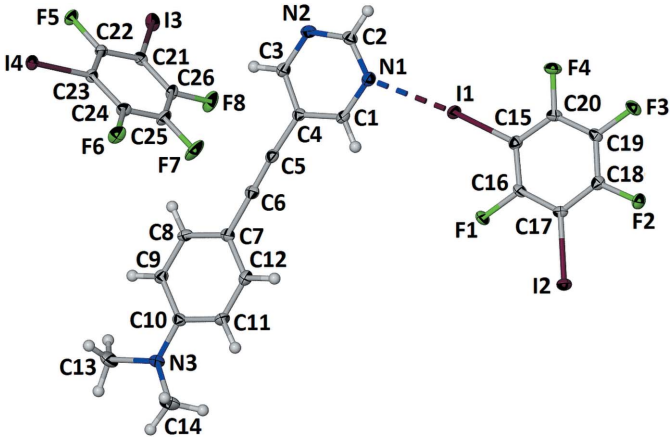


Figure 1
The molecular structure of the title compound with displacement ellipsoids drawn at 50% and the halogen bond shown as a dashed line.

(13DIFP), only one of the 13DIFP molecules is halogen bonded to the APEP. The APEP and the halogen-bonded 13DIFP molecule are essentially coplanar: the interplanar angle between the pyrimidine ring and the aminophenyl ring is 4.24 (15)° and the interplanar angle between the pyrimidine ring and the halogen-bonded 13DIFP molecule is 6.63 (15)°. The two unique C—I···N halogen bonds that combine to form

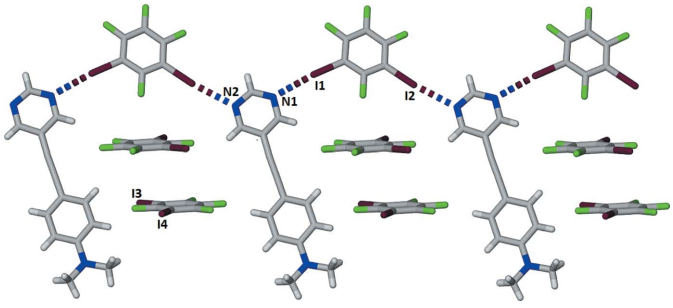


Figure 2
Partial view of a chain of halogen-bonded APEP and 13DIFB molecules with pairs of 13DIFB molecules shown between APEP molecules.

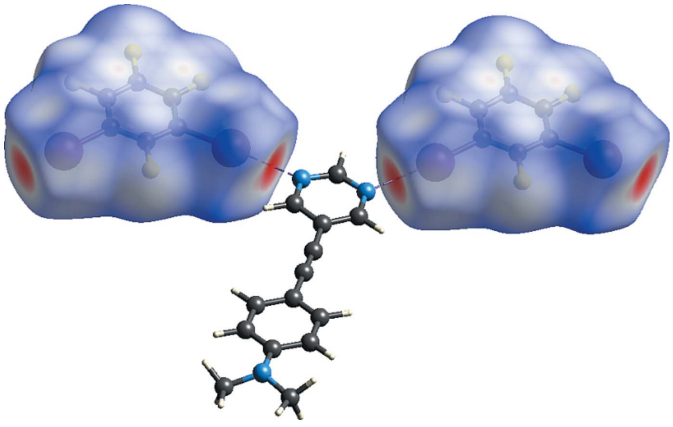


Figure 3
Hirshfeld surface highlighting the halogen-bonding interactions to pyrimidine APEP.

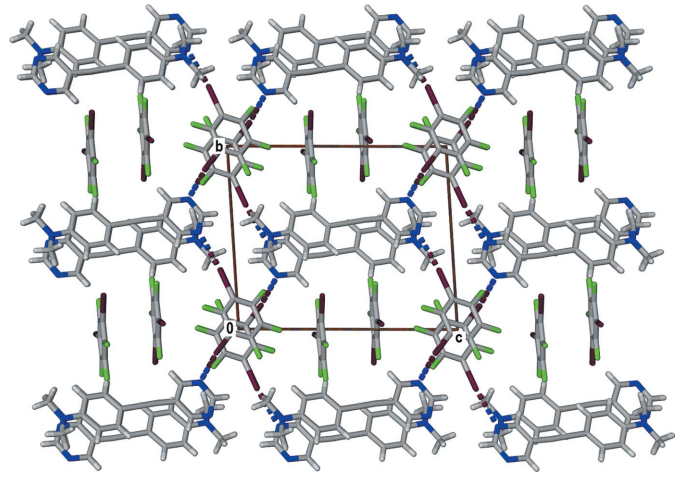


Figure 4
View of crystal packing of the title compound viewed along the *a*-axis direction.

a zigzag alternating halogen-bonded chain, shown in Fig. 2, have separations of I1···N1 and I2···N2^{i} = 2.853 (2) and 2.901 (2) Å and angles C15—I1···N1 and C17—I2···N2^{i} = 174.8 (9) and 173.8 (8)°, respectively [symmetry code: (i) −1 + *x*, −1 + *y*, *z*]. These distances and angles are similar to those previously reported in the 1:1 co-crystal formed between these two molecules of 2.920 (2) Å and 178.27 (6)° (Nwachukwu *et al.*, 2020). The Hirshfeld surface (Spackman *et al.*, 2021) of the halogen-bonded 13DIFB molecules shown in Fig. 3 highlights these two interactions.

In the extended structure, the APEP molecules are offset π-stacked in a head-to-tail manner such that the halogen-bonded 13DIFB molecules are also alternately π-stacked as shown in Fig. 4. With this arrangement, the second non-halogen-bonded 13DIFB molecule is located as a π-stacked pair in channels that lie parallel to the *a*-axis direction (Fig. 4).

The pair of loosely π-stacked 13DIFB molecules interact with the surrounding molecules as shown in the Hirshfeld surface plot in Fig. 5. This highlights a close I···π contact to a

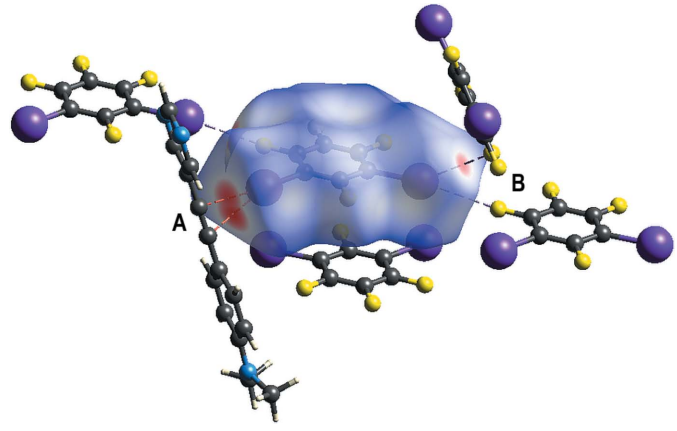


Figure 5
Hirshfeld surface highlighting the close contacts to the solvate 13DIFB molecule.

neighboring alkyne group with I4···C6^{ii} and I4···C5^{ii} [symmetry code: (ii) $1 - x, 2 - y, 1 - z$] separations of 3.276 (3) and 3.316 (3) Å, respectively. These are significantly less than the sum of the van der Waals radii of 3.68 Å at 89 and 90%, respectively. The second I atom has close I···F contacts to two neighboring 13DIFB molecules with I3···F6^{iii} and I3···F3^{iv} separations of 3.2142 (17) and 3.30129 (15) Å as compared to the sum of the van der Waals radii of 3.38 Å [symmetry codes: (iii) $1 + x, y, z$; (iv) $x, 1 + y, -1 + z$].

Synthesis and crystallization

The pyrimidine APEP (8.3 mg) was dissolved in 2 ml of dichloromethane in a screw-cap vial. Three equivalents of 13DIFB were added and the solvent was allowed to slowly evaporate until crystals formed when the vial was sealed to prevent further loss of solvent.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1.

Acknowledgements

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Table 1
Experimental details.

Crystal data	
Chemical formula	$C_{14}H_{13}N_3{\cdot}2C_6F_4I_2$
M_r	1026.99
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	100
a, b, c (Å)	9.1574 (5), 12.0339 (6), 14.0667 (7)
α, β, γ (°)	91.989 (1), 96.924 (1), 102.996 (1)
V (Å^3)	1496.35 (13)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	4.24
Crystal size (mm)	0.52 × 0.28 × 0.20
Data collection	
Diffractometer	Bruker APEXI CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2014)
T_{min}, T_{max}	0.518, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	19410, 6594, 6107
R_{int}	0.023
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.641
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.020, 0.046, 1.09
No. of reflections	6594
No. of parameters	372
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.69, −0.56

Computer programs: *SMART* and *SAINT* (Bruker, 2014), *SHELXT2018/2* (Sheldrick, 2015*a*), *SHELXL2018/3* (Sheldrick, 2015*b*), and *X-SEED* (Barbour, 2020).

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full crystallographic data

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5-{[4-(Dimethylamino)phenyl]ethynyl}pyrimidine–1,2,3,5-tetrafluoro-4,6-diiodobenzene (1/2)

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5-{[4-(Dimethylamino)phenyl]ethynyl}pyrimidine bis(1,2,3,5-tetrafluoro-4,6-diiodobenzene)

Crystal data

$C_{14}H_{13}N_3·2C_6F_4I_2$
M_r = 1026.99
Triclinic, $P\overline{1}$
a = 9.1574 (5) Å
b = 12.0339 (6) Å
c = 14.0667 (7) Å
α = 91.989 (1)°
β = 96.924 (1)°
γ = 102.996 (1)°
V = 1496.35 (13) Å^3
Z = 2
$F(000)$ = 948
D_x = 2.279 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9920 reflections
θ = 2.3–27.1°
μ = 4.24 mm^{-1}
T = 100 K
Irregular cut block, colourless
0.52 × 0.28 × 0.20 mm

Data collection

Bruker APEXI CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 8.3660 pixels mm^{-1}
phi and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2014)
T_{min} = 0.518, T_{max} = 0.746
19410 measured reflections
6594 independent reflections
6107 reflections with $I > 2\sigma(I)$
R_{int} = 0.023
θ_{max} = 27.1°, θ_{min} = 2.2°
h = −11→11
k = −15→15
l = −17→18

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.020
$wR(F^2)$ = 0.046
S = 1.09
6594 reflections
372 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0204P)^2 + 0.5553P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.69 e Å^{-3}
$\Delta\rho_{min}$ = −0.56 e Å^{-3}

Special details

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

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
I1	0.49323 (2)	0.32275 (2)	0.93280 (2)	0.02074 (5)
F1	0.21264 (18)	0.11841 (13)	0.85256 (11)	0.0253 (4)
N1	0.6063 (3)	0.52854 (19)	0.84397 (16)	0.0228 (5)
C1	0.5221 (3)	0.5211 (2)	0.75898 (19)	0.0203 (6)
H1	0.442392	0.455214	0.742023	0.024*
I2	0.02348 (2)	−0.12845 (2)	0.89212 (2)	0.01983 (5)
F2	0.23180 (18)	−0.14839 (13)	1.08815 (11)	0.0245 (3)
N2	0.7521 (3)	0.70747 (19)	0.80721 (16)	0.0228 (5)
C2	0.7169 (3)	0.6221 (2)	0.8639 (2)	0.0215 (6)
H2	0.776741	0.628608	0.924803	0.026*
I3	1.23452 (2)	0.97142 (2)	0.34507 (2)	0.02347 (5)
F3	0.47643 (17)	−0.00515 (14)	1.18660 (11)	0.0240 (3)
N3	−0.0078 (3)	0.5104 (2)	0.17456 (18)	0.0288 (6)
C3	0.6668 (3)	0.6985 (2)	0.7221 (2)	0.0229 (6)
H3	0.689419	0.757418	0.679287	0.027*
I4	0.70571 (2)	1.18190 (2)	0.39166 (2)	0.01903 (5)
F4	0.58522 (17)	0.20184 (14)	1.12306 (11)	0.0256 (4)
C4	0.5460 (3)	0.6057 (2)	0.69404 (19)	0.0176 (5)
F5	1.03550 (16)	1.15246 (12)	0.36927 (11)	0.0219 (3)
C5	0.4513 (3)	0.5954 (2)	0.6039 (2)	0.0203 (6)
F6	0.56017 (17)	0.91354 (14)	0.39466 (14)	0.0306 (4)
C6	0.3687 (3)	0.5801 (2)	0.5296 (2)	0.0199 (5)
F7	0.67827 (19)	0.72914 (14)	0.38368 (16)	0.0402 (5)
C7	0.2714 (3)	0.5631 (2)	0.44040 (19)	0.0192 (5)
F8	0.97066 (19)	0.75248 (14)	0.36268 (14)	0.0338 (4)
C8	0.2961 (3)	0.6402 (2)	0.36941 (19)	0.0200 (5)
H8	0.378242	0.705295	0.381043	0.024*
C9	0.2039 (3)	0.6246 (2)	0.2823 (2)	0.0203 (6)
H9	0.223836	0.678728	0.235226	0.024*
C10	0.0812 (3)	0.5295 (2)	0.2628 (2)	0.0202 (5)
C11	0.0557 (3)	0.4526 (2)	0.3355 (2)	0.0236 (6)
H11	−0.027198	0.387958	0.324617	0.028*
C12	0.1480 (3)	0.4689 (2)	0.4219 (2)	0.0239 (6)
H12	0.127870	0.415619	0.469581	0.029*
C13	0.0052 (4)	0.6021 (3)	0.1095 (2)	0.0473 (10)
H13A	−0.025722	0.666905	0.138573	0.071*
H13B	−0.060174	0.575019	0.048978	0.071*
H13C	0.110369	0.626297	0.097130	0.071*
C14	−0.1542 (3)	0.4298 (3)	0.1657 (3)	0.0378 (8)
H14A	−0.139652	0.353862	0.180913	0.057*
H14B	−0.204986	0.426549	0.099927	0.057*
H14C	−0.216383	0.454809	0.210428	0.057*
C15	0.4006 (3)	0.1649 (2)	0.98576 (19)	0.0193 (5)
C16	0.2772 (3)	0.0880 (2)	0.93589 (18)	0.0179 (5)
C17	0.2162 (3)	−0.0179 (2)	0.96755 (18)	0.0174 (5)

C18	0.2848 (3)	−0.0463 (2)	1.05331 (19)	0.0186 (5)
C19	0.4083 (3)	0.0263 (2)	1.10472 (18)	0.0176 (5)
C20	0.4647 (3)	0.1320 (2)	1.07115 (19)	0.0188 (5)
C21	1.0096 (3)	0.9535 (2)	0.36423 (18)	0.0171 (5)
C22	0.9461 (3)	1.0476 (2)	0.37107 (18)	0.0162 (5)
C23	0.7959 (3)	1.0382 (2)	0.38056 (18)	0.0167 (5)
C24	0.7064 (3)	0.9287 (2)	0.3845 (2)	0.0201 (6)
C25	0.7661 (3)	0.8338 (2)	0.3796 (2)	0.0246 (6)
C26	0.9165 (3)	0.8463 (2)	0.3691 (2)	0.0207 (6)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.02265 (9)	0.01765 (9)	0.01957 (9)	−0.00020 (7)	0.00227 (7)	0.00274 (7)
F1	0.0277 (9)	0.0261 (9)	0.0181 (8)	0.0016 (7)	−0.0051 (7)	0.0070 (7)
N1	0.0279 (13)	0.0181 (11)	0.0208 (12)	0.0025 (10)	0.0016 (10)	0.0021 (9)
C1	0.0222 (14)	0.0143 (12)	0.0224 (14)	0.0011 (10)	0.0016 (11)	−0.0002 (10)
I2	0.01730 (9)	0.02003 (9)	0.01945 (9)	0.00009 (7)	0.00027 (7)	−0.00083 (7)
F2	0.0278 (9)	0.0195 (8)	0.0241 (8)	−0.0002 (6)	0.0041 (7)	0.0074 (6)
N2	0.0216 (12)	0.0219 (12)	0.0209 (12)	−0.0008 (9)	−0.0009 (10)	−0.0006 (10)
C2	0.0225 (14)	0.0240 (14)	0.0178 (13)	0.0069 (11)	0.0000 (11)	−0.0014 (11)
I3	0.01585 (9)	0.02765 (10)	0.03083 (10)	0.00845 (7)	0.00992 (7)	0.00949 (8)
F3	0.0245 (8)	0.0328 (9)	0.0135 (7)	0.0048 (7)	−0.0003 (6)	0.0060 (7)
N3	0.0262 (13)	0.0250 (13)	0.0287 (13)	−0.0008 (10)	−0.0095 (11)	0.0027 (11)
C3	0.0248 (14)	0.0195 (13)	0.0227 (14)	0.0020 (11)	0.0021 (11)	0.0031 (11)
I4	0.02028 (9)	0.01707 (9)	0.02182 (9)	0.00801 (7)	0.00392 (7)	0.00142 (7)
F4	0.0234 (8)	0.0289 (9)	0.0181 (8)	−0.0044 (7)	−0.0027 (7)	−0.0003 (7)
C4	0.0180 (13)	0.0159 (12)	0.0190 (13)	0.0052 (10)	0.0018 (10)	−0.0016 (10)
F5	0.0188 (8)	0.0159 (7)	0.0305 (9)	0.0005 (6)	0.0071 (7)	0.0045 (6)
C5	0.0225 (14)	0.0145 (12)	0.0236 (14)	0.0043 (10)	0.0027 (11)	−0.0004 (11)
F6	0.0127 (8)	0.0240 (9)	0.0551 (12)	0.0025 (6)	0.0081 (8)	0.0028 (8)
C6	0.0207 (13)	0.0178 (13)	0.0222 (14)	0.0080 (10)	0.0021 (11)	−0.0034 (11)
F7	0.0230 (9)	0.0150 (8)	0.0807 (15)	−0.0028 (7)	0.0133 (9)	0.0034 (9)
C7	0.0176 (13)	0.0199 (13)	0.0211 (13)	0.0081 (10)	0.0004 (11)	−0.0032 (11)
F8	0.0280 (9)	0.0184 (8)	0.0603 (12)	0.0122 (7)	0.0135 (9)	0.0039 (8)
C8	0.0162 (13)	0.0177 (13)	0.0238 (14)	0.0012 (10)	0.0009 (11)	−0.0037 (11)
C9	0.0195 (13)	0.0187 (13)	0.0222 (14)	0.0026 (10)	0.0034 (11)	0.0019 (11)
C10	0.0182 (13)	0.0196 (13)	0.0225 (14)	0.0064 (10)	−0.0023 (11)	−0.0016 (11)
C11	0.0206 (14)	0.0186 (13)	0.0270 (15)	−0.0023 (11)	−0.0020 (12)	0.0013 (11)
C12	0.0274 (15)	0.0175 (13)	0.0259 (15)	0.0032 (11)	0.0023 (12)	0.0031 (11)
C13	0.057 (2)	0.041 (2)	0.0320 (18)	−0.0005 (17)	−0.0209 (17)	0.0090 (16)
C14	0.0239 (16)	0.0400 (19)	0.0421 (19)	0.0014 (14)	−0.0120 (14)	−0.0023 (15)
C15	0.0206 (13)	0.0180 (13)	0.0188 (13)	0.0020 (10)	0.0052 (11)	0.0017 (10)
C16	0.0189 (13)	0.0228 (13)	0.0127 (12)	0.0072 (11)	0.0004 (10)	0.0006 (10)
C17	0.0147 (12)	0.0193 (13)	0.0167 (13)	0.0014 (10)	0.0017 (10)	−0.0020 (10)
C18	0.0191 (13)	0.0188 (13)	0.0181 (13)	0.0026 (10)	0.0064 (10)	0.0026 (10)
C19	0.0173 (13)	0.0235 (14)	0.0125 (12)	0.0051 (10)	0.0026 (10)	0.0021 (10)
C20	0.0166 (13)	0.0218 (13)	0.0158 (13)	0.0001 (10)	0.0017 (10)	−0.0018 (10)

C21	0.0126 (12)	0.0230 (13)	0.0168 (13)	0.0052 (10)	0.0041 (10)	0.0036 (10)
C22	0.0166 (12)	0.0167 (12)	0.0147 (12)	0.0022 (10)	0.0020 (10)	0.0017 (10)
C23	0.0166 (12)	0.0166 (12)	0.0184 (13)	0.0061 (10)	0.0034 (10)	0.0003 (10)
C24	0.0123 (12)	0.0212 (13)	0.0264 (14)	0.0025 (10)	0.0038 (11)	0.0014 (11)
C25	0.0205 (14)	0.0151 (13)	0.0370 (17)	0.0007 (11)	0.0053 (12)	0.0018 (12)
C26	0.0233 (14)	0.0149 (13)	0.0256 (14)	0.0068 (11)	0.0052 (11)	0.0031 (11)

Geometric parameters (Å, º)

I1—C15	2.099 (3)	F8—C26	1.336 (3)
F1—C16	1.348 (3)	C8—C9	1.382 (4)
N1—C2	1.330 (3)	C8—H8	0.9500
N1—C1	1.331 (3)	C9—C10	1.405 (4)
C1—C4	1.390 (4)	C9—H9	0.9500
C1—H1	0.9500	C10—C11	1.408 (4)
I2—C17	2.099 (2)	C11—C12	1.375 (4)
F2—C18	1.347 (3)	C11—H11	0.9500
N2—C2	1.328 (3)	C12—H12	0.9500
N2—C3	1.335 (4)	C13—H13A	0.9800
C2—H2	0.9500	C13—H13B	0.9800
I3—C21	2.074 (2)	C13—H13C	0.9800
F3—C19	1.350 (3)	C14—H14A	0.9800
N3—C10	1.382 (3)	C14—H14B	0.9800
N3—C13	1.451 (4)	C14—H14C	0.9800
N3—C14	1.456 (4)	C15—C20	1.382 (4)
C3—C4	1.392 (4)	C15—C16	1.386 (4)
C3—H3	0.9500	C16—C17	1.383 (4)
I4—C23	2.086 (2)	C17—C18	1.382 (4)
F4—C20	1.343 (3)	C18—C19	1.371 (4)
C4—C5	1.432 (4)	C19—C20	1.383 (4)
F5—C22	1.344 (3)	C21—C26	1.387 (4)
C5—C6	1.196 (4)	C21—C22	1.389 (4)
F6—C24	1.336 (3)	C22—C23	1.378 (4)
C6—C7	1.428 (4)	C23—C24	1.394 (4)
F7—C25	1.341 (3)	C24—C25	1.376 (4)
C7—C8	1.391 (4)	C25—C26	1.377 (4)
C7—C12	1.401 (4)		
C2—N1—C1	116.2 (2)	N3—C14—H14A	109.5
N1—C1—C4	122.7 (2)	N3—C14—H14B	109.5
N1—C1—H1	118.7	H14A—C14—H14B	109.5
C4—C1—H1	118.7	N3—C14—H14C	109.5
C2—N2—C3	116.5 (2)	H14A—C14—H14C	109.5
N2—C2—N1	126.5 (3)	H14B—C14—H14C	109.5
N2—C2—H2	116.7	C20—C15—C16	117.2 (2)
N1—C2—H2	116.7	C20—C15—I1	120.76 (19)
C10—N3—C13	118.6 (2)	C16—C15—I1	122.0 (2)
C10—N3—C14	118.7 (3)	F1—C16—C17	118.4 (2)

C13—N3—C14	116.1 (3)	F1—C16—C15	118.2 (2)
N2—C3—C4	122.2 (3)	C17—C16—C15	123.4 (2)
N2—C3—H3	118.9	C18—C17—C16	116.9 (2)
C4—C3—H3	118.9	C18—C17—I2	121.17 (19)
C1—C4—C3	115.8 (2)	C16—C17—I2	121.86 (19)
C1—C4—C5	121.1 (2)	F2—C18—C19	118.1 (2)
C3—C4—C5	123.1 (2)	F2—C18—C17	120.1 (2)
C6—C5—C4	176.0 (3)	C19—C18—C17	121.8 (2)
C5—C6—C7	179.2 (3)	F3—C19—C18	120.7 (2)
C8—C7—C12	117.9 (2)	F3—C19—C20	119.9 (2)
C8—C7—C6	120.9 (2)	C18—C19—C20	119.4 (2)
C12—C7—C6	121.2 (3)	F4—C20—C15	120.5 (2)
C9—C8—C7	121.6 (2)	F4—C20—C19	118.3 (2)
C9—C8—H8	119.2	C15—C20—C19	121.2 (2)
C7—C8—H8	119.2	C26—C21—C22	117.7 (2)
C8—C9—C10	120.7 (3)	C26—C21—I3	120.75 (19)
C8—C9—H9	119.6	C22—C21—I3	121.58 (19)
C10—C9—H9	119.6	F5—C22—C23	118.5 (2)
N3—C10—C9	121.2 (3)	F5—C22—C21	118.6 (2)
N3—C10—C11	121.4 (2)	C23—C22—C21	122.9 (2)
C9—C10—C11	117.4 (2)	C22—C23—C24	117.4 (2)
C12—C11—C10	121.5 (2)	C22—C23—I4	121.67 (19)
C12—C11—H11	119.3	C24—C23—I4	120.92 (19)
C10—C11—H11	119.3	F6—C24—C25	118.3 (2)
C11—C12—C7	120.9 (3)	F6—C24—C23	120.6 (2)
C11—C12—H12	119.6	C25—C24—C23	121.2 (2)
C7—C12—H12	119.6	F7—C25—C24	120.3 (2)
N3—C13—H13A	109.5	F7—C25—C26	119.8 (2)
N3—C13—H13B	109.5	C24—C25—C26	119.8 (2)
H13A—C13—H13B	109.5	F8—C26—C25	118.5 (2)
N3—C13—H13C	109.5	F8—C26—C21	120.5 (2)
H13A—C13—H13C	109.5	C25—C26—C21	121.0 (2)
H13B—C13—H13C	109.5		