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# 5-Bromo-2-iodo-1,3-dimethylbenzene

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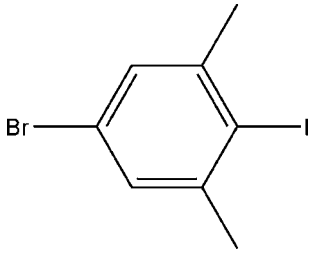
Key indicators: single-crystal X-ray study; $T$ = 294 K; mean $\sigma$(C–C) = 0.013 Å; $R$ factor = 0.059; $wR$ factor = 0.133; data-to-parameter ratio = 20.2.

The asymmetric unit of the title compound, $C_8H_8BrI$, contains three independent molecules. In each molecule, the Br, I and C atoms of the methyl groups lie in the benzene ring plane. Intramolecular C—H···I hydrogen bonds result in the formation of three planar five-membered rings, which are nearly coplanar with the adjacent rings.

## Related literature

For general background, see: Hu *et al.* (2001). For bond-length data, see: Allen *et al.* (1987).




## Experimental

### Crystal data

$C_8H_8BrI$
$M_r$ = 310.94
Triclinic, $P\overline{1}$
$a$ = 10.282 (2) Å
$b$ = 11.314 (2) Å
$c$ = 12.951 (3) Å
$\alpha$ = 69.27 (3)°
$\beta$ = 89.11 (3)°
$\gamma$ = 83.70 (3)°
$V$ = 1400.1 (6) Å$^3$
$Z$ = 6
Mo $K\alpha$ radiation
$\mu$ = 7.64 mm$^{-1}$
$T$ = 294 (2) K
0.10 × 0.10 × 0.10 mm

### Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: $\psi$ scan (North *et al.*, 1968)
$T_{min}$ = 0.466, $T_{max}$ = 0.466
5802 measured reflections
5481 independent reflections
2809 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.042
3 standard reflections
frequency: 120 min
intensity decay: none

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.133
$S$ = 1.06
5481 reflections
271 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.76 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.72 e Å$^{-3}$

**Table 1**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C1—H1$A$···I1 | 0.96 | 2.70 | 3.316 (11) | 122 |
| C10—H10$A$···I2 | 0.96 | 2.70 | 3.303 (10) | 122 |
| C18—H18$A$···I3 | 0.96 | 2.63 | 3.252 (10) | 123 |

Data collection: *CAD-4 Software* (Enraf–Nonius, 1985); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXTL* (Bruker, 2000).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2404).

## References

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# supporting information

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## 5-Bromo-2-iodo-1,3-dimethylbenzene

**Rui Liu, Yu-Hao Li, Wei Luo, Shan Liu and Hong-Jun Zhu**

### S1. Comment

The title compound, (I), contains two different halogen groups, which can react with different groups to prepare various function organic compounds by the different reaction activity of Br and I. It is a kind of aromatic organic intermediate that can be used for many fields such as aromatic conductive polymer, organometallic chemistry (Hu *et al.*, 2001). We herein report its crystal structure.

The asymmetric unit of (I) contains three independent molecules (Fig. 1), in which the bond lengths and angles (Table 1) are within normal ranges (Allen *et al.*, 1987). The Br, I and C atoms of the methyl groups lie in the benzene ring planes. The intramolecular C—H···I hydrogen bonds (Table 2) result in the formations of three planar five-membered rings; B (I1/H1A/C1/C4/C5), D (I2/H10A/C10—C12) and F (I3/H18A/C18—C20). Rings A (C3—C8), C (C11—C16) and E (C19—C24) are, of course, planar and the dihedral angles between them are A/B = 1.29 (3)°, C/D = 1.73 (3)° and E/F = 1.77 (2)°. So, the adjacent rings are also nearly co-planar.

As can be seen from the packing diagram, (Fig. 2), the molecules are stacked along the *b* axis. The $\pi$-$\pi$ interactions of benzene rings with a face-to-face stacking distance of 3.636 Å are also found.

### S2. Experimental

For the preparation of the title compound, a mixture of 4-bromo-2,6-dimethyl- aniline (4.0 g, 20 mmol), concentrated sulfuric acid (40 mmol, 2.24 ml) and water (100 ml) was stirred in an ice bath. When the mixture was below 278 K, the solution of sodium nitrite (1.75 g, 25 mmol) and water (100 ml) was added dropwise. Then, the mixture was added to a solution of KI (3.3 g, 20 mmol) and water (50 ml) with stirring. The solid residue was extracted with boiling hexane (40 ml) and hexane was distilled off. The product was recrystallized from ethanol. The crystals were obtained by dissolving (I) in ethanol (20 ml) and evaporating ethanol slowly at room temperature for about 10 d.

### S3. Refinement

H atoms were positioned geometrically, with C—H = 0.93 and 0.96 Å for aromatic and methyl H, respectively, and constrained to ride on their parent atoms, with $U_{iso}$(H) = $xU_{eq}$(C), where $x$ = 1.5 for methyl H, and $x$ = 1.2 for aromatic H atoms.

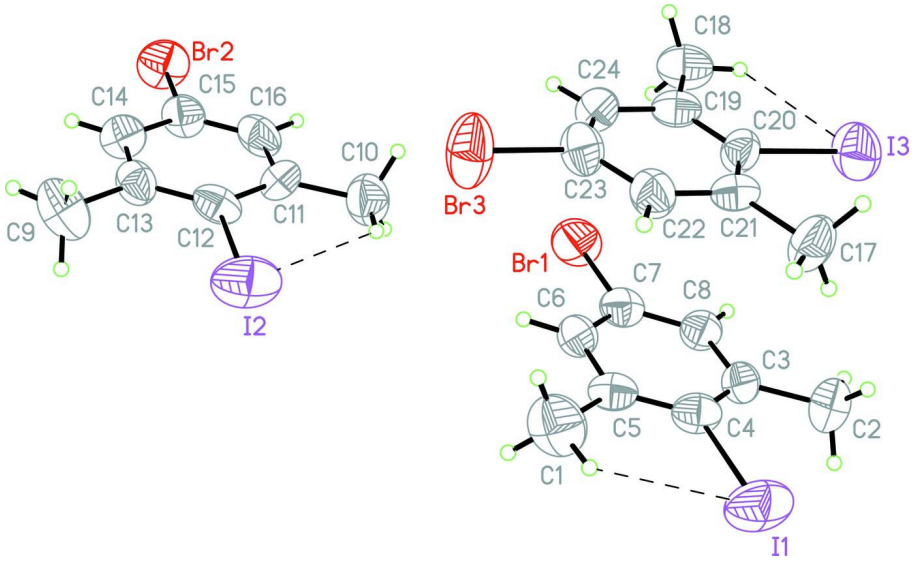


**Figure 1**

The molecular structure of the title molecule with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. Hydrogen bonds are shown as dashed lines.

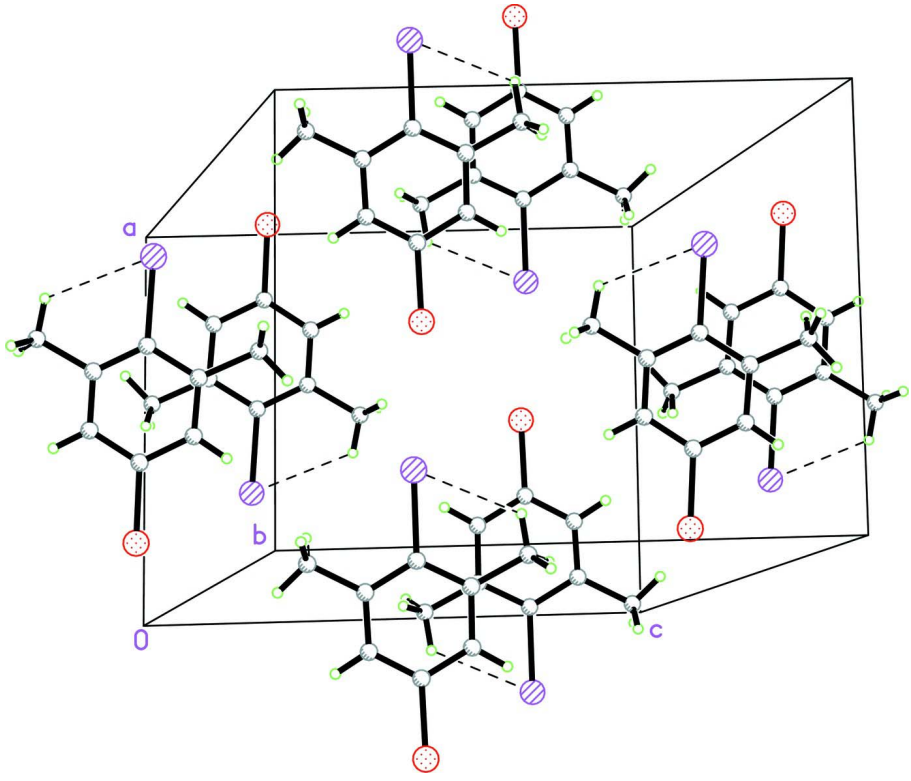


**Figure 2**

A packing diagram of (I). Hydrogen bonds are shown as dashed lines.

## 5-Bromo-2-iodo-1,3-dimethylbenzene

*Crystal data*

$C_8H_8BrI$
$M_r = 310.94$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 10.282$ (2) Å
$b = 11.314$ (2) Å
$c = 12.951$ (3) Å
$\alpha = 69.27$ (3)°
$\beta = 89.11$ (3)°
$\gamma = 83.70$ (3)°
$V = 1400.1$ (6) Å$^3$
$Z = 6$
$F(000) = 864$
$D_x = 2.213$ Mg m$^{-3}$
Melting point: 307 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 25 reflections
$\theta = 10$–13°
$\mu = 7.64$ mm$^{-1}$
$T = 294$ K
Block, colorless
0.10 × 0.10 × 0.10 mm

*Data collection*

Enraf–Nonius CAD-4 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega/2\theta$ scans
Absorption correction: $\psi$ scan (North *et al.*, 1968)
$T_{min} = 0.466$, $T_{max} = 0.466$
5802 measured reflections
5481 independent reflections
2809 reflections with $I > 2\sigma(I)$
$R_{int} = 0.042$
$\theta_{max} = 26.0°$, $\theta_{min} = 1.7°$
$h = -12 \rightarrow 12$
$k = -12 \rightarrow 13$
$l = 0 \rightarrow 15$
3 standard reflections every 120 min
intensity decay: none

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.059$
$wR(F^2) = 0.133$
$S = 1.06$
5481 reflections
271 parameters
0 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
$w = 1/[\sigma^2(F_o^2) + (0.050P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.76$ e Å$^{-3}$
$\Delta\rho_{min} = -0.72$ 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)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| I1 | 0.26694 (7) | 0.30503 (8) | 0.13847 (7) | 0.0898 (3) |
| I2 | 0.77050 (7) | 0.30518 (8) | 0.67167 (8) | 0.0901 (3) |

| | | | | |
|---|---|---|---|---|
| I3 | 0.74437 (8) | −0.00666 (8) | 0.03475 (6) | 0.0798 (3) |
| Br1 | 0.90853 (10) | 0.36368 (12) | 0.15368 (10) | 0.0785 (4) |
| Br2 | 1.40828 (10) | 0.38917 (12) | 0.62860 (10) | 0.0782 (4) |
| Br3 | 0.75298 (12) | 0.00304 (14) | 0.54991 (9) | 0.0891 (4) |
| C1 | 0.4494 (11) | 0.3088 (11) | 0.3459 (8) | 0.086 (4) |
| H1A | 0.3588 | 0.3038 | 0.3332 | 0.129* |
| H1B | 0.4573 | 0.3817 | 0.3661 | 0.129* |
| H1C | 0.4847 | 0.2332 | 0.4046 | 0.129* |
| C2 | 0.4834 (10) | 0.3314 (10) | −0.0588 (8) | 0.075 (3) |
| H2A | 0.5506 | 0.3421 | −0.1127 | 0.113* |
| H2B | 0.4144 | 0.3999 | −0.0856 | 0.113* |
| H2C | 0.4491 | 0.2520 | −0.0459 | 0.113* |
| C3 | 0.5415 (9) | 0.3319 (8) | 0.0497 (7) | 0.050 (2) |
| C4 | 0.4687 (8) | 0.3180 (8) | 0.1459 (8) | 0.051 (2) |
| C5 | 0.5241 (9) | 0.3211 (8) | 0.2418 (8) | 0.051 (2) |
| C6 | 0.6560 (9) | 0.3308 (8) | 0.2456 (7) | 0.048 (2) |
| H6A | 0.6955 | 0.3292 | 0.3103 | 0.058* |
| C7 | 0.7295 (9) | 0.3430 (8) | 0.1529 (8) | 0.051 (2) |
| C8 | 0.6722 (9) | 0.3438 (8) | 0.0557 (7) | 0.054 (2) |
| H8A | 0.7234 | 0.3525 | −0.0059 | 0.064* |
| C9 | 0.9707 (9) | 0.3346 (9) | 0.8546 (8) | 0.073 (3) |
| H9A | 1.0325 | 0.3445 | 0.9050 | 0.109* |
| H9B | 0.9362 | 0.2545 | 0.8875 | 0.109* |
| H9C | 0.9006 | 0.4024 | 0.8382 | 0.109* |
| C10 | 0.9673 (10) | 0.3129 (10) | 0.4659 (8) | 0.070 (3) |
| H10A | 0.8774 | 0.2996 | 0.4818 | 0.105* |
| H10B | 1.0117 | 0.2411 | 0.4518 | 0.105* |
| H10C | 0.9714 | 0.3883 | 0.4020 | 0.105* |
| C11 | 1.0326 (9) | 0.3283 (8) | 0.5637 (7) | 0.048 (2) |
| C12 | 0.9713 (9) | 0.3258 (8) | 0.6616 (8) | 0.053 (2) |
| C13 | 1.0378 (10) | 0.3385 (8) | 0.7501 (7) | 0.053 (2) |
| C14 | 1.1692 (9) | 0.3532 (8) | 0.7396 (7) | 0.055 (3) |
| H14A | 1.2160 | 0.3591 | 0.7982 | 0.066* |
| C15 | 1.2316 (9) | 0.3594 (9) | 0.6444 (8) | 0.055 (2) |
| C16 | 1.1665 (9) | 0.3466 (8) | 0.5572 (8) | 0.058 (3) |
| H16A | 1.2113 | 0.3502 | 0.4934 | 0.070* |
| C17 | 0.5044 (9) | −0.0355 (10) | 0.2075 (8) | 0.068 (3) |
| H17A | 0.4380 | −0.0454 | 0.2619 | 0.102* |
| H17B | 0.5147 | −0.1090 | 0.1861 | 0.102* |
| H17C | 0.4790 | 0.0389 | 0.1440 | 0.102* |
| C18 | 0.9888 (9) | 0.0237 (10) | 0.1763 (8) | 0.072 (3) |
| H18A | 0.9751 | 0.0152 | 0.1062 | 0.108* |
| H18B | 1.0562 | −0.0406 | 0.2178 | 0.108* |
| H18C | 1.0150 | 0.1062 | 0.1647 | 0.108* |
| C19 | 0.8630 (9) | 0.0082 (7) | 0.2397 (7) | 0.047 (2) |
| C20 | 0.7480 (9) | −0.0034 (8) | 0.1963 (7) | 0.048 (2) |
| C21 | 0.6322 (8) | −0.0216 (8) | 0.2552 (7) | 0.049 (2) |
| C22 | 0.6335 (9) | −0.0184 (9) | 0.3618 (8) | 0.058 (3) |

| | | | | |
|---|---|---|---|---|
| H22A | 0.5577 | −0.0273 | 0.4028 | 0.070* |
| C23 | 0.7527 (10) | −0.0012 (9) | 0.4076 (7) | 0.056 (3) |
| C24 | 0.8632 (8) | 0.0125 (8) | 0.3466 (7) | 0.047 (2) |
| H24A | 0.9400 | 0.0249 | 0.3765 | 0.056* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| I1 | 0.0426 (4) | 0.0927 (6) | 0.1290 (8) | −0.0114 (4) | 0.0064 (4) | −0.0322 (5) |
| I2 | 0.0441 (4) | 0.0918 (6) | 0.1307 (7) | −0.0115 (4) | 0.0106 (4) | −0.0342 (5) |
| I3 | 0.0972 (6) | 0.0946 (6) | 0.0534 (4) | −0.0077 (5) | 0.0096 (4) | −0.0345 (4) |
| Br1 | 0.0446 (6) | 0.0942 (9) | 0.1125 (10) | −0.0111 (6) | 0.0070 (6) | −0.0554 (7) |
| Br2 | 0.0446 (6) | 0.0999 (9) | 0.0907 (9) | −0.0137 (6) | 0.0124 (6) | −0.0333 (7) |
| Br3 | 0.0792 (8) | 0.1468 (12) | 0.0609 (7) | −0.0395 (8) | 0.0175 (6) | −0.0538 (8) |
| C1 | 0.085 (9) | 0.101 (9) | 0.076 (8) | −0.019 (7) | 0.026 (7) | −0.034 (7) |
| C2 | 0.077 (8) | 0.089 (8) | 0.066 (7) | −0.011 (6) | −0.015 (6) | −0.034 (6) |
| C3 | 0.051 (6) | 0.045 (6) | 0.058 (6) | −0.006 (4) | −0.005 (5) | −0.023 (5) |
| C4 | 0.041 (6) | 0.048 (6) | 0.061 (6) | −0.005 (4) | 0.009 (5) | −0.014 (5) |
| C5 | 0.043 (5) | 0.048 (6) | 0.057 (6) | 0.002 (4) | 0.008 (5) | −0.014 (5) |
| C6 | 0.049 (6) | 0.055 (6) | 0.041 (5) | −0.004 (5) | 0.007 (4) | −0.019 (5) |
| C7 | 0.045 (6) | 0.038 (5) | 0.069 (7) | −0.010 (4) | 0.003 (5) | −0.018 (5) |
| C8 | 0.042 (6) | 0.069 (7) | 0.053 (6) | 0.000 (5) | 0.005 (5) | −0.028 (5) |
| C9 | 0.070 (7) | 0.084 (8) | 0.078 (7) | −0.039 (6) | 0.047 (6) | −0.040 (6) |
| C10 | 0.070 (7) | 0.081 (8) | 0.072 (7) | −0.014 (6) | −0.002 (6) | −0.039 (6) |
| C11 | 0.042 (5) | 0.053 (6) | 0.043 (5) | −0.005 (4) | −0.007 (4) | −0.010 (4) |
| C12 | 0.043 (6) | 0.047 (6) | 0.071 (7) | −0.006 (4) | 0.016 (5) | −0.026 (5) |
| C13 | 0.067 (7) | 0.048 (6) | 0.043 (6) | −0.008 (5) | 0.010 (5) | −0.017 (5) |
| C14 | 0.045 (6) | 0.062 (6) | 0.051 (6) | −0.011 (5) | 0.014 (5) | −0.012 (5) |
| C15 | 0.036 (5) | 0.071 (7) | 0.062 (6) | −0.010 (5) | 0.013 (5) | −0.029 (5) |
| C16 | 0.064 (7) | 0.059 (6) | 0.054 (6) | −0.002 (5) | 0.020 (5) | −0.024 (5) |
| C17 | 0.049 (6) | 0.093 (8) | 0.068 (7) | −0.014 (6) | −0.009 (5) | −0.033 (6) |
| C18 | 0.047 (6) | 0.082 (8) | 0.084 (8) | 0.001 (5) | 0.018 (6) | −0.030 (6) |
| C19 | 0.045 (6) | 0.034 (5) | 0.050 (6) | −0.002 (4) | 0.009 (4) | −0.002 (4) |
| C20 | 0.050 (6) | 0.056 (6) | 0.037 (5) | −0.003 (5) | −0.003 (4) | −0.017 (4) |
| C21 | 0.038 (5) | 0.048 (6) | 0.058 (6) | 0.005 (4) | 0.000 (5) | −0.015 (5) |
| C22 | 0.056 (6) | 0.068 (7) | 0.058 (6) | −0.004 (5) | 0.005 (5) | −0.032 (5) |
| C23 | 0.067 (7) | 0.061 (6) | 0.043 (6) | −0.017 (5) | 0.012 (5) | −0.021 (5) |
| C24 | 0.039 (5) | 0.061 (6) | 0.038 (5) | −0.007 (4) | 0.009 (4) | −0.015 (4) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| I1—C4 | 2.102 (9) | C10—H10C | 0.9600 |
| Br1—C7 | 1.881 (9) | C11—C12 | 1.399 (12) |
| C1—C5 | 1.513 (13) | C11—C16 | 1.412 (12) |
| C1—H1A | 0.9600 | C12—C13 | 1.401 (12) |
| C1—H1B | 0.9600 | C13—C14 | 1.378 (12) |
| C1—H1C | 0.9600 | C14—C15 | 1.364 (12) |
| C2—C3 | 1.537 (11) | C14—H14A | 0.9300 |

| | | | |
|---|---|---|---|
| C2—H2A | 0.9600 | C15—C16 | 1.380 (12) |
| C2—H2B | 0.9600 | C16—H16A | 0.9300 |
| C2—H2C | 0.9600 | I3—C20 | 2.106 (8) |
| C3—C8 | 1.372 (11) | Br3—C23 | 1.861 (9) |
| C3—C4 | 1.413 (12) | C17—C21 | 1.508 (11) |
| C4—C5 | 1.387 (12) | C17—H17A | 0.9600 |
| C5—C6 | 1.376 (12) | C17—H17B | 0.9600 |
| C6—C7 | 1.382 (11) | C17—H17C | 0.9600 |
| C6—H6A | 0.9300 | C18—C19 | 1.515 (11) |
| C7—C8 | 1.395 (12) | C18—H18A | 0.9600 |
| C8—H8A | 0.9300 | C18—H18B | 0.9600 |
| I2—C12 | 2.100 (9) | C18—H18C | 0.9600 |
| Br2—C15 | 1.879 (9) | C19—C20 | 1.356 (11) |
| C9—C13 | 1.498 (12) | C19—C24 | 1.402 (11) |
| C9—H9A | 0.9600 | C20—C21 | 1.399 (11) |
| C9—H9B | 0.9600 | C21—C22 | 1.394 (12) |
| C9—H9C | 0.9600 | C22—C23 | 1.431 (12) |
| C10—C11 | 1.515 (12) | C22—H22A | 0.9300 |
| C10—H10A | 0.9600 | C23—C24 | 1.365 (11) |
| C10—H10B | 0.9600 | C24—H24A | 0.9300 |

| | | | |
|---|---|---|---|
| C5—C1—H1A | 109.5 | C11—C12—C13 | 122.8 (9) |
| C5—C1—H1B | 109.5 | C11—C12—I2 | 117.3 (7) |
| H1A—C1—H1B | 109.5 | C13—C12—I2 | 119.9 (7) |
| C5—C1—H1C | 109.5 | C14—C13—C12 | 118.1 (8) |
| H1A—C1—H1C | 109.5 | C14—C13—C9 | 119.9 (9) |
| H1B—C1—H1C | 109.5 | C12—C13—C9 | 122.0 (9) |
| C3—C2—H2A | 109.5 | C15—C14—C13 | 120.8 (9) |
| C3—C2—H2B | 109.5 | C15—C14—H14A | 119.6 |
| H2A—C2—H2B | 109.5 | C13—C14—H14A | 119.6 |
| C3—C2—H2C | 109.5 | C14—C15—C16 | 121.2 (9) |
| H2A—C2—H2C | 109.5 | C14—C15—Br2 | 120.2 (7) |
| H2B—C2—H2C | 109.5 | C16—C15—Br2 | 118.6 (7) |
| C8—C3—C4 | 117.2 (8) | C15—C16—C11 | 120.7 (8) |
| C8—C3—C2 | 118.9 (9) | C15—C16—H16A | 119.6 |
| C4—C3—C2 | 123.9 (9) | C11—C16—H16A | 119.6 |
| C5—C4—C3 | 122.3 (8) | C21—C17—H17A | 109.5 |
| C5—C4—I1 | 119.4 (7) | C21—C17—H17B | 109.5 |
| C3—C4—I1 | 118.2 (7) | H17A—C17—H17B | 109.5 |
| C6—C5—C4 | 119.0 (9) | C21—C17—H17C | 109.5 |
| C6—C5—C1 | 116.9 (9) | H17A—C17—H17C | 109.5 |
| C4—C5—C1 | 124.0 (9) | H17B—C17—H17C | 109.5 |
| C5—C6—C7 | 119.7 (9) | C19—C18—H18A | 109.5 |
| C5—C6—H6A | 120.2 | C19—C18—H18B | 109.5 |
| C7—C6—H6A | 120.2 | H18A—C18—H18B | 109.5 |
| C6—C7—C8 | 120.9 (8) | C19—C18—H18C | 109.5 |
| C6—C7—Br1 | 120.6 (7) | H18A—C18—H18C | 109.5 |
| C8—C7—Br1 | 118.4 (7) | H18B—C18—H18C | 109.5 |

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| C3—C8—C7 | 120.9 (9) | C20—C19—C24 | 118.0 (8) |
| C3—C8—H8A | 119.5 | C20—C19—C18 | 123.2 (9) |
| C7—C8—H8A | 119.5 | C24—C19—C18 | 118.7 (8) |
| C13—C9—H9A | 109.5 | C19—C20—C21 | 123.6 (8) |
| C13—C9—H9B | 109.5 | C19—C20—I3 | 118.8 (7) |
| H9A—C9—H9B | 109.5 | C21—C20—I3 | 117.5 (6) |
| C13—C9—H9C | 109.5 | C22—C21—C20 | 117.8 (8) |
| H9A—C9—H9C | 109.5 | C22—C21—C17 | 118.3 (8) |
| H9B—C9—H9C | 109.5 | C20—C21—C17 | 123.8 (8) |
| C11—C10—H10A | 109.5 | C21—C22—C23 | 119.3 (8) |
| C11—C10—H10B | 109.5 | C21—C22—H22A | 120.4 |
| H10A—C10—H10B | 109.5 | C23—C22—H22A | 120.4 |
| C11—C10—H10C | 109.5 | C24—C23—C22 | 119.9 (8) |
| H10A—C10—H10C | 109.5 | C24—C23—Br3 | 121.3 (7) |
| H10B—C10—H10C | 109.5 | C22—C23—Br3 | 118.8 (7) |
| C12—C11—C16 | 116.3 (8) | C23—C24—C19 | 121.2 (8) |
| C12—C11—C10 | 125.5 (9) | C23—C24—H24A | 119.4 |
| C16—C11—C10 | 118.1 (8) | C19—C24—H24A | 119.4 |

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| C8—C3—C4—C5 | 2.5 (13) | C12—C13—C14—C15 | 2.0 (14) |
| C2—C3—C4—C5 | −178.9 (9) | C9—C13—C14—C15 | −178.8 (8) |
| C8—C3—C4—I1 | 178.2 (7) | C13—C14—C15—C16 | −2.3 (15) |
| C2—C3—C4—I1 | −3.1 (12) | C13—C14—C15—Br2 | 176.4 (7) |
| C3—C4—C5—C6 | −3.7 (14) | C14—C15—C16—C11 | 0.7 (15) |
| I1—C4—C5—C6 | −179.4 (6) | Br2—C15—C16—C11 | −177.9 (7) |
| C3—C4—C5—C1 | 179.0 (9) | C12—C11—C16—C15 | 0.9 (13) |
| I1—C4—C5—C1 | 3.3 (13) | C10—C11—C16—C15 | −179.1 (9) |
| C4—C5—C6—C7 | 2.9 (14) | C24—C19—C20—C21 | −5.4 (13) |
| C1—C5—C6—C7 | −179.6 (8) | C18—C19—C20—C21 | 178.0 (9) |
| C5—C6—C7—C8 | −0.9 (13) | C24—C19—C20—I3 | 178.9 (6) |
| C5—C6—C7—Br1 | 177.3 (7) | C18—C19—C20—I3 | 2.2 (12) |
| C4—C3—C8—C7 | −0.4 (13) | C19—C20—C21—C22 | 4.8 (14) |
| C2—C3—C8—C7 | −179.2 (8) | I3—C20—C21—C22 | −179.4 (6) |
| C6—C7—C8—C3 | −0.3 (14) | C19—C20—C21—C17 | −179.5 (9) |
| Br1—C7—C8—C3 | −178.6 (7) | I3—C20—C21—C17 | −3.7 (12) |
| C16—C11—C12—C13 | −1.1 (13) | C20—C21—C22—C23 | −2.1 (14) |
| C10—C11—C12—C13 | 178.9 (9) | C17—C21—C22—C23 | −178.1 (8) |
| C16—C11—C12—I2 | 177.9 (6) | C21—C22—C23—C24 | 0.3 (14) |
| C10—C11—C12—I2 | −2.1 (12) | C21—C22—C23—Br3 | 179.9 (7) |
| C11—C12—C13—C14 | −0.3 (14) | C22—C23—C24—C19 | −1.0 (14) |
| I2—C12—C13—C14 | −179.3 (7) | Br3—C23—C24—C19 | 179.5 (6) |
| C11—C12—C13—C9 | −179.5 (8) | C20—C19—C24—C23 | 3.4 (13) |
| I2—C12—C13—C9 | 1.5 (12) | C18—C19—C24—C23 | −179.8 (8) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C1—H1*A*···I1 | 0.96 | 2.70 | 3.316 (11) | 122 |

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|---|---|---|---|---|
| C10—H10*A*···I2 | 0.96 | 2.70 | 3.303 (10) | 122 |
| C18—H18*A*···I3 | 0.96 | 2.63 | 3.252 (10) | 123 |