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

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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, \( \text{C}_{14}\text{H}_{13}\text{N}_{3}/\text{C}_{6}\text{F}_{4}\text{I}_{2} \). In the extended structure, two unique \( \text{C}−\text{I}⋯\text{N} \) halogen bonds from one of the 1,2,3,5-tetrafluoro-4,6-diiodobenzene molecules to the pyrimidine \( \text{N} \) atoms of the 5-[[4-(dimethylamino)phenyl]ethynyl]pyrimidine molecule generate \{110\} chains and layers of these chains are \( \pi \)-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 \( \text{C}−\text{I}⋯\pi(\text{alkyne}) \) contacts.

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, \( \text{C}_{14}\text{H}_{13}\text{N}_{3} \) (APEP) and 1,2,3,5-tetrafluoro-4,6-diiodobenzene, \( \text{C}_{6}\text{F}_{4}\text{I}_{2} \),
(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 a zigzag alternating halogen-bonded chain, shown in Fig. 2, have separations of I1···N1 and I2···N2i = 2.853 (2) and 2.901 (2) Å and angles C15—I1···N1 and C17—I2···N2i = 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
neighboring alkyne group with $14 \cdots C_6^{ii}$ and $14 \cdots CS^{ii}$ [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 $1 \cdots F$ contacts to two neighboring 13DIFB molecules with $13 \cdots F_6^{iii}$ and $13 \cdots F_3^{iv}$ 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.

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Table 1
Experimental details.

| Crystal data | C_{14}H_{13}N_{3}\cdot 2C_{6}F_{4}I_{2} |
|--------------|----------------------------------|
| Chemical formula | 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) |
| $\alpha$, $\beta$, $\gamma$ (°) | 91.989 (1), 96.924 (1), 102.996 (1) |
| $V$ (Å³) | 1496.35 (13) |
| $Z$ | 2 |
| Radiation type | Mo $K\alpha$ |
| $\mu$ (mm$^{-1}$) | 4.24 |
| Crystal size (mm) | 0.52 $\times$ 0.28 $\times$ 0.20 |

| Data collection | Bruker APEXI CCD |
|-----------------|-----------------|
| Diffractometer | 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 | Bruker APEXI CCD |
|-----------------|-----------------|
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, $S$ | 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, 2015a), SHELXL2018/3 (Sheldrick, 2015b), and X-SEED (Barbour, 2020).

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full crystallographic data

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

Crystal data
C14H13N3·2C6F4I2  Z = 2
Mr = 1026.99  F(000) = 948
Triclinic, P  Dm = 2.279 Mg m−3
a = 9.1574 (5) Å  Mo Kα radiation, λ = 0.71073 Å
b = 12.0339 (6) Å  Cell parameters from 9920 reflections
θ = 2.3–27.1°  θmax = 27.1°, θmin = 2.2°
c = 14.0667 (7) Å
α = 91.989 (1)°  h = −11→11
β = 96.924 (1)°  k = −15→15
γ = 102.996 (1)°  l = −17→18
V = 1496.35 (13) Å3

Data collection
Bruker APEXI CCD diffractometer 19410 measured reflections
Radiation source: fine-focus sealed tube 6594 independent reflections
Graphite monochromator 6107 reflections with I > 2σ(I)
Detector resolution: 8.3660 pixels mm−1 θmax = 27.1°, θmin = 2.2°
phi and ω scans
Absorption correction: multi-scan
(SADABS; Bruker, 2014)
Tmin = 0.518, Tmax = 0.746

Refinement
Refinement on F²
Least-squares matrix: full
R[F² > 2σ(F²)] = 0.020
wR(F²) = 0.046  Hydrogen site location: inferred from
S = 1.09  neighbour sites
6594 reflections  H-atom parameters constrained
372 parameters
0 restraints
Primary atom site location: dual

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)  |
| N4| 0.5460 (3)  | 0.6057 (2)  | 0.69404 (19)| 0.0176 (5)  |
| C4| 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)  |
| F5| 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)  |
|   | \(U_{11}^1\) | \(U_{22}^1\) | \(U_{33}^1\) | \(U_{12}^1\) | \(U_{13}^1\) | \(U_{23}^1\) |
|---|---|---|---|---|---|---|
| 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) | 0.00207 (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) |
### Geometric parameters (Å, °)

|        |        |        |        |        |        |        |        |
|--------|--------|--------|--------|--------|--------|--------|--------|
| 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—C12| 0.9500  |
| N2—C3  | 1.335 (4) | C13—H13A| 0.9800 |
| C2—H2  | 0.9500  | C13—H13B| 0.9800 |
| C3—C4  | 2.074 (2) | C13—H13C| 0.9800 |
| C3—C6  | 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) |
| C4—C5  | 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)  C15—C20—C19 121.2 (2)
C8—C7—C6 120.9 (2)  C26—C21—C22 117.7 (2)
C12—C7—C6 121.2 (3)  C26—C21—I3 120.75 (19)
C9—C8—C7 121.6 (2)  C26—C21—I3 121.58 (19)
C9—C8—H8 119.2  C15—C20—C19 121.2 (2)
C7—C8—H8 119.2  C15—C20—C19 121.2 (2)
C8—C9—C10 120.7 (3)  C26—C21—I3 120.75 (19)
C8—C9—H9 119.6  C26—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—C24 117.4 (2)
C12—C11—H11 119.3  C22—C23—I4 121.67 (19)
C10—C11—H11 119.3  C24—C23—I4 120.92 (19)
C11—C12—C7 120.9 (3)  F6—C24—C25 118.3 (2)
C11—C12—H12 119.6  F6—C24—C23 120.6 (2)
C7—C12—H12 119.6  C25—C24—C23 121.2 (2)
N3—C13—H13A 109.5  F7—C25—C24 120.3 (2)
N3—C13—H13B 109.5  F7—C25—C26 119.8 (2)
H13A—C13—H13B 109.5  C24—C25—C26 119.8 (2)
N3—C13—H13C 109.5  F8—C26—C25 118.5 (2)
H13A—C13—H13C 109.5  F8—C26—C21 120.5 (2)
H13B—C13—H13C 109.5  C25—C26—C21 121.0 (2)